



November 17 (Sun) – 21 (Fri), 2024 Paradise Hotel, Busan, Korea

Organized by

The Surface Analysis Society of Japan





Korean Society of Surface Analysis

This symposium is supported by grants from **BUSAN TOURISM ORGANIZATION**



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Preface

PSA-24

Applications of Practical Surface Analysis on Advanced Industries

Practical Surface Analysis (PSA) is an international conference in Asian area held alternately in Japan and Korea every three years since 1998 to promote research exchange among scientists participating in ISO/TC-201 in the field of surface chemical analysis. PSA-24 (9th International Symposium on Practical Surface Analysis) will be held two years later than originally scheduled in 2022 due to the COVID-19 pandemic.

Surface analysis technology currently plays a key role in product development and quality improvement in various high-tech industries such as semiconductors, batteries, displays, automobiles, and electronic products. PSA is an international conference on practical surface analysis to promote the industrial applications of surface analysis methods.

As the Chairman of the PSA-24 Organizing Committee, I am very pleased that PSA will be held in Busan, following Jeju, Gyeongju, and Daejeon. Through this academic conference, we hope to revitalize research on the basic theory and standardization of surface analysis and to promote exchanges between surface analysis researchers for various industrial applications such as semiconductors, energy, and bio.

Busan is Korea's largest and most famous port city, and it will be a great opportunity to enjoy delicious Korean food and see the historical and cultural sites of the Busan area. We hope that this will be a great opportunity to plan a new future through academic exchange while taking a long-awaited break at the beautiful Paradise Hotel located on the beach.

Preface

Continuing the tradition of focusing on practical application and standardization

On behalf of all committee members of PSA-24, it is a great pleasure to write this preface to the proceedings of the PSA-24, which will be held in Busan, Korea, in November 2024. The PSA International Symposium was held in Matsue in 1998 and has have been held alternately in Korea and Japan every three years. It has been 26 years since the 1st PSA International Symposium. Through the PSA Symposia, the researchers and engineers of Japan and Korea, as well as Western countries and Asia, have cultivated the friendship.

After the last PSA-19 Symposium was held in Sapporo, the COVID-19 pandemic hit the world. I am overwhelmed with emotion that we are able to hold a face-to-face symposium for the first time in five years, overcoming various difficulties. I believe that our friendship will not be broken no matter what happens.

PSA is a symposium that emphasizes practical application in name and in reality. We have shown each other surface analysis techniques that anyone can use easily, conveniently, and effectively. And the surface analysis has played a key role in the progress of advanced industries.

The next stage of practical application is standardization. The standardization is one of the universal truths, on which the modern science and technology based. Both the practical application and standardization of surface analysis led to breakthroughs in materials research and process development. It is expected that PSA will continue these traditions and make even greater progresses in the future.

To that end, we would like to work with all of you to make the PSA International Symposium to be held at PSA-24 Busan a great success. We look forward to your participation in this groundbreaking event. We look forward to seeing you again soon.

Dr. Katsuaki Yanagiuchi Chairperson, Organizing Committee, PSA-24

Preface

PSA-24

Dear Esteemed Colleagues,

It is my distinct honor to extend a warm invitation to you for the upcoming PSA-24 (Practical Surface Analysis-24) International Conference. As President of the Korean Society for Surface Analysis, I am thrilled to welcome you to the dynamic city of Busan, South Korea, for what promises to be an extraordinary gathering of minds in our field.

PSA-24 stands as a beacon of innovation, encompassing a broad spectrum of cutting-edge research domains. From the intricacies of materials science and semiconductor technology to the frontiers of energy materials, biomedical applications, and environmental science, our conference serves as a nexus for groundbreaking discoveries and collaborative breakthroughs.

At the heart of our conference lie the revolutionary analytical techniques that drive our field forward. PSA-24 will showcase the latest advancements in XPS, AES, SIMS, TEM, SEM, FIB, APT, and RBS. These powerful tools are not merely instruments; they are gateways to understanding the fundamental nature of materials at the atomic and molecular levels, enabling us to push the boundaries of what's possible in surface analysis.

We are honored to host an illustrious lineup of world-renowned speakers who will share their insights and latest findings. Complementing the academic program, our state-of-the-art exhibition will feature cutting-edge equipment and innovations from industry leaders, offering a unique opportunity to bridge theoretical knowledge with practical applications.

Beyond the realm of scientific discourse, PSA-24 offers a wonderful opportunity to immerse yourself in Korea's rich cultural tapestry. Busan, with its fascinating blend of modernity and tradition, provides the perfect backdrop for both intellectual stimulation and cultural exploration. I encourage you to savor our renowned cuisine, explore our historical landmarks, and experience the warmth of Korean hospitality.

This conference is more than a gathering of scientists; it's a crucible for forging new friendships, sparking collaborations, and shaping the future of surface analysis. Your participation, expertise, and passion are the catalysts that will make PSA-24 an unforgettable and transformative event.

As we stand at the forefront of scientific and technological innovation, PSA-24 offers a unique platform to share knowledge, challenge assumptions, and collectively envision the future of our field. The insights gained and connections made here have the potential to drive advancements that will resonate far beyond our individual laboratories.

I look forward to welcoming you to Busan with open arms. Together, let us embark on this exciting journey of discovery, innovation, and collaboration. PSA-24 is not just a conference; it's a milestone in our shared scientific odyssey.

Thank you for your dedication to advancing our field. See you soon in Busan for what promises to be an extraordinary PSA-24!

Warmest regards,

Dr. Jae-Pyoung Ahn

President, Korean Society for Surface Analysis

Organization

Q

PSA-24 Organizing Committee

Organizing Committee	K. J. Kim (Chair, KRISS, Korea) J. P. Ahn (KIST, Korea) S. Y. Park (Semilab, Korea) Y. H. Lee (KIST, Korea) S. J. Cho (Park Systems, Korea) W. J. Yoon (ThermoFisher Scientific, Korea) Y. Park (Kyung HeeUniv., Korea) C. S. Jeon (Samsung Electronics, Korea) D. Fujita (JSCA, Japan) S. Ichimura (WasedaUniv., Japan) M. Suzuki (SA consul., Japan) S. Tanuma (NIMS, Japan)	 K. Yanagiuchi (Chair, TDK, Japan) J. M. Yang (NNFC, Korea) S. R. Lee (LGD, Korea) H. G. Shin (POSTECH, Korea) S. D. Cho (Surface Systems Korea, Korea) J. Lee (KBSI, Korea) C. W. Yang (SungkyunkwanUniv., Korea) Y. Abe (Mitsubishi Chem., Japan) Y. Homma (Tokyo Univ. of Sci., Japan) K. Miura (NIMS, Japan) S. Suzuki (Tohoku Univ., Japan) K. Yoshihara (NIMS, Japan)
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Conference Venue

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Paradise Hotel Busan

296, Haeundae haebyeon-ro, Haeundae-gu, Busan, Korea



Busan is the 2nd largest city and number one trading hub in Korea, with a population of 3.4 million and a total area of 770.17 square kilometers as of 2022.

Since opening Korea's first international port in 1876, the city has become a hub of trade, commerce and industry

Global events including the Asia-Pacific Economic Cooperation conference, Busan International Film Festival and Busan Fireworks Festival, as well as various sea-related festivals are held throughout the year. The city is also a tourist destination and home to Asia's largest department store, Haeundae beach, and a yacht marina.

Located on the southern tip of the Korean Peninsula, Busan is a historic city that served as the temporary capital during the Korean War and refuge for men, women and children fleeing the North to build new lives.



		Nov. 19	(Tue)		Nov. 20	(Med)		Nov. 2	(Thu)	Į	Nov. 22 (Fri)
_	Time/Place	PSA-24 (Eng)	KoSSA (Kor)	Time/Place	PSA-24 (Eng)	KoSSA (Kor)	Time/Place	PSA-24 [Eng]	KoSSA (Eng)	Time/Place	PSA-24 (Eng)
the second se		Capri Room	Grand Ballroom I		Capri Room	Grand Ballroom I		Capri Room	Grand Ballroom I		Capri Room
	00:60-00:80	Registr	ation	08:00-09:00	Regist	ration	08:00-03:00	Regist	ration	08:00-03:00	Registration
1				00 00 00	Plenary Lecture 3.						
1	09:00-10:20 [53, 58]	Satoka A0YAGI In-Hui Hwang Setosehi T0Y0DA	Yeonjin Yi Kyung-Tae Ko	00:40-00:40	Sung-Chan Jo		09:00-10:20 [56, 512]	Hyun-Wook Lee Hasmat Khan Huoiun Kim	Yunseok Kim Jungchul Lee Ithium Dark	09:00-10:20 (S7)	Jun-ichiro SAMESHIMA Maciai Mazur
1			Jeongjin Kim Siwoo Noh	09:50-10:10	Bre	ak		IIIN IIIN			
	10:30-10:50	Break	0				10:20-10:40	Break	Break	10:20-10:40	Break
	10:50-12:10 (S4, S9)	Chales Clifford Si-Young Choi Daniel Khaykelson	Break Sung-Dae Kim Jiwon Park Jung In Yeo	10:10-12:10 (S5, S11)	Hurard Morris Hwi Je Woo Chanwon Jung Dongchul Ihm Pyuck-Pa Choi	Un Jeong Kim Sooji Nam Seokjoon Yun Yoon Mi Choi	10:40-12:10 (S6, S12)	Masahiro Terashima Hyun-Woo Gong Hongjin Park Alireza Razazzadeh	Dong Hyeon Kim Junghoon Jahng Young-Jun Yu	10:40-11:40 S7	Tanguy Terlier HeeJin Lim
(Hic)	12:10-13:30	Luncheon Seminar (Ametek Korea)	Luncheon Seminar (KRATOS)	12:10-13:30	Luncheon (GSEM)	Luncheon Seminar (SPECS)	12:10-13:30	Pho Luncheon Semin:	o & r (Park Systems)	11:40-12:00	Closing Ceremony
1.22	13:30-15:30 (S4,59)	John Sader Tsutsumi Kenichi Young Min Kim Benedikt Paul Klein SeHo Kim	Young Heon Kim Ju-Young Kim Jungjae Park Break	13:30-15:10 [56, 511]	Chris Blomfield Takahiro Suzuki Tanguy Tertier	Kwangseuk Kyhm Chaejeong Heo Jung hwa Seo			Eunpa Kim Sangmin An Manhee Lee Taesung Lee	Time/Place	Nov. 17 (Sun) PSA-24 (Eng) Sicily Room
	15:30-15:40	Break		15:10-15:30	Bre	ak	13:30-18:20 [S12]	Excursion		18:00-21:00	Welcome Reception
×	15:40-17:20 [55, 510]	Wooyoung Jung Yoshiyuki Yamashita Yongsup Park Adam Bushell	Kyeryung Kim Myoung Choul Choi Yun Jung Jang Kyungsu Park						51. Sta 52. The	andardization eory and simu	and pre-standardize ulation
	17:20-17:30	Bre	jk	15:30-18:20	Poster 5 leven nu	iession mbers)			54. Nov	ta anatysis an vel technique	id treatment s and instrumentatio
							Blue : Invi Black: Ori	ited Speaker (30 al Speaker (20 m	minl S5. Apr inl S6. Apr S7. Apr	plications I (d plications II (e plications III ()	evice and materials) snergy) bio and organic)
	17:30-19:20	Poster S lodd nur	ession nbersl	18:20-18:30	Bre	ak		PSA-24	S8. Ele S9. Ele	ectron Spectro ectron Microso	oscopy (Korean only) copy (Korean only)
				18:30-20:00	Ban	luet		KoSSA PSA-24+K	510. lo 511. Ph 555A 512. Na	in Beam Techi hoton Beam T ano Scientific	nology (Korean only echnology (Korean Symposium Korea (

Schedule

9th International Symposium on Practical Surface Analysis

Floor Plan

PSA-24



Exhibition



Booth No.	Company Name	Booth No.	Company Name
1	LOTISKOREA (주)로티스코리아	2	Surface Systems Korea (주)서페이스시스템스코리아
3, 4	Thermo Fisher Scientific	5	R-DEC / KASHIYAMA 에스와이사이언스
6	ULVAC-PHI INC. 우신크라이오백(주)	7	HB SOLUTION 에이치비솔루션(주)
8, 9	Park Systems 파크시스템스(주)	10	AMETEK KOREA / CAMECA 아미텍코리아㈜ 카메카
11	COXEM (주)코셈	12, 13	KRATOS Analytical Ltd. /(주)아이엔에이코리아 SPECS Surface Nano Analysis GmbH /(주)아이엔에이코리아
14	ZEISS ZEISS 코리아	15	Leica Microsystems 라이카 마이크로시스템즈
16	HITACHI ELECTRON MICROSCOPES (주)이공교역	17, 18	GSEM (주)지에스이엠
19	Oxford Instruments 옥스포드 인스트루먼츠	20	SCINCO (주)신코
21	KRIMPA 한국소재물성평가원	22	ASTA Corp. 주식회사 아스타
23	JEOL (주)지올코리아	24	TESCAN KOREA 테스칸코리아
25	Bruker Korea Co.,Ltd 브루커코리아(주)	26	SEMIAN 세미안
27	Quantum Design		

Booth Stamp Event Guide



How to Enter the Event:

STEP 1

Visit more than 10 booths and collect stamps (Booth Exhibition: 2F Lobby & Grand Ballroom).



Fill out your personal information on the entry ticket and place it in the submission box at the registration desk.



The prize draw will take place during the closing ceremony.

Signature Prize Draw Ceremony:

- Time: 11:40 AM 12:00 PM, November 22 (Friday), Closing Ceremony
- Note: You must be present at the time of the draw; otherwise, your entry will be void.

🔄 <u>Prizes:</u>

Apple iPad Air 2024 (128GB, Wi-Fi) Apple Watch 10 GPS Apple Beats Studio Pro Wireless Headphones

• Welcome Reception

Welcome reception is scheduled in the evening of November 17 (Sun), 2024. Before coming to welcome reception, visit the registration desk.

🛐 Registration on November 17 (Sun)

The registration desk will be opened from 4PM to 7PM of November 17 (Sun) in front of Conference Room at the second floor.

S <u>Welcome Reception</u>

Welcome reception will be held from 6PM to 9PM of November 17 (Sun) in the Conference Room at the first floor (Sicily Room).

Social program

O Banquet

Banquet will be held in the evening of November 20 (Wed), 2024 in the Grand Ballroom and Capri Room at the 2nd floor of Paradise hotel.

Playing Pieces

- 1. Dancing Queen A global pop hit by ABBA, this song exudes the excitement of dancing and youth, known for its upbeat melody and joyful chorus.
- 2. Arirang A beloved Korean folk song symbolizing resilience and unity, "Arirang" is often regarded as Korea's unofficial national anthem, evoking nostalgia and deep cultural pride.
- 3. Boat Song (배띄워라) This traditional Korean song celebrates maritime heritage, with lyrics encouraging ships to set sail, symbolizing courage and adventure.
- 4. Jang Taryeong A Korean folk tune filled with vibrant rhythm, "Jang Taryeong" is typically performed with traditional Korean instruments and celebrates rural life and community.
- 5. Tiger is Coming (범내려온다) This popular fusion of Korean traditional beats with modern rhythms represents strength and charisma, often performed by crossover bands.
- 6. Beautiful Country (아름다운 나라) A patriotic Korean song celebrating the natural beauty and cultural richness of Korea, conveying pride and love for the homeland.

Each piece brings a unique blend of tradition and contemporary style to the banquet.



Poster Presentation and Best Poster Voting Guide

Poster Presentation and Best Poster Voting Guide

S Poster Setup Schedule

Odd-numbered posters: By the morning of November 19, 2024 (Tuesday) **Even-numbered posters:** By the morning of November 20, 2024 (Wednesday)

Note:

All posters must be removed immediately after your session concludes. Any posters left behind will be collected at 9:00 AM the following morning, and we are not responsible for any left-behind items. Your understanding and cooperation are appreciated.

Poster Presentation & Judging Schedule:

Odd-numbered posters: 17:30 - 19:20, November 19 (Tuesday) **Even-numbered posters:** 15:30 - 18:20, November 20 (Wednesday)

Please ensure you are present during these times for evaluations.

Sydney Room, 2nd floor, Paradise Hotel, Busan

S Poster Numbers:

Poster numbers are listed in the abstract booklet and will also be posted at the entrance of the poster exhibition area.

C

Best Poster Voting Guide

S Voting Period: During the poster presentation.

🛐 <u>Results Announcement:</u>

- Best Poster of PSA-24 (Powell Prize) : During banquet on Nov. 20 (Wed.)
- Best Poster of KoSSA : After finishing the conference.

How to Vote:

Select one outstanding poster based on the following schedule:

- November 19 (Tuesday): Vote for ODD-numbered posters.
- November 20 (Wednesday): Vote for EVEN-numbered posters.

You will receive a voting ticket in your name badge for easy access.

Note: The final awardees will be chosen based on both the vote results and the judges' evaluations. Winners will receive certificates and a small prize after the event.

Excursion

Excursion

Excursion is scheduled in the afternoon of Nov. 21 (Thu), 2024.

S Application Form for the Excursion

The schedule of the excursion

- -1:30 Meeting at the lobby
- 1:30-2:30 move
- 2:30-3:20 Gamcheon Village
- 3:20-3:50 move
- 3:50-4:20 Orukdo Skywalk
- 4:20-5:00 move
- 5:00-5:50 Haedongyounggungsa Temple
- 5:50-6:30 Back to Hotel

Destination of Excursion

1. Gamcheon Village

Colorful roofs that seem to touch the sky, A warmth that covers the whole village, here is Gamcheon Culture Village in Busan.

While the village's beautiful landscape gave it the nickname of the Machu Picchu of Korea, the town was a part of the painful history of Busan. Refugees settled in Gamcheon Village during the Korean War and cultivated the mountainous region to make a living. In 2009, students, artists, and residents decorated the village as a part of the Village Art Project, and the town grew into a leading tourist attraction of Busan since then.



2. Orukdo Skywalk

The Busan Sea, encountered between sandy beaches and coastal roads, offers a special view of the ocean. Walk along the three major skywalks of Busan to enjoy the sky and ocean from high above.

Opened in 2013, Oryukdo Skywalk is located at the end of a 35 m-long coastal cliff. The clear glass floor looking down on the sea is made of bulletproof glass that can withstand heavy loads. The emerald waters off the coast of Oryukdo Islets, where the East Sea meets the South Sea, are spectacular. The waves breaking under the transparent glass floor against the coastal cliffs present a dizzyingly beautiful spectacle, while the sea unfolds before one's eyes and dazzles with its color.

Excursion

PSA-24



3. Haedongyounggungsa Temple

Haedong Yonggungsa Temple is situated on the coast of the north-eastern portion of Busan. This superb attraction offers visitors the rare find of a temple along the shore line as most temples in Korea are located in the mountains. Haedong Yonggungsa Temple was first built in 1376 by the great Buddhist teacher known as Naong during the Goryeo dynasty.

The main sanctuary of the temple was reconstructed in 1970 with careful attention paid to the colors that were traditionally used in such structures. On the right-hand side, inside a cave, is a uniquely designed Buddhist sanctum, while situated just in front of the main sanctuary is a three-story pagoda with four lions. The four lions symbolize joy, anger, sadness, and happiness. Other special sites at the temple are the 108 stairs and stone lanterns lining the rocky landscape. After going down the 108 steps, one will be delighted with the beauty of the temple. Midway down the 108 steps one can stop and enjoy the calming sounds of the waves, and view the majestic sunrise.



🛐 Accompanying person's program

While there is no separate program for accompanying persons, you are welcome to join the tour programs. Please download the application form and send it via email to secretary-psa24@surfaceanalysis.kr.

Information about Korea tourism

You can find information about Korea tourism here. English Site - http://english.visitkorea.or.kr/enu/index.kto Japanese Site - http://japanese.visitkorea.or.kr/jpn/index.kto You can find information about Busan tourism here. English Site - https://www.visitbusan.net/en/index.do

Corporate and Institutional Sponsors of PSA-24

We would like to express our deepest gratitude to the following companies and organizations for their generous support and contributions to PSA-24. Their involvement has made this event possible and greatly enhanced the quality of our program.



Nov. 18 (Mon), 2024

08:00-19:00 Registration 09:00-09:20 Opening Remark

Plenary Talk 1

Chair: Yongsup Park (Kyung Hee University, Korea)

PL-01_09:20-10:05 A Perspective on XPS Challenges, Needs and Opportunitie Donald Baer (Pacific Northwest National Laboratory)

Plenary Talk 2

Chair: Yongsup Park (Kyung Hee University, Korea)

PL-02_10:05-10:50 Evolution and Revolution in Secondary Ion Mass Spectrometry Ian Gilmore (National Physical Laboratory)

S1. Standardization and Pre-standardization _11:10-14:30

11:10-12:10 Chair: Seung Mi Lee (KRISS, Korea)

S1-01_11:10-11:40 A Roadmap to HAXPES Standardisation David Cant (National Physical Laboratory)

S1-02_11:40-12:10 Standardization of Medium Energy Ion Scattering Spectrometry Wonja Min (HB Solution)

12:10-13:30 Luncheon Seminar: Thermo Fisher Scientific

13:30-14:30 Chair: David Cant (National Physical Laboratory, UK)

S1-03_13:30-14:00 Standardization Activities in ISO TC 201 (Surface Chemical Analysis) Hidehiko NONAKA (Tsukuba University)

Nov. 18 (Mon), 2024

S1-04_14:00-14:30

Quantitative Analysis of Binary Alloy Films by Surface Analysis

Seung Mi Lee (Korea Research Institute of Standards and Science)

14:30-14:45 Break

S2. Theory and Simulation _14:45-17:30

14:45-16:15 Chair: Samuel Bertolini Da Silva Oliveira (Université catholique de Louvain, Belgium)

S2-01_14:45-15:15 Parameters Needed for Simulations of Electron Transport in Condensed Matter Aleksander Jablonski (Polish Academy of Sciences)

S2-02_15:15-15:45

Innovative Sample Structure Prediction Using Bayesian Estimation and XPS Simulator HIroshi Shinotsuka (National Institute for Materials Science (NIMS))

S2-03_15:45-16:15

Molecular Dynamics Simulations of Gas Cluster Induced Protein Desorption, Transfer and Soft/reactive Landing Samuel Bertolini Da Silva Oliveira (Université Catholique de Louvain)

16:15-16:30 Break

16:30-17:30 Chair: Aleksander Jablonski (Polish Academy of Sciences, Poland)

S2-04_16:30-17:00

Smart Algorithm for Three-Dimensional AFM Imaging of High Aspect Ratio Nanostructures Yongho Seo (Sejong University)

S2-05_17:00-17:30

Nondestructive Nanoscopy through Bifurcation-Controlled Nonlinear Dynamics of Micro-Cantilever Manhee Lee (Chungbuk National University)

17:30-17:45 Break

Nov. 18 (Mon), 2024

PSA-24

S3. Data Analysis and Treatment _17:45-19:35

17:45-19:35 Chair: Satoka AOYAGI (Seikei University, Japan)

S3-01_17:45-18:15 Towards a Common Data File Format for Hyperspectral Images Alex Henderson (The University of Manchester)

S3-02_18:15-18:45 XPS/HAXPES, and NAP-XPS, for Characterization of Nano-Structured Materials Sven Tougaard (University of Southern Denmark, DK-5230 Odense M, Denmark)

S3-03_18:45-19:05 Surface composition of Sc and ScN by XPS Stanislav Cichon (Institute of Physics, the Czech Academy of Sciences)

S3-04_19:05-19:35 Transformative Data Insights: Advanced Hybrid Nano-Metrology for High-Resolution Material Characterization Sang-Joon Cho (Park Systems)

Nov. 19 (Tue), 2024

S3. Data Analysis and Treatment _09:00-10:20

09:00-10:20 Chair: Sang-Joon Cho (Park Systems, Korea)

S3-05_09:00-09:30 Data-driven Analysis of Spectrum and Image Data Satoka AOYAGI (Seikei University)

S3-06_09:30-09:50 X-ray Emission Spectroscopy Data Processing and Analysis Using Artificial Intelligence In-Hui Hwang (POSTECH)

S3-07_09:50-10:20 Towards advanced interface visualization in multi layer stacks: Big data and and simulation approaches using angle-resolved XPS Satoshi TOYODA (Scienta Omicron Japan)

10:20-10:50 Break

S4. Novel Techniques and Instrument _10:50-15:30

10:50-12:10 Chair: Young Min Kim (Sungkyunkwan University, Korea)

S4-01_10:50-11:20 Scanning Probe Microscopy: from Research to International Standards Chales Clifford (National Physical Laboratory)

S4-02_11:20-11:50 Electron Microscopic Understanding toward Highly-Performed Cathode Si-Young Choi (POSTECH)

S4-03_11:50-12:10 Structural Insights into Non-Crystalline ("Amorphous") Thin Silicone-Nitride Films Daniel Khaykelson (Weizmann Institute of Science)

12:10-13:30 Luncheon Seminar: Ametek Korea

13:30-15:30 Chair: Chales Clifford (National Physical Laboratory, UK)

S4-04_13:30-14:00 Suspended Microchannel Resonators John Sader (Caltech)

Nov. 19 (Tue), 2024

S4-05_14:00-14:20

PSA-24

Applications of New Hyper Spectral Map Method by Auger Electron Spectroscopy Tsutsumi Kenichi (JEOL Ltd.)

S4-06_14:20-14:50 Machine Learning-assisted Electron Spectroscopic Imaging for Chemical Analysis of Energy-related Materials Young-Min Kim (Sungkyunkwan University)

S4-07_14:50-15:10 Practical Determination of the Transmission Function of a Near Ambient Pressure Hemispherical Electron Analyzer Benedikt Paul Klein (Korea Basic Science Institute)

S4-08_15:10-15:30 Designing Energy Materials Guided by 3D Atomic-Resolution Tomography SeHo Kim (Korea University)

15:30-15:40 Break

S5. Applications I (Device and Materials) _15:40-17:20

15:40-17:20 Chair: Richard Morris (IMEC, Belgium)

S5-01_15:40-16:10 Innovative Applications of Surface Analysis for 3D Semiconductor Structures Wooyoung Jung (SK hynix)

S5-02_16:10-16:30

Photoelectron Holographic Study of Atomic Site Occupancy of the Si Dopant in k-Ga2O3(001) Yoshiyuki Yamashita (NIMS)

S5-03_16:30-16:50 Interface Energy Level Offset in Organic Solar Cells Measured by UPS and IPES and Its Correlation with Voc and CT Energy Yongsup Park (Kyung Hee University)

S5-04_16:50-17:20 Correlative XPS Multi-technique sample analysis Adam Bushell (Thermo Fisher Scientific)

17:20-17:30 Break

17:30-19:20 Poster Session

Nov. 19 (Tue), 2024

S8. Electron Spectroscopy _09:00-10:50

09:00-10:50 Chair: Jouhahn Lee (Korea Basic Science Institute, Korea)

S8-01_09:00-09:30

Electronic Structure of Halide Perovskites: Insights from Photoelectron Spectroscopy Measurement Techniques Yeonjin Yi (Yonsei University)

S8-02_09:30-10:00 Investigation on Electronic Structure of Exotic Layered Chalcogenide Materials Kyung-Tae Ko (Korea Basic Science Institute)

S8-03_10:00-10:30

Probing the Surface Electronic Structure and Reaction Intermediate using Synchrotron-Based AP-XPS Jeongjin Kim (Pohang Accelerator Laboratory, POSTECH)

S8-04_10:30-10:50

Recent Advances in Soft and Tender X-ray Photoemission Spectroscopies at the Pohang Accelerator Laboratory Siwoo Noh (Korea University/ PAL)

10:50-11:00 Break

S9. Electron Microscopy _11:00-14:50

Chair: Sangmin An (Jeonbuk National University, Korea)

S9-01_11:00-11:30 Understanding Dislocation Dynamics in Advanced Steels via Transmission Electron Microscopy Sung-Dae Kim (Pukyong National University)

S9-02_11:30-11:50 대기 중 단일 입자의 모양 및 성분 분석 Jiwon Park (Korea Research Institute of Chemical Technology)

S9-03_11:50-12:10 Gate-dependent Interactions between Fe Atoms on Graphene Jung In Yeo (Chung-Ang University)

12:10-13:30 Luncheon Seminar: KRATOS

Nov. 19 (Tue), 2024

S9-04_13:30-14:00

In situ and Operando Transmission Electron Microscopy Study of One-dimensional InAs-based Compound Semiconductor Nanowires

Young Heon Kim (Chungnam National University)

S9-05_14:00-14:30 Recent Advancements in Elasto-visco-plastic Self-consistent Model and its Application to Various Polycrystal Metals Youngung Jeong (Changwon National University)

S9-06_14:30-14:50

Real-Time Investigation of Corrosion Behaviors in Zn-Mg-Al Alloys Using Liquid-Phase TEM Jungjae Park (Research Institute of Industrial Science & Technology)

14:50-15:10 Break

S10. Ion Beam Technology _15:10-16:50

Chair: Taeeun Hong (Korea Basic Science Institute, Korea)

S10-01_15:10-15:40

Status and Utilization of Tandem Accelerator-Based Ion Beam Analysis System of KAERI Kyeryung Kim (Korea Atomic Energy Research Institute)

S10-02_15:40-16:00 Development of Gas Cluster Ion Beam and Application to the Surface Processing in X-ray Mirror Myoung Choul Choi (Korea Basic Science Institute)

S10-03_16:00-16:30 Effect of Ag Incorporation on CIGS Solar Cells Using Surface Analytical Techniques Jang Yun Jung (Korea Institute of Science and Technology)

S10-04_16:30-16:50 Advantages of Non-Destructive Depth Profile Analysis Using TOF-MEIS Over Destructive Method Kyungsu Park (HB SOLUTION)

16:50-17:30 Break

17:30-19:20 Poster Session

Nov. 20 (Wed), 2024

Plenary Talk 3

Chair: Taeeun Hong (Korea Basic Science Institute, Korea)

PL-03_09:00-09:50

Advanced Surface Analysis for the Perspective in Display/Semiconductor Industry Sung-Chan Jo (Samsung Display)

09:50-10:10 Break

S5. Applications I (Device and Materials) _10:10-12:10

Chair: Tae-Gon Kim (Hanyang University Korea)

S5-05_10:10-10:40

Atom Probe Tomography: Application and Challenges within the Semiconductor Field Richard Morris (IMEC)

S5-06_10:40-11:00 Nano Imaging of Ultrafast Exciton Dynamics in 2-Dimensional Materials with s-SNOM Hwi Je Woo (Korea Research Institute of Standards and Science)

S5-07_11:00-11:20 Investigation of 3D Atomic Distributions in Functional Materials through Atom Probe Tomography Chanwon Jung (Pukyoung National University)

S5-08_11:20-11:50 Advancements and Challenges in Surface Metrology and Inspection for the 3D Integration Era Dongchul Ihm (Samsung Electronics)

S5-09_11:50:12:10 Characterization of Colloidal Pd Nanoparticles using Atom Probe Tomography Pyuck-Pa Choi (Korea Advanced Institute of Science and Technology)

12:10-13:30 Luncheon Seminar: GSEM

Nov. 20 (Wed), 2024

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S6. Applications II (Energy) _13:30-15:10

13:30-14:40 Chair: Masahiro Terashima (ULVAC PHI, Japan)

S6-01_13:30-13:50 Using High-throughput XPS Analysis in Determining Na-Fe-Mn-O Cathode Materials Chemistry Chris Blomfield (Kratos Analytical Ltd.)

S6-02_13:50-14:20 Investigation on XPS Charge Neutralization Method for Carbon-Based Battery Materials Takahiro Suzuki (Cataler Corporation)

S6-03_14:20-14:40 Novel Strategies for the Characterization of the Next-generation Energy Storage Materials by ToF-SIMS: from an In-situ Exploration to an Operando Measurement Tanguy Terlier (Rice University)

14:40-15:30 Break

15:30-18:20 Poster Session

S11. Photon Beam Technology _10:10-15:00

10:10-12:00 Chair: Kwangseuk Kyhm (Pusan National University, Korea)

S11-01_10:10-10:40 Optical Properties of Low Dimenstional investigated by Light-Matter Interactions Un Jeong Kim (Dongguk University)

S11-02_10:40-11:10 Analysis of Tellurium/Indium Zinc Tin Oxide Heterostructures and Their Device Applications Sooji Nam (Electronics and Telecommunications Research Institute)

S11-03_11:10-11:40 Bottom-up Synthesis of 2D Materials for Future Electronics Seokjoon Yun (University of Ulsan)

S11-04_11:40-12:00 Molecular-level structural understanding of temperature induced phase transitions in bromine functionalized metal organic framework

Yoon Mi Choi (Korea research Institute of Chemical Technology)

12:10-13:30 Luncheon Seminar: SPECS

Nov. 20 (Wed), 2024

13:30-15:00 Chair: Un Jeong Kim (Dongguk University, Korea)

S11-05_13:30-14:00 Ultrafast Spectroscopy and Microscopy on Nanostructures Kwangseuk Kyhm (Pusan National University)

S11-06_14:00-14:30 Label-free Spectroscopic Detection of Biomolecules for Diagnosing Alzheimer's Disease Chaejeong Heo (Sungkyunkwan University)

S11-07_14:30-15:00 Photoelectron Spectroscopic Study of the Interfacial Electronic Structures of Metal-Ion Containing Polyelectrolytes on ITO Substrates Jung hwa Seo (University of Seoul)

15:00-15:30 Break

15:30-18:20 Poster Session

Nov. 21 (Thu), 2024

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S6. Applications II (Energy) _09:00-12:10

09:00-10:10 Chair: Hyun-Wook Lee (Ulsan National Institute of Science and Technology, Korea)

S6-04_09:00-09:30 Observation of the Nucleation and Growth of Lithium Metal Dodecahedra in Anode-free Lithium Batteries Hyun-Wook Lee (Ulsan National Institute of Science and Technology)

S6-05_09:30-09:50 Surface Engineering and Regulation of a Photoelectrode for Solar Rechargeable Zn-Air Batteries Hasmat Khan (Pusan National University)

S6-06_09:50-10:10 The Solidification Effect of Using Benzenesulfonyl Fluoride Assistants for Liquid Electrolyte in Lithium-Sulfur Batteries Hyejun Kim (Sungkyunkwan University)

10:10-10:40 Break

10:40-12:10 Chair: Soohyung Park (Korea Institute of Science and Technology, Korea)

S6-07_10:40-11:10 Chemical State and Energy Band Structure Analysis for Interface Modification in All-Solid-State Battery Materials Masahiro Terashima (ULVAC PHI)

S6-08_11:10-11:30 Unveiling the Longevity Mechanism of Si/Graphite Composite Anodes in Sulfide-based All Solid-State Batteries: Interplay of Nanostructure Evolution and Interface Stability Hyun-Woo Gong (Korea Institute of Science and Technology)

S6-09_11:30-11:50

Single-Atom Platinum Catalyst for CO Oxidation on Multi-Component Vanadia/Titania Support Hongjin Park (Chungnam National University)

S6-10_11:50:12:10

Ru-Based High Entropy Oxide as Acid Stable Electrocatalyst for Oxygen Evolution Reaction Alireza Razazzadeh (Pusan National University)

12:10-13:30 Photo & Luncheon Seminar: Park Systems

13:30-18:20 Excursion

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S12. Nano Scientific Symposium Korea (NSSK) _09:00-15:20

Chair: Sang-Joon Cho (Park Systems, Korea)

S12-01_09:00-09:30 Improved Sensitivity of Atomic force Microscopy Images by Machine Learning Yunseok Kim (Sungkyunkwan University)

S12-02_09:30-10:00 Unconventional Micro-/Nanofabrication via High Temperature Annealing Jungchul Lee (Korea Advanced Institute of Science and Technology)

S12-03_10:00-10:20 Ultra-sensitive and Nanoscale Imaging of Individual Biomarkers in a Single Neuronal Cell Using Force-Based AFM Ikbum Park (Korea Research Institute of Chemical Technology)

10:20-10:40 Break

S12-04_10:40-11:10 The Nanoscale Lattice Deformations in Two-dimensional Materials Dong Hyeon Kim (HanYang University)

S12-05_11:10-11:40 Advances and Challenges in Dynamic Photo-induced Force Microscopy Junghoon Jahng (Korea Research Institute of Standards and Science)

S12-06_11:40-12:10 Charge Trapping Memory Based on 2D Materials Heterostructures Young-Jun Yu (Chungnam National University)

12:10-13:30 Photo & Luncheon Seminar

S12-07_13:30-14:00 The Present and Future of Scanning Probe Technology for Advanced Semiconductor Device Manufacturing Eunpa Kim (Samsung)

S12-08_14:00-14:30 Atomic Force Microscope-based Analysis of the Nanoscale Materials and Fabrication of the Microscale Probes Sangmin An (Jeonbuk National University)

S12-09_14:30-15:00 Quartz Tuning Fork-based Microviscometry for Selecting High-quality Sperm from Semen Manhee Lee (Chungbuk National University)

S12-10_15:00-15:20 Tip Displacement Detection Technology AFM Using Quadrature Phase Differential Interferometry Taesung Lee (Oxford Instruments)

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S7. Applications III (Bio and Organics) _09:00-11:40

09:00-10:20 Chair: Tanguy Terlier (Rice University, USA)

S7-01_09:00-09:30 Unraveling of Complex Poxvirus Structure using Cryo-Electron Microscopy Jaekyung Hyun (Sungkyunkwan University)

S7-02_09:30-10:00 Mass Imaging Analyses for Practically Utilized Polymers and Bio Materials Jun-ichiro SAMESHIMA (Toray Research Center, Inc.)

S7-03_10:00-10:20 Arrays of Spherical Cap Particles: Fabrication of Substrates for Cell Cultures by Dewetting of Thin Polymer Films Maciej Mazur (University of Warsaw)

10:20-10:40 Break

10:40-11:40 Chair: Jaekyung Hyun (Sungkyunkwan Universit, Korea)

S7-04_10:40-11:10 Multiplexing Analysis Using Microarray by ToF-SIMS: a High Throughput Exploration Tool for Rapid Chemical Screening Tanguy Terlier (Rice University)

S7-05_11:10-11:40 Time-of-flight secondary ion mass spectrometry imaging of biological samples HeeJin Lim (Korea Basic Science Institute)

Closing Ceremony

POSTER PRESENTATION I / November 19 (Tue)

P-01	Particle dispersibility evaluation: An approach to quantifying impressions	Ogata Shuji (Nissan Chemical Corp.)
P-03	Development of evaluation method for ligand conjugation of Fe3O4 and AuNPs using mass images and statistical analysis	Jin Gyeong Son (KRISS)
P-05	Porous Carbon Interlayer Derived from Traditional Korean Paper for Li–S Batteries	Yunju Choi (Korea Basic Science Institute)
P-07	Evaluation of CSR-based Tool-to-tool matching of LEAP 6000XR in Samsung Electronics	Hosun Jun (Samsung Electronics)
P-09	Exploring Beyond Linear Relations in Catalyst Performance	Kihyun Shin (Hanbat National University)
P-11	Understanding CO Oxidation at Au9/MO _x Interfaces: Reaction Mechanisms and Catalytic Efficiency through DFT	Jongseok Kim (Chungnam National University)
P-13	Quantitative Analysis of Cu ⁰ , Cu ⁺ and Cu ²⁺ Compounds with Multiple Core-level XPS Spectra Decomposition Method	Hiroshi Okumura (Mitsubishi Materials Corporation)
P-15	계면 분석을 통한 InGaZnO 산화물 TFT 소자 Hysteresis 원인 연구	Minjee Ko (LG Display)
P-17	4 characteristics and film physical properties for good performance SiNx encapsulation films	Jungmin bae (LG Display)
P-19	Analysis of impurities on the substrate surface using FT-IR microscopy	dongchan LEE (AICT)
P-21	Atomic force microscope-guided 3D printed carbon nanotube nanowires with in situ Raman spectroscopy	Sangmin An (Jeonbuk National University)
P-23	Characteristics of Magnesium–Ion–Implanted Gallium Nitride for Power Semiconductor Applications	Jang Taehun (Korea Basic Science Institute)
P-25	Characterization of Individual Airborne Particles Using Complementary Analytical Methods with Combined SEM/EDS, Fluorescence Microscope, and O-PTIR	Jiwon Park (KRICT(Korea Research Institute of Chemical Technology))
P-27	Hydrogen-Inclusive Compositional Analysis of SiOCH Thin Films	Sung-Jin Chang (NNFC)
P-29	Hydrogen Diffusion Model in Austenite Steel Containing Martensite Structure	Hiromi Kato (Seikei University)
P-31	Influence of Electron Beam Acceleration Voltage on Critical Dimension Measurements in Semiconductor Metal Lines Using Scanning Electron Microscopy	Taeksoo Shin (Sungkyunkwan University)
P-33	Analysis of Palladium Diffusion from ENEPIG Surface Finish into Solder Joint	JaeJun YOON (Sungkyunkwan university)

P-35	In-situ characterization of interface layer between ZnO overlayer and AI metal by XPS and HAXPES	Hisao Makino (Kochi University of Technology)
P-37	Development of a Humidity Sensor Based on CaCu3Ti4O12/NaCl Using the Aerosol Deposition Method	ZhangYuanBo (KwangWoon University)
P-39	Atomic Layer Deposition of Ru-Ir Thin Films for Advanced Interconnects	Jihye Baek (Pusan National University)
P-41	Development of a Humidity Sensor Based on CaCu3Ti4O12/NaCl Using the Aerosol Deposition Method	Zhang YuanBo (KwangWoon University)
P-43	Indium-Gallium-Zinc-Oxide Based Negative Capacitance Field Effect Transistors for Low Power Consumption	JiHyeon Min (Dongguk University)
P-45	Fluorescence and electrochemical dual-mode detection of norepinephrine with a portable smartphone assay using nitrogen-doped Ti_3C_2 MXene quantum dots via instant microwave-assisted synthesis	Murugesan chandran (Gachon University)
P-47	Plasma Enhanced Atomic Layer Deposition for High–Performance Scaled Indium Oxide Thin Film Transistors	Jaewon Park (Dongguk Univ.)
P-49	Highly Conductive and Stretchable AgNW/PEDOT:PSS Heater via Laser Patterning Process for Soft Heater	Jeong Eun Byun (Pusan National University)
P-51	Control of Microstructure and Micropatterning of Carbon-based Functional Materials for Soft Electronics	Jung Woo Lee (Pusan National University)
P-53	Analysis of Pore within SiOCH Films on Si Substrate	Sung-Jin Chang (NNFC)
P-55	Correlation Between Micropatterned Strain Domains in Graphene on Copper Substrates and Facet Structures	Joonhee Moon (Korea Basic Science Institute)
P-57	Enhanced Capacitance Density and Leakage Current Performance of BaTiO ₃ /BaTiO ₃ -Ag Double-Layer Structure	Jeon Jwa-Bin (KwangWoon Univ.)
P-59	Surface Engineering of Ti ₂ N MXene Quantum Dots for Nano Thermometry	Afrizal Lathiful Fadli (Sungkyunkwan University)
P-61	Application of Neural Network Algorithms of Semiconducting Metal Oxide (SMO) gas sensors to Gas Sensing Discrimination Tasks	Huisu Shin (Hongik University)
P-63	Hydrophobic Surface Modification of MgO for Application as Heat–Dissipating Filler in Electric Vehicle Batteries	Seyoung Park (Kyonggi University)
P-65	Fabrication of MoS ₂ Patterns Using a Laser Direct Writer and Emulation of Neuromorphic Device Characteristics	Park Hyehyeon (sejong university)
P-67	Unraveling the sodium storage mechanism of NASICON-type cathode for sodium-ion battery	Junpyo Hur (KAIST)
P-69	Engineering Alloyed Transition Metal Dichalcogenides Nanosheets towards Efficient Electrocatalytic Hydrogen Evolution Reaction	In Hye Kwak (Korea Basic Science Institute (KBSI))

P-71	Fabrication of electrodeposited three-dimensional nickel nanocup array electrode	Jungyu Sung (Kwangwoon University)
P-73	Surface Properties of Organic Halide Perovskite Thin Films Degraded by Electron Beam Irradiation	Hyeonho Park (Department of Physics, Jeonbuk Natl. Univ.)
P-75	Fine-tuning strategy of supported Au single atom catalyst : atomic-precision hybrid oxide interface modulation	Kim Minkyeong (Chungnam National University)
P-77	Electrochemical characteristics of dense PVDF-PEGDME polymer electrolytes for solid state lithium batteries	Jong-Pil Kim (aKorea Basic Science Institute Busan Center)
P-79	Interpretation of ToF–SIMS depth profiles of mycelium coils in an orchid mycorrhiza of <i>Cephalanthera falcata</i> using sparse autoencoder	Hikaru Yamaguchi (Seikei University)
P-81	Evaluation of diclofenac permeation into human skin using ToF-SIMS	Atsumi Shinozaki (Seikei University)
P-83	3D Distribution Imaging Analysis of Components Using Orbitrap/TOF Hybrid SIMS	Jiyeong Sung (KBSI)
P-85	Red fluorescent copper nanocluster for fluorescence, smartphone, and electrochemical sensor array to detect the monkeypox A29 protein	Dhanasekaran Barkavi (Gachon University)
P-87	Quartz tuning fork-based viscometry for separating bovine sperm in a biomimetic cervix environment	dongwon kim (chungbuk national university)
P-89	High-Throughput Quantitative Analysis of Amino Acids in Freeze-Dried Drops Using Time-of-Flight Secondary Ion Mass Spectrometry	Heejin Lim (Korea Basic Science Institute)
P-91	Investigation of Antenna Effect: Enhanced Luminescence of Terbium(III) with Glucoconjugated Ligands	Parmeshthi Parikh (BITS Pilani, Pilani Campus)
P-93	Analysis of natural pigments using various instrument and their statistical processing	Lee youngseo (KIST)
P-95	Accelerator Mass Spectrometry-based Quantitative Tracing of Phenol and its Derivatives in Soil and Plants	Gwan-Ho Lee (KIST)
P-97	Device-level XPS Analysis for Physical and Electrical Characterization of Oxide-Channel Thin-Film Transistors	Gyungtae Kim (National Nanofab Center)
P-99	Design of the High Heat Load Front-End for the 4th Generation Synchrotron in Korea	Hyung-seok Choi (Pohang Accelerator Laboratory)
P-101	Synthesis and application of tungsten disulfide for energy storage devices	Hae Kyung Jeong (Daegu University)
P-103	Study on Reversible Multicolor Chromism through Humidity for Short Organic Spacer-based Perovskites: Focusing In-situ Observation	Aelim Ha (Yonsei University)

P-105	Electronic Structure of Silver Phenyl Selenolates [AgSePh], and Their Dependency on Thickness: A Investigation via Photoemission Spectroscopy	SeungHwan Kim (KIST (Korea Institute of Science and Technology))
P-107	Spacer-Assisted Growth of Thin Single-Crystalline Two-dimensional Perovskite Membranes	Sooyeon Pak (Korea Institute of Science and Technology)
P-109	Cryo-TEM Observation of Ice I	Ji Su Park (KAIST)
P-111	Defect Analysis of Semiconductor Devices Using SEM, FIB, PFIB : Practical Cases and Results	Junyoung Won (Advanced Institute of Convergence Technology(AICT))
P-113	In-Situ Observation of Ag2S-Catalyzed ZnS Nanowire Growth via VLS-SLV Mechanisms	Jung Han kim (Dong-A University)
P-115	Isotropic electrical field-driven MEMS chip for electrochemical in situ TEM application	Min Wook Pin (Research Institute of Industrial Science & Technology (RIST))
P-117	Advanced Electron Microscopy Analysis of High–Ni single crystal NCM cathode	Joon Ha Chang (Research Institute of Industrial Science and Technology)
P-119	Calculation of light element (Li,C,O) ionization ratio measured by 2D–ERDA method using TOF–MEIS and electrostatic deflector	Chang Seon Park (HB Solution)
P-121	Semiconductor Analysis by Atom Probe Tomography	Lee Bong Ho (DGIST)
P-123	Optimization of SIMS Energy Slit for Dopant Distribution Analysis in SiC Power Semiconductors	Minji Kang (Korea Basic Science Institute)
P-125	Determining the Radius and Cone Angle of a Probe Tip Using an AFM Tip Characterizer	Young Bum Kim (KimsReference Corp.)
P-127	Sub-picoliter drug delivery into living cells	Jinwan Cho (Chungbuk national university)
P-129	Study on Crystallinity and Phase Changes of NCA Cathode Material Using Advanced XRD Analysis	Sangyong Lee (Advanced Institute of Convergence Technology)
POSTER PRESENTATION II / November 20 (Wed)

P-02	Optimal Mass Spectra Preprocessing to Extract Mass–Specific Features and Application to Classification	Jin Gyeong Son (KRISS)
P-04	Fabrication and Analysis of Electrode from Rapid Alkaline Depolymerization of PET into Na2TP with High Performance MXene (Ti3C2TX) on Nickel Foam Substrate for Hydrogen Evolution Reaction.	Rahul Ramkumar (Pusan National University)
P-06	LDI–TOF Mass Spectrometry for Composition Differentiation of Transition Metal Dichalcogenides	Taewan Kim (ASTA)
P-08	2024년도 TC201 표면화학분석 국가표준 개발 성과 및 향후계획	Son Jeong Hyo (KOTITI)
P-10	First Principles Study on CO2 Hydrogenation over Pd Catalysts: Elucidating the Role of C–O Bond Activation	Yejung Choi (Chungnam National University)
P-12	Analysis of electron backscatter diffraction raw data, Kikuchi patterns, using machine learning	Kazuma Takeishi (Seikei University)
P-14	Effect of pixel binning on principal component extraction in PCA-based denoise of AES spectrum image	Fuyuki Nabeshima (JEOL Ltd.)
P-16	Study on the correlation with the characteristic and role of inorganic films for LTPO TFT	SERA KWON (LG Display)
P-18	Peculiarities of XPS analysis of ScN based thin films	Stanislav Cichoň (Institute of Physics, the Czech Academy of Sciences, Prague, Czechia)
P-20	Evaluation of quantitative analysis of OrbiSIMS spectra using ANNbased supervised learning method.	Shun Shibayama (Seikei University)
P-22	Development of a hybrid quartz tuning fork-atomic force microscope combined with a scanning electron microscope	Sangmin An (Jeonbuk National University)
P-24	Formation of electrochemical solid/liquid interface with hygroscopic electrolyte for ambient pressure hard X-ray photoelectron spectroscopy	Beomgyun Jeong (Korea Basic Science Institute)
P-26	Highly Sensitive Low Energy Inverse Photoemission Spectroscopy for the Unoccupied State Measurement of Organic Semiconductors	Yongsup Park (Kyung Hee University)
P-28	Evaluation of the image fusion data of hydrogen distribution by operando hydrogen microscope and crystal structure distributions	Yuki Sano (Seikei University)
P-30	Surface-Analysis Approaches to Elucidate Chromium Ion Adsorption on Glycoconjugate-derived Metallopolymer	Anuvasita Parikh (BITS Pilani Pilani Campus India)

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P-32	CO cryo-sorption as a surface-sensitive spectroscopic probe of the active site density of single-atom catalysts	Benedikt Paul Klein (Korea Basic Science Institute)
P-34	Ultra-high Breakdown Field of Ga ₂ O ₃ Film via Nozzle Tilting of Aerosol Deposition Method	Jun-Woo Lee (Kwangwoon University)
P-36	CsPbBr ₃ /Al ₂ O ₃ composite; Large-scale synthesis; Thermostability; Green-emitting phosphor	Seok-Hun Kim (Dong-Eui University)
P-38	Enhancing the Initial Nucleation Behavior of ALD-Iridium Thin Films via a Surface Pretreatment Process	Myung-Jin Jung (Pusan National University)
P-40	Evaluation of PEALD AI2O3 according to deposition temperature for thin-film transistor applications	Jo Hojeong (Dongguk Univ.)
P-42	Impurity Reduction Leading to Enhanced Properties in Atomic Layer Deposited Ru Films by Introducing Additional Reactant for Cu Alternative Interconnects	Jeongha Kim (UNIST)
P-44	3D integration of CMOS inverters composed of IGZO and Te through a via-hole-less structure	Dongbin Lee (Dongguk University)
P-46	Development of highly conductive NbC _x thin films using PEALD for diffusion barrier applications in Cu and Ru interconnects	Chaehyun Park (UNIST)
P-48	Highly Breathable and Stretchable Temperature Sensor Using Mesh–Shaped Textile and Partially Reduced Graphene Oxide	Hyun Jin Kang (Pusan National University)
P-50	Effect of density and crystal structure of InOx samples on D–SIMS depth profiles	Ki-Cheol Song (KIST)
P-52	Research on Silicon Oxynitride Thin Films Deposited by PECVD Processes with Low–GWP Gas	Woo Cheol Jang (UNIST)
P-54	Controlled Reduction of the Graphene Oxide for Temperature Sensing	YeongJun YUN (Pusan National University)
P-56	Crystal Structure Determination of Coordination Polymers Using Combined Computational Simulation and Powder XRD Analysis	Sung-Chul Kim (Korea Institute of Science and Technology)
P-58	Analysis of ZnO/HfO ₂ thin film grown Discrete Feeding Method using ToF–SIMS and GIXRD	Haegyeong Kim (UNIST)
P-60	Fabrication of Titanium Carbonitride (Ti ₃ CN) MXene Quantum Dots for Optical Detection of Fe ³⁺ ions	Muhammad Annas Syhukri Bin Mohd Ariffin (Sungkyunkwan University)
P-62	Machine Learning-Assisted Discrimination Strategy of Acetone and Hydrogen Based on Hybrid SnO2/WO3 Breath Sensors	Heesu Hwang (Hongik University)
P-64	Nonequilibrium electrical conductivity-induced particle aggregation in slurry	Jeongmok Cho (Chungbuk National University)

P-66	Enhancing Sodium-Ion Battery Performance: Advanced Synthesis Methodology for Prussian White Cathodes	JaeEun Joo (KAIST)
P-68	Phase evolution induced by irreversible reactions in metal sulfide anodes	Jacob Choe (Korea Advanced Institute of Science and Technology)
P-70	Unveiling the Surface Reaction Mechanisms of Nickel Nitride@ N-doped Carbon for Hydrogen and Oxygen Evolution Through In-situ Raman Spectroscopy	Uk Sim (Korea Institute of Energy Technology (KENTECH))
P-72	Enhanced Electrochemical Properties of Li _{1.6} Ni _{0.6} Co _{0.2} Mn _{0.2} Cathode Thin Film by Post-annealing Process in Oxygen Atmosphere	SAAC LEE (materials science and enginnering)
P-74	Oxidative Stability of PEO based Polymer Electrolyte	Suhyeon Kim (KyungHee University)
P-76	Structure and electrochemical properties of Li-Ti-O anode material for Li-ion battery	Jong Bae Park (Korea Basic Science Institute)
P-78	New Strategy to Improve the Accuracy of Quantitative Analysis of Energy Dispersive Spectroscopy	Wan-Gil Jung (KBSI)
P-80	Characterization of ocean plastics using ToF-SIMS and machine learning	Miku Kimura (Seikei University)
P-82	Surface Analysis of CaCO ₃ Nanoparticles Modified by a Silane Coupling Agent Methyltrimethoxysilane	JongChoo Lim (Dongguk University)
P-84	Bimetal MOF based electrochemical sensor for the detection of serotonin in serum	Veerapandian Mekala (Gachon University)
P-86	Infrared Nano-Spectroscopy of Single Extracellular Vesicles via Photo-Induced Force Microscopy	Mingu Kang (Korea Research Institute of Standards and Science)
P-88	Post-functionalization of diazonium-modified surfaces in the presence of redox inhibitor	Sojin Park (Kwangwoon University)
P-90	Nanoscopic Investigation of Real-Time Conformational Dynamics of Condensins using High-Speed Atomic Force Microscopy	Lim Kee Siang (WPI Nano Life Science Institute, Kanazawa University)
P-92	Application of AFM Measurements in Various Environments	Jihye Lee (KIST)
P-94	Verification of therapeutic effect through Accelerator Mass Spectrometry based single cell level quantification of hESC-endothelial cells distributed into an ischemic model	Oh Min-Seok (korea institute of science and technology)
P-96	Cutting-edge analysis technology for various materials of the semiconductor industrial research field by X-ray Photoelectron Spectroscopy in AICT	Gyung Hyun Kim (Advanced Institute of Convergence Technology)

PSA-24

P-98	Alloying of ReS ₂ and VS ₂ Nanosheets for Enhanced Electrocatalytic Hydrogen Evolution Reaction	Ik Seon Kwon (Pohang Accelerator Laboratory)
P-100	Study on Oxygen Vacancies in Oxide Semiconductors under Thermal Treatment using XPS	Ae Jin Choi (Korea Institute of Science and Technology)
P-102	Influence of Neutralizer on the ITO Surface in XPS Analysis	Kang Hee Kyoung (Korea Institute of Science and Technology)
P-104	Mechanism of Light-induced Surface Degradation in Two-Dimensional Halide Perovskites: Impact of Light during Fabrication and a Passivation Strategy	Kitae Kim (Yonsei University)
P-106	Round Robin Test for the Calibration of Magnification and Offset in SEM and AFM Measurements using a Nanostructured Certified Reference Material	Young Su Park (Kimsreference Corp.)
P-108	Comparative study of time-resolved electroluminescence and photoluminescence of light emitting devices	Weon-Sik Chae (Korea Basic Science Institute)
P-110	In-situ liquid phase TEM for revealing suppression effect of Mo etching by solid by-products	Sanghyeon Ji (KAIST)
P-112	Automatic analysis program for the TEM diffraction patterns(REDI, RIST Electron Diffraction Interpreter)	Sung KANG (RIST)
P-114	ZnS/Diamond-Like Carbon Heterostructure Nanowires: Synthesis and Characterization	Jung Han Kim (Dong-A University)
P-116	Impact of n-Doping on Defect States and Energy Level in Two-Dimensional Hybrid Organic-Inorganic Ruddlesden-Popper Perovskites	Eunki Yoon (Yeonsei Univ.)
P-118	Depth Profiling of Thick Samples Excluding Sputtering Damage Using TOF-MEIS and Ar Sputter	Jwasoon Kim (HB-Solution Co. Ltd)
P-120	Determination of Screening model for Quantitative analysis in ToF-MEIS for 150 keV He^{+}	Haejoon Hahm (HB Solution)
P-122	Elemental distribution analysis of nanoparticles by atom probe tomography	Ji Yeong Lee (Korea Institute of Science and Technology)
P-124	Enhancing nanoscale resolution in AFM images using deep learning algorithm	Jeongwoo Yang (Sungkyunkwan University)
P-126	Evaluation of atomic-level interfacial layer using AFM	Kim Minhyung (Sungkyunkwan University (SKKU))
P-128	Calibration of lateral piezoelectric coefficient in atomic force microscopy	Kim Jina (Sungkyunkwan University (SKKU))
P-130	Enhancement of valley polarization of monolayer transition metal dichalcogenides by plasmonic surface lattice resonance	Changwon Seo (Sungkyunkwan University)

C-001 /	Operando Electrochemistry: NAP-XPS on electrolyte/electrode interfaces – studies of liquid electrolytes and their interfaces to battery cathodes for Lithium ion battery applications	Andreas Thissen (SPECS Surface Nano Analysis GmbH)
C-002	Quantification and reporting of XPS data taken under Near Ambient Pressure conditions – chances and challenges in acquision speed, beam damage, sensitivity, reliability, reproducibility and repeatability	Paul Dietrich (SPECS Surface Nano Analysis GmbH)
C-003	Using lab-based HAXPES for angle resolved XPS reconstructed depth profiles of thin-films	C.J. Blomfield (Kratos Analytical Ltd)
C-004	Using cryo-XPS for XPS analysis of lithium-sulfur battery materials	C.J. Blomfield (Kratos Analytical Ltd)

9th International Symposium on Practical Surface Analysis

Capri Room

Plenary Talk

Chair: Yongsup Park (Kyung Hee University, Korea) Taeeun Hong (Korea Basic Science Institute, Korea)



PL-1 Invited

A Perspective on XPS Challenges, Needs, and Opportunities

Donald R. Baer*

Pacific Northwest National Laboratory, Richland WA 99352 Richland WA, USA *don.baer@pnnl.gov or pakiara@aol.com

The number of published papers using XPS has been growing at an exponential rate [1] while the percentage of those papers appearing in surface science or analysis related journals has been decreasing [2].

This has led to two types of challenges for the XPS community. Increasingly incorrectly analyzed [3] and reported [4] XPS data is appearing in the literature. Unfortunately, a significant amount of faulty data is appearing in high profile journals. Secondly, many users are not taking full advantage of the information that XPS can provide about surfaces and the near surface region of samples. XPS can provide highly useful, and sometimes unique electrical and other property information about the surface region of many types of materials. In addition, there are challenges and opportunities associated with newer XPS technologies [5] such as higher energy XPS (HAXPES) or higher pressure (near ambient pressure) XPS (NAP-XPS). My views on XPS were developed by a career of research that required highly reproducible quantitative surface analysis (AES, XPS and AFM) as well gathering of information that was either uncommon or that required unusual sample preparation and handling. This talk will briefly address: the frequency and nature of problems with XPS data in the literature [3], the scarcity of adequate reporting of data and analysis parameters [4], the status of efforts to address these issues [6, 7], an overview of types of underused nanostructure [8], optical [9] and electronic property [10, 11] information XPS can provide, and thoughts on needs and opportunities associated with HAXPES [5] and NAP-XPS. Addressing these needs and challenges requires efforts by all members of the surface analysis community including knowledge of resources available for XPS analysis, and helping new and casual XPS users recognize problematic data analysis.

^[1] D.R. Baer et al. J. Vac Sci. Technol. A **39** (2021) 021601.

^[2] G.H. Major et al., J. Vac Sci. Technol. A 41 (2023) 038501.

^[3] G.H. Major et al., J. Vac Sci. Technol. A 38 (2020) 061204.

^[4] G.H. Major et al., J. Vac Sci. Technol. A 41 (2023) 043201

^[5] A. Herrera-Gomez et al., Surf. Interface Anal. (2024) doi:https://doi.org/10.1002/sia.7340

^[6] D.R. Baer et al. Surf. Interface Anal. 55 (2023) 480-488.

^[7] J.W. Pinder et al., App. Surf. Anal. Reports 19 (2024) 100534.

^[8] S. Tougaard, Surf. Interface. Anal. 50 (2018) 657-666.

^[9] J.F. Watts, J.E Castle, Surf. Interface. Anal. 56 (2024) 408-424.

^[10] H, Cohen, Appl Phys. Lett. 85 (2004)1271-1273.

^[11] P.A. Gokturk et al., J. Vac Sci. Technol. A 38 (2020) 040805



Evolution and revolution in SIMS

lan S. Gilmore

National Physical Laboratory, Teddington, Middlesex, TW11 0LW, UK *Ian.gilmore@npl.co.ukp

Since the origins of secondary ion mass spectrometry (SIMS), almost nine decades ago, the field has evolved along distinct pathways where a process of natural selection has seen the emergence and decline of techniques as they, in turn, are superseded by new innovations. This has resulted in today's powerful SIMS instruments that are having extraordinary impact in almost every area of materials science and increasingly in the life-sciences[1]. However, independent evolutionary lineages have led to segmentation of the community. Recent advances in instrumentation and advances in fundamental understanding are now beginning to show prospects for evolutionary convergence.

To put this in context, advances driven by a fundamental analytical challenge will be discussed. Techniques, like nuclear magnetic resonance, provide high confidence in identification but with limited information on localisation. Whilst techniques like electron microscopy, give high confidence in localisation but low confidence in identification. This has been termed the "molecular uncertainty principle" [2]. In 2017, NPL introduced the OrbiSIMS technology [3] with an objective to simultaneously provide molecular identification and localisation as close to this limit as possible. Since then, the number of OrbiSIMS instruments around the world has increased significantly and the community of users and range of applications has grown. In this presentation, we briefly introduce the OrbiSIMS and use examples of the applications in advanced materials [4] and life-sciences [5] to highlight a convergence of "static SIMS" and "dynamic SIMS" as some of the traditional barriers begin to disappear. [6] In a look to the future, further advances in mass spectrometers are expected, for example multiple reflection Time of Flight analysers, ion mobility and other novel hybrid analysers as well as improved sensitivity using quantum detection.

^[1] N. P. Lockyer et al. Secondary ion mass spectrometry, Nat Rev Methods Primers 4, 32 (2024)

^[2] A Ali et al, Single cell metabolism: current and future trends. Metabolomics, 2022. 18 (10)

^[3] M K Passarelli et al., The 3D OrbiSIMS-label-free metabolic imaging with subcellular lateral resolution and high mass-resolving power, Nature Methods, 2017. 14 (12): p. 1175-

^[4] G F Trindade et al., Direct identification of interfacial degradation in blue OLEDs using nanoscale chemical depth profiling. Nature Communications, 2023. 14 (1): p. 8066.

^[5] F Zani et al., The dietary sweetener sucralose is a negative modulator of T cell-mediated responses. Nature, 2023. 615 (7953): p. 705-711.

^[6] Y. Zhou et al, OrbiSIMS depth profiling of semiconductor materials-Useful yield and depth resolution J. Vac. Sci. Technol. A 1 September 2024; 42 (5): 053208



Advanced Surface Analysis for the Perspective in Display/Semiconductor Industry

Sung-Chan Jo

Samsung Display Co., Ltd *corresponding. enigma.jo@samsung.com

Surface analysis has been one of the most sophisticated analytical methodologies from the very moment when the matters for monitoring the surface started to matter. After Heisenberg suggested the famous "Uncertainty Principle", classical optical approaches had to admit their limitations and the researchers had dived deep down to the fundamental theories to expand the realm of "tangible" surface probing techniques. The density of the analytical samples and the interferences from surroundings were another serious headache, which eventually led to the acknowledgement of the importance of ultimate vacuum conditions. All the necessities naturally snowball the cost and the applications in the practical area were once very much limited.

Semiconductor business switched the situations substantially and display industry had pushed the necessities further up decades later. When LSI (Large Scale Integrated circuit) and VLSI (Very Large Scale Integrated circuit) were introduced to the market, the quality controls and optimization of the processes were not to be possible without morphological and qualitative characterization. That is where electron microscopic techniques played an inevitable role and the pricy tags were rationalized. Other instrumental approaches such as XPS (X-Ray Photoelectron Spectrometry) and SIMS (Secondary Ion Mass Spectrometry), once only found in academic treatise, became serious players also after the devices require much more materials for the functionality. The situation becomes even further more complex in display industry as many organic layers remain in the final products.

As the world sees more affluent market society, customers get to lay their hands on diverse products with unheard-of functions. The number of pure materials that should cover such functional differences cannot easily fulfill the needs one by one. As a result, many reveal "new" materials but not totally new and products are not utilizing pure stuff by themselves ever any more.

Afterwards, the strength and inevitability of surface science is not found in the tiny thin niche that simply mediates important bodies but seen in the thin layers that allows huge shift in certain properties of a physical structure.

In this presentation, the role of surface analysis is delivered in the field of semiconductor and display. As such businesses are now confronted with much more complicated problems than before, the direction will be discussed through current issues. The importance of combined efforts from different areas is put much emphasis on as well. 9th International Symposium on Practical Surface Analysis

Capri Room, Grand Ballroom I

Luncheon Seminar





12:10-13:30, Nov. 18 (Mon) Capri Room

Introducing the Iliad - the first fully integrated advanced analytical (S)TEM

Paolo Longo, Sorin Lazar, Maria Meledina, Jain Noopur, Peter Tiemeijer, Maarten Wirix.

Thermo Fisher Scientific, Eindhoven, The Netherlands *paolo.longo@thermofisher.com

Over the last decades we have witnessed a tremendous development in advanced transmission electron microscopy. To name a few, probe correctors have become more powerful and now in combination with ultra-brightness electron sources 60 - 70pm spatial resolution in STEM can be routinely reached with nearly 1nA probe current, improvements in energy resolution have led to phonon spectroscopy, EDS detector systems have become 6x more efficient and sensitive with the latest generation leading to low-dose data collection and in-situ analytical studies, detectors are now capable to count electrons dramatically reducing the contribution of instrumental noise and that has led to the revolution in cryo-EM.

Very recently with the market introduction of the Iliad (S)TEM microscope platform, Thermo Fisher Scientific has brought, for the very time, full microscope hardware and software integration that now extends and includes the Iliad EELS spectrometer and energy filter and the NanoPulser the Ultrafast Electrostatic Beam Blanker ESBB. Multimodal integration of EELS, EDS and the NanoPulser ensures the most advanced and effective electron dose optimization strategies. EELS data collection is extended with the ease-of-use of Velox software ecosystem making the most challenging experiments now accessible to every user including novices. Nearly every component in the Iliad platform can be fully accessed via Python scripting using Autoscript and that opens the possibility of creating new data collection workflows as well as the adoption of Artificial Intelligence based data collection and processing strategies.



12:10-13:30, Nov. 19 (Tue) Capri Room

The new CAMECA NanoSIMS-HR

Aurélien Thomen^{*}, Marc Debliqui, Céline Defouilloy, Laurent Arnoldi, Nicolas Saquet, Sarah Vitcher Fichou, Jérôme Farcy, and Ludovic Renaud

> CAMECA,29 Quai des Grésillons, Gennevilliers 92230, France *aurelien.thomen@ametek.com

CAMECA introduces the new NanoSIMS-HR product as the successor of the NanoSIMS 50L secondary ion mass spectrometer characterized by its high lateral resolution, high transmission, and high mass resolution. Several improvements have been made compared to the established NanoSIMS 50L:

(1) A more accurate imaging capability thanks to an improved Cs^+ source reducing the lateral resolution down to ≤ 30 nm and thus dramatically limiting lateral dilution of isotopic and elemental composition of the measured surface.

(2) A more accurate depth profiling capability thanks to a primary beam energy from 16 keV to 2 keV reducing the ultimate depth resolution down to 12 nm/dec.

(3) A capability to image elemental and isotopic compositions of volatile-rich samples such as fluid inclusions, soft materials, and biological samples with a cryogenic system.

(4) A capability to measure highly reactive samples such as Lithium batteries using a customized glovebox providing a low-humidity and inert atmosphere.

(5) An overall analysis throughput improvement thanks to an ultra-accurate sample stage reproducibility delivering a 10-fold decrease in acquisition time of unattended chained analysis and a remote sample holder exchange between the analysis chamber and the 8-slots storage room within 5 minutes.

New results of isotopic analysis of fluid inclusions in quartz will be presented at the conference.



The New NanoSIMS-HR



12:10-13:30, Nov. 19 (Tue) Grand Ballroom I

Latest developments in X-ray photoelectron spectroscopy and their application to new materials discovery

CJ Blomfield^{*}, JDP Counsell, AJ Roberts

Kratos Analytical Ltd, Wharfside, Trafford Wharf Rd, Manchester, M17 1GP, UK *chris.blomfield@kratos.co.uk

X-ray photoelectron spectroscopy is a mature surface analysis technique and the Kratos Axis Supra⁺ is a well established instrument for both high throughput routine analysis as well as cutting edge research applications.

Recent developments of the ESCApe datasystem aid automated turnkey operation of the spectrometer to provide consistent results, independent of the operators experience with the aim of producing more reliable and statistically consistent data

Examples of the capabilities of small area analysis combined with the Gas Cluster Ion Source (GCIS) for depth profiling medical devices, illustrated with analysis of bio-degradable stents will be shown. Higher energy X-ray sources for slightly deeper surface analysis which also permits the excitation of deeper core levels will be illustrated through analysis of Hf based thin films.

Analysis of battery related materials by XPS is becoming more common and examples will illustrate the benefits of sample cooling to retain critical surface chemistry. A new cryo-XPS capability will also be introduced with examples of analysis of organic solvents at UHV conditions.



12:10-13:30, Nov. 20 (Wed) Capri Room

The latest progress of CIQTEK electron microscope technology

YITONG LIU

CIQTEK Co., Ltd. *lyt@ciqtek.com

This report will introduce the characteristics of several CIQTEK "star products" and the latest technological progress of CIQTEK electron microscopes, mainly including SEM3200 normal scanning electron microscope, SEM5000X ultra-high resolution field emission scanning electron microscope, FIB-SEM DB550 dual-beam electron microscope and HEM6000 high-speed scanning electron microscope. In the field of normal scanning electron microscopes, CIQTEK can now achieve a level comparable to international brands, with the flagship model being SEM3200; in field emission electron microscopes, SEM5000X shows the highest resolution level of CIQTEK SEM, which is positioned as a high-end electron microscope product; the FIB dual-beam electron microscope DB550 adopts self-developed electron column and ion column, which can realize the processing of any cross-section of the sample and easily prepare TEM samples; HEM6000 is a high-speed scanning electron microscope that can realize cross-scale and large-scale sample imaging. It adopts a unique column design, which ensures resolution while achieving an imaging speed of more than 5 times that of a conventional field emission scanning electron microscope. In the future, CIQTEK will continue to deepen the research in the field of electron microscopes and expect to bring more advanced products and better services to everyone.



12:10-13:30, Nov. 20 (Wed) Grand Ballroom I

Novel instrumentation for routine surface chemical analysis of challenging samples

Paul Dietrich, Francesca Mirabella and Andreas Thissen*

SPECS Surface Nano Analysis GmbH, Voltastrasse 5, 13355 Berlin, Germany *andreas.thissen@specs.com

Over the last decades XPS under Near Ambient Pressure (NAP) conditions has demonstrated its promising potential in a wide variety of applications, especially for measurements of challenging samples. Starting from operando studies of surface reactions in catalysis, the applications soon have been enhanced towards studies of processes at liquid surfaces, mainly using freezing/melting cycles, liquid jets or liquid films on rotation disks or wheels. Since more than 15 years, the need for basic studies off fundamental solid-liquid interface chemistry has attracted growing interest. Dip-and-pull experiments at synchrotron sources finally also demonstrated, that in-situ and operando XPS in electrochemical experiments can be realized, significantly contributing to the basic understanding of modern energy converting or storing devices, like batteries, fuel cells, etc.

The development of pure laboratory NAP-XPS systems with optimized sample environments, like special sample holders, Peltier coolers and operando liquid cells combined with full automation and process control provides possibilities for preparation and analysis of a multitude of liquid samples or solid-liquid interfaces on a reliable daily base. Finally with EnviroESCA a tool for routine analysis of samples by NAP-XPS has been established in several laboratories.

But liquids are not the only challenging samples. Analysis examples from the categories food, biomaterials porous insulators, and related materials will be presented in different atmospheres, even including plasma environments.

Changing gears, also the interest of semiconductor researchers in XPS with higher information depths is constantly increasing. Thus, a new concept for non-destructive depth profiling with variable energy XPS will be presented. The tool that allows for such analyses is the EnviroMETROS. It is a fully automated routine analysis machine for XPS depths profiling allowing for different sample sizes, even including 8" and 12" wafers.



12:10-13:30, Nov. 21 (Thu) Grand Ballroom I

Converging AFM Solutions: Pioneering Nanotechnology for Advanced Industries

Sang-Joon Cho*

Park Systems Corp., Republic of Korea *corresponding.msjcho@parksystems.co.kr

The rapid advancement of industries, particularly the semiconductor sector, has outpaced traditional research methods and technological developments in academia. To sustain this momentum, research methodologies and technological innovations must evolve in tandem. This necessity has brought scanning probe microscopy (SPM) technology, capable of providing detailed nanometer-scale information, into the spotlight. Among these technologies, the versatile Atomic Force Microscopy (AFM) has found numerous applications within the semiconductor industry.

In this seminar, we will explore SPM's unparalleled capabilities in nanoscale imaging and characterization, showcasing its transformative impact across disciplines-from materials science to biological research. Through compelling case studies, we will demonstrate how SPM-driven collaborations are accelerating innovation in semiconductor development and enhancing the relevance of academic research. These outcomes will also equip students with the skills needed for high-demand careers in a fast-evolving landscape.

Join us to discover how this powerful technology is not just bridging the nano-world, but also closing the crucial gap between theoretical knowledge and practical application, propelling both academia and industry towards new frontiers of excellence in the semiconductor era.

9th International Symposium on Practical Surface Analysis

Capri Room

S1. Standardization and Pre-standardization

Chair: Seung Mi Lee (KRISS, Korea) David Cant (National Physical Laboratory, UK)





A Roadmap to HAXPES Standardisation

David J H Cant^{1*}, Benjamen P Reed¹, Ben F Spencer², Wendy R Flavell², and Alexander G Shard¹

¹National Physical Laboratory, Hampton Road, Teddington, UK 2The University of Manchester, Oxford Road, Manchester, UK *david.cant@npl.co.uk

Electron spectroscopy techniques such as X-ray Photoelectron Spectroscopy (XPS) and Auger Electron Spectroscopy (AES) have been in active use for more than 50 years. During this time, a wealth of analytical methods, protocols, calibration techniques and general metrology have been developed, in particular for XPS using Al K α X-rays at 1486 eV, which are the most commonly used. Although issues remain in the day-to-day application of these techniques by non-expert users, the metrology of the technique can be considered relatively mature. Throughout this development, the translation of this work into international standards has been consistent as calibration and analysis methods have been formalized through bodies such as ASTM International and the International Organization for Standardization (ISO). With the publishing of the first intensity calibration standard for XPS this year (ISO 5861), standards are now available for all the core metrology necessary to conduct basic, quantitative XPS.

New measurement techniques, non-standard applications, and developments in instrument technology, however, can lead to new metrology needs. With the development of off-the-shelf laboratory-based instrumentation for high-energy XPS (HAXPES), and its ensuing proliferation, the existing body of standards must be updated to cover the new systems now commonly available and in use around the world. For some standards, only minor updates are required, as with the recently revised standard for the use of sensitivity factors in XPS (ISO 18118). For other aspects however, such as energy scale and intensity calibration, new developments or extensions to the existing metrology are required, and interlaboratory comparisons needed, before standardization can be achieved[1-2]. Here we present a roadmap for HAXPES standardization, to be developed through the Electron Spectroscopies subcommittee (SC7) of ISO TC/201 - Surface Chemical Analysis. The key requirements for reliable, quantitative HAXPES measurements will be outlined, as well as the intended route by which these requirements will be achieved, validated, and standardized.

Herrera-Gomez A, Cant DJH, Conard T, et al. New challenges associated with hard X-ray photoelectron spectroscopy (report on the 2023 ASTM E42-ASSD AVS workshop). Surf Interface Anal. 2024; 1-7. doi:10.1002/sia.7340

^[2] Kateryna Artyushkova, Stuart R. Leadley, Alexander G. Shard; Introduction to reproducible laboratory hard x-ray photoelectron spectroscopy. J. Vac. Sci. Technol. A 1 September 2024; 42 (5): 052801. doi:10.1116/6.0003740



Standardization of Medium Energy Ion Scattering Spectrometry

Jiho Song, ILC participants, and P. L. Grande, Won Ja Min*

HB solution, Techno 8ro 33, Yuseong-gu Daejeon, Republic o Korea, 34028 *wj.min@hb-solution.co.kr

MEIS (Medium Energy Ion Scattering) is a surface analysis technology that allows quantitative depth profiling of ultra-thin films with single atomic layer resolution.[1] In recent years, as the layer used in industry have become ultra-thin, the demand for MEIS analysis is increasing. As the scope of MEIS use is expanding, standardization of MEIS analysis and measurement are needed to ensure consistency of MEIS analysis.

To obtain a compositional depth profile from a MEIS spectrum, the spectrum is usually fitted using an ion scattering simulator after measurement. From 2015 to 2017, two interlaboratory comparisons (ILCs) using HfO₂ films with nominal thicknesses of 1, 3, 5 and 7 nm were performed at 12 institutions to standardize the analytical parameters used in the fitting process. The results of this study confirmed that accurate electronic stopping cross section is important for quantitative MEIS analysis. When using electronic stopping cross section based on experimental data, the standard deviation of results was 7.3% for composition, 4.5% for thickness and 7.0% for Hf quantity. This is a significant improvement compared to the results using SRIM (Stopping and Range of Ion in Matter) 95 (standard deviation of 5.3% for composition, 15.3% for thickness, and 13.3% for Hf content).[2] From these results, ISO 23170 "Non-destructive depth profiling of nanoscale heavy metal oxide thin films on Si substrates with medium energy ion scattering" was published.

Measurement parameters must also be well established to obtain valid results. For this purpose, an VAMAS interlaboratory comparative study was proposed from 2023, using PtxNi1-x alloy samples (nominal x = 0, 0.2, 0.35, 0.5, 0.65, 0.8, 1) of approximately 7 nm thick. We proposed four parameters as important measurement conditions: beam energy, scattering angle, mcp detector voltage, and no multiple hits condition. 8 groups participated, the content of Pt and Ni and the ratio of Pt/Ni were analyzed from the data sent by the participants to confirm the dispersion of results between laboratories. We would like to standardize the method of establishing measurement parameters from the analysis results of this ILC.

^[1] W.K. Chu, James W. Mayer and Marc-A. Nicolet, Backscattering Spectrometry (Academic Press, Orlando, 1978).

^[2] W.J. Min, G. Marmitt, RRT Participants, P.L. Grande and D.W. Moon, Surf. Interface Anal., 51 (2019) 712.



Standardization Activities in ISO TC 201 (Surface Chemical Analysis)

Hidehiko NONAKA^{*}

University of Tsukuba, 1-1-1 Tennodai Tsukuba, Ibaraki 305-8577, Japan *nonaka.hidehiko.gn@u.tsukuba.ac.jp

ISO TC 201 was established in 1991 as one of the ISO technical committees to promote the standardization in the field of surface chemical analysis. The committee has been managed by JISC, the Japanese Industrial Standards Committee, as secretariat, and currently consists of thirteen participating (P-) members (the member bodies of countries), and twelve observing (O-) members. The scope of the TC includes analytical techniques in which beams of electrons, ions, neutral atoms or molecules, or photons are incident on the specimen material and scattered or emitted electrons, ions, neutral atoms or molecules, or photons are detected as well as techniques in which probes are scanned over the surface and surface-related signals are detected [1]. The specific analytical methods within the scope include Auger electron spectroscopy, X-ray photoelectron spectroscopy, secondary ion mass spectrometry, glow discharge spectroscopy, X-ray Reflectometry and X-ray Fluorescence Analysis, and scanning probe microscopy. The TC is actively expanding the scope of methods related to surface chemical analysis, such as confocal fluorescence microscopy and Surface Plasmon Resonance spectroscopy.

The parent TC and its subcommittees and working groups have developed more than 120 standards including the revised editions, 83 of which are currently in effect and available at the ISO online store or elsewhere. The standards standardize what is essential when performing surface chemical analysis, including the terminology, determination of measurement conditions, guidelines for sample preparation, calibration methods, reporting formats, industrial applications and so on. After a standard is published, it is reviewed every five years and updated as necessary to meet the needs of the user industry at that time. The standards have become increasingly important as guidelines for correct acquisition and interpretation of measurement data, since nowadays, because of the automation of analytical equipment, measurements can be made without knowing the details of the principles and techniques of the measurement methods [2].

The structure, history, strategy and recent activities of TC 201 will be discussed from the perspective of the former chair of the TC.

^[1] https://www.iso.org/committee/54618.html.

^[2] Donald R. Baer, Gary E. McGuire, Kateryna Artyushkova, Christopher D. Easton, Mark E. Engelhard, and Alexander G. Shard, J. Vac. Sci. Technol. A39 (2021) 021601.



Quantitative Analysis of Binary Alloy Films by Surface Analysis Methods in CCQM-SAWG

Seung Mi Lee*

Korea Research Institute of Standards and Science, 267 Gajeong-ro, Yuseong-gu, Daejeon 34113, Korea *seungmi.lee@kriss.re.kr

The quantitative analysis of alloy films has been an important subject for key comparison (KC) of the Surface Analysis Working Group (SAWG) of the Consultative Committee for Amount of Substance (CCQM). The equivalence of measurement has been established by National Metrology Institutes (NMIs), which participate in the KCs. In SAWG, two KCs for the quantitative analyses have been performed: K67 for Fe_xNi_{1-x} alloy films[1] and K129 for Cu(In,Ga)Se₂ films[2].

Among various methods for surface analysis, Auger electron spectroscopy (AES) and X-ray photoelectron spectroscopy (XPS) are generally used for the surface compositional analysis of multi-element alloy films. However, accurate composition analysis is difficult due to matrix effects which are affected by the atomic density, attenuation lengths of electrons, and the electron backscattering factor in the matrix materials. Isotope dilution inductively coupled plasma mass spectrometry (ID ICP-MS) is a primary method to determine the composition of alloy films. In a recent study for Ag_xCu_{1-x} alloy films, the mole fractions measured by Rutherford backscattering spectroscopy (RBS) and ID ICP-MS showed a great agreement within a 0.4% difference.[3] It suggests that RBS may act as a practical reference for the quantitative analysis of alloy films, although it requires more evidence from the measurements of other materials.

Currently, the quantitative analysis of Pt_xNi_{1-x} alloy films is being studied by eight NMIs as a pilot study P229 by CCQM-SAWG. The mole fractions of the five Pt_xNi_{1-x} alloy films were certified by ID ICP-MS and RBS and used as the basis for the quantification of alloy films. In this CCQM pilot study, the mole fractions of Pt_xNi_{1-x} alloy films were measured by various surface analysis methods such as XPS, X-ray fluorescence (XRF) and scanning electron microscopy (SEM) with energy dispersive X-ray spectrometry (EDX). Nine data sets from eight countries were collected. The current status of our analysis and the feasibility of RBS data as the practical reference in the quantitative analysis of alloy films will be shown in this presentation.

^[1] K. J. Kim et al., Metrologia 47 (2010) 08011.

^[2] K. J. Kim et al., Metrologia 53 (2016) 08011.

^[3] T. G. Kim et al., Metrologia 58 (2021) 065004.

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Capri Room

S2. Theory and Simulation

Chair: Samuel Bertolini Da Silva Oliveira (Université catholique de Louvain, Belgium) Aleksander Jablonski (Polish Academy of Sciences, Poland)





Parameters needed for simulations of electron transport in condensed matter

A. Jablonski^{*}

Institute of Physical Chemistry, Polish Academy of Sciences, ul. Kasprzaka 44/52, 01-224 Warsaw, Poland *e-mail: ajablonski@ichf.edu.pl

The Monte Carlo (MC) approach is a universal tool for describing electron transport in condensed matter and for developing descriptive formulas applicable to quantitative applications of XPS and other electron spectroscopies. Any MC simulation strategy requires implementation of samplers that generate certain parameters that are needed for determining an electron trajectory in the surface region of a sample material. Two parameters are of considerable importance in MC strategies: (i) the cross sections for elastic scattering of electrons by atoms in the surface region, and (ii) the electron inelastic mean free path (IMFP).

The probability of elastic scattering by a certain angle is related to the differential cross-section (DCS). While numerous sources of DCSs are available, the DCS can also be conveniently expressed as a series of Legendre polynomials. For this representation, we need the expansion coefficients A_l , l = 0, 1, 2, The DCSs from the series expansion are accurate typically within 5-6 decimals for energies up to 20 keV.. The relevant calculations turn out to be very fast. Furthermore, the dependence of the A_l coefficients on electron energy is very smooth which facilitates interpolation to a needed energy. Practical MC simulations require a sampler of elastic scattering angles for elements of interest and for a wide energy range. A suitable sampler based on the vector of A_l coefficients has recently been developed. Care was taken to ensure high accuracy for electron energies of hard X-ray photoelectron spectroscopy (HAXPES)..

A frequently used source of IMFPs is the TPP-2M predictive formula that was derived from a set of calculated IMFPs for energies up to 2 keV. A new IMFP predictive formula, designated as the JTP equation, has recently been developed from a set of calculated IMFPs for 100 materials and for electron energies between 50 eV and 200 keV [1]. It was shown that the accuracy of the new predictive formula was distinctly better than accuracy of the TPP-2M equation.

IMFPs can also be determined by elastic peak electron spectroscopy (EPES). These values are derived from measurements of the signal intensity of electrons elastically backscattered from a surface at a given electron energy. Measurements are typically made of the ratios of backscattered electrons from the sample of interest and a chosen reference material for which the IMFP is known. MC or other calculations are required to determine the elastic backscattered intensities from both materials. The accuracy of the derived IMFPs is estimated to be about 10% for electron energies above about 200 eV, and this value can be tentatively recommended as the lower limit of applicability of EPES.

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Innovative Sample Structure Prediction using Bayesian Estimation and XPS Simulator

Hiroshi Shinotsuka^{1*}, Kenji Nagata¹, Hideki Yoshikawa¹, Hayaru Shouno², and Masato Okada³

¹National Institute for Materials Science, 1-1 Namiki, Tsukuba, 305-0044, Japan ²The University of Electro-Communications, 1-5-1 Chofugaoka, Chofu, Tokyo 182-8585, Japan ³The University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa, Chiba 277-8561, Japan *SHINOTSUKA.Hiroshi@nims.go.jp

In recent years, the application of data science techniques has become increasingly prevalent in the analysis of measurement data. In the case of X-ray photoelectron spectroscopy (XPS), it is possible to simulate spectra using the Simulation of Electron Spectra for Surface Analysis (SESSA) simulator, given information about the sample structure, type of incident X-ray, and the geometric configuration of the measurement apparatus. Traditionally, manually adjusting the simulation parameters is a labor-intensive task. To address this challenge, we have developed a framework that incorporates the SESSA simulator into Bayesian estimation to solve the inverse problem of XPS [1]. This framework automates the tedious task of manually tuning the sample structure parameters within the simulator, allowing us to derive a comprehensive understanding of the distribution of plausible sample structures from the measured XPS data.

As an example, we performed virtual experiments of angle-resolved XPS on a four-layered sample, and estimated the sample structures based on the XPS intensity data obtained from experiments. We succeeded in not only obtaining an optimal solution, but also visualizing the distribution of the solution through the Bayesian posterior probability distribution.

This method of combining simulators with Bayesian estimation for data analysis is expected to become more widespread in the future, offering a more efficient and comprehensive understanding of measurement data.

H. Shinotsuka, K. Nagata, M. Siriwardana, H. Yoshikawa, H. Shouno, M. Okada, J. Electron Spectroscopy and Related Phenomena. 267 (2023) 147370. https://doi.org/10.1016/j.elspec.2023.147370.



Molecular dynamics simulations of gas cluster induced protein desorption, transfer and soft/reactive landing

S. Bertolini and A. Delcorte

Université Catholique de Louvain

The bombardment of a protein film target by an energetic argon cluster ion beam induces the emission of neutral and ionized molecules in the gas phase. The ions can be used for an analytical purpose, after their extraction, separation and detection using a mass spectrometer [1]. Recently, it was shown that the whole emitted flux can also be transferred onto a collector in the vacuum environment, without damaging their structure and bioactivity, a soft-landing process allowing to build (bio)molecular multilayers with nanometric thickness resolution (iBEAM method). Using cluster-induced soft-landing, bioactive lysozymes (14 kDa), trypsin (24 kDa) and glucose oxidase (65 kDa) were successfully transferred on silicon, gold and polymeric collectors [2].

In this contribution, we focus on the elucidation of the mechanisms of cluster-induced desorption and soft or reactive landing, via molecular dynamics (MD) simulations employing a reactive force field (ReaxFF). First, we investigated the influence of the target surface nature and the Ar cluster beam properties (including size and velocity) on the emission process, particularly focusing on protein fragmentation, denaturation, and desorption of non-covalent clusters [3,4]. The simulations revealed a correlation between lysozyme fragmentation and the cluster energy per atom (E/n), as well as an additional influence of cluster size for a given E/n. The organic target's structure significantly affects emission, with a softer desorption occurring as the amount of organic material increases. For lysozyme bilayers, non-covalent aggregates could be desorbed with minimal protein denaturation [3]. For a larger enzyme, glucose oxidase, our results show that intact desorption only occurs when the molecule is lying on a protein "mattress", while only enzyme fragments are emitted when the substrate is gold. Second, our simulations elucidated the landing mechanisms of lysozymes and their fragments on various collectors (gold and hydrogen-terminated graphite) [5]. The findings emphasize the conditions necessary for soft and reactive landing on rigid surfaces, considering factors such as protein structure, energy, incidence angle, and adhesion forces with the collector substrate. The insights obtained in this second series of simulations are broadly applicable to other soft and reactive landing techniques used for biomolecules, including ESI and MALDI. Overall, our ReaxFF-based MD simulations provide a theoretical framework to the desorption and soft-landing of proteins induced by large gas clusters, crucial for the prediction and explanation of the experimental observations.

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Smart Algorithm for Three-Dimensional AFM Imaging of High Aspect Ratio Nanostructures

Imtisal Akhtar and Yongho Seo

Faculty of Nanotechnology & Advanced Materials Engineering and HMC, Sejong University, Seoul 05006, Republic of Korea E-mail address: yseo@sejong.edu

Three-dimensional (3D) imaging of nanostructures with high aspect ratio features is crucial for advancements in nanoscience and technology. Various experimental methods have been proposed to enhance 3D imaging capabilities, including novel probes and algorithms such as the flared tip method and probe tilting approach. However, current methods primarily focus on imaging deep trenches, with limited exploration into precise imaging of arbitrarily shaped structures.

In this study, we introduce a tuning fork-based atomic force microscopy (AFM) technique that addresses these challenges by utilizing a novel 3D scanning algorithm. We achieved high-resolution measurements of depth and sidewall topography in porous materials, such as anodic aluminum oxide, and silicon nanopillars (protrusions). The AFM probe, fabricated with a carbon nanotube and tungsten tip, exhibited a high aspect ratio (ranging from 5 to 25). This allowed us to image hole depths up to 1 μ m in silicon via holes.

The 3D scanning algorithm is based on sidewall contact within a hole, following the rim of the sidewall in the XY plane. This approach is fundamentally different from conventional raster scanning. As a result, we obtained artifact-free images of the sidewall and bottom edge of the hole. Our findings demonstrate the potential of an intelligent scanning algorithm, combined with a high-aspect-ratio probe, to accurately characterize 3D topographical nanostructures.

This technique offers significant potential for non-destructive imaging across a wide range of industrial applications. The experimental results provide compelling evidence that this method can be extended to complex nanostructures with arbitrary morphologies. Unlike previous methods, which relied on highly specialized probes limited to specific nanostructures like trenches, our approach has the unique advantage of being able to image a diverse array of morphological features, whether they are above or below the primary scanning surface.

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Nondestructive Nanoscopy through Bifurcation-Controlled Nonlinear Dynamics of Micro-Cantilever

Manhee Lee^{1*}, Sang-Joon Cho^{2*}

¹Department of Physics, Research Institute for Nanoscale Science and Technology, Chungbuk National University, Cheongju 2864, South Korea

> ²Park Systems Corporation, 109 Gwanggyo-ro, Yeongtong-gu, Suwon 16229, Gyeonggi, Korea *mlee@cbnu.ac.kr, msjcho@parksystems.com

Atomic force microscopy (AFM) [1] has demonstrated the ability to image surfaces and subsurfaces of conductors, semiconductors, and insulators at atomic resolution. This imaging capability of AFM is provided by a highly sensitive micro-cantilever that can probe universal atomic forces between the tip and the sample, such as van der Waals forces, Pauli and ionic repulsions. To detect these atomic interactions, the tip is approached to the sample surface within a few nanometers, while scanning over the sample. Imaging at such a close proximity often causes damage to both the tip and the sample, limiting the reproducibility and reliability of AFM [2]. Therefore, achieving non-contact, nondestructive imaging is a challenge in atomic force microscopy.

Here, we demonstrate theoretically and experimentally non-contact, nondestructive atomic force microscopy. In essence, we implement a fast and accurate feedback control system, while monitoring the phase shift and amplitude change of the cantilever motion, to ensure that the dynamic regime of the cantilever remains within the range of attractive van der Waals interaction [3]. We show that the tip condition did not change after tens of consecutive scans over a sample, and all scanned images were nearly identical to the first image obtained. Atomic force microscopy is now a nondestructive, reliable, and reproducible imaging tool, which could be used for dimensional metrology in semiconductor manufacturing and material characterization.

Keywords: atomic force microscopy, noncontact imaging, nonlinear dynamics, bifurcation, amplitudemodulation.

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S3. Data Analysis and Treatment

Chair: Satoka AOYAGI (Seikei University, Japan) Sang-Joon Cho (Park Systems, Korea)





Towards a common data file format for hyperspectral images

Alex Henderson

The University of Manchester, Oxford Road, Manchester, UK alex.henderson@manchester.ac.uk

Most funding organisations in Europe, USA, and increasingly worldwide, require data from projects they support, be published in an open manner. The acknowledged best-practice for this is to follow the 'FAIR Guiding Principles for scientific data management and stewardship' [1]. These principles lay out recommendations for both the way data should be presented, and the metadata relating to the experiments or studies that produced those data. The FAIR Principles define four interlinked categories, by which data should be Findable, Accessible, Interoperable and Reusable.

In the surface analysis community we may share our data, but it is not easily interoperable or reusable by those outside our immediate circle. This not only prevents our data being reused by others in their own research, but also inhibits the development of third-party data analysis packages which could grow the technique in unforeseen directions. In other fields, such as astronomy, microscopy, and climate studies, file format solutions have been developed that the SIMS community could benefit from.

It is important to note that FAIR does not imply Open. However, even in scenarios where data cannot be openly shared, for example in a commercial setting, it can still be beneficial to allow data to flow within the business; for example, between sites, and to more easily access open source software.

The FAIRSpectra Initiative [2] aims to present options in a vendor-neutral environment and develop an open conversation to benefit the field as a whole.

In this presentation we explore some of these options for storing the hyperspectral data, and discuss their benefits. In addition, we present the metadata requirements the community must agree upon to facilitate take-up of any proposed solution.

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XPS/HAXPES, and NAP-XPS, for Characterization of Nano-Structured Materials

Sven Tougaard

Department of Physics, Chem. and Pharm., University of Southern Denmark, Odense M, Denmark email: svt@sdu.dk

Quantitative characterization of nanostructures by analysis of the inelastic background in photoelectron spectroscopy (XPS and HAXPES) is now a widely used method. [1] In the talk, we report on recent advancements of this method. First, we discuss the application to characterize core-shell nanoparticles (CSNPs) and show that both the shell thickness and its heterogeneity can be accurately determined, and it also correctly proves if the shell material fully encapsulates the core or if part of the core is uncoated [2]. Further, we recently showed how the method can be applied to very accurately correct ambient pressure XPS for the spectral distortion caused by the gas [3].



The only input in the method, besides the IMFP, is the cross section for inelastic electron scattering. For cases with stacks of layered materials that have widely different cross sections, this quantity is taken as the weighted average of the involved materials. [4] For cases where the involved cross sections are unknown, we recently showed that an optimized cross section, that is determined as part of the fitting procedure, can reliably be determined without any knowledge of the sample composition [5].

The method is non-destructive, and the probing depth is considerably larger than the usually quoted 3 IMFP because the inelastically scattered electrons originate from larger depths than the electrons in the peak and it is typically ~8 IMFP but can be ~20 IMFP in cases where the background can be followed over several hundred eV. The latter is often the case with HAXPES because the separation between deep lying core electrons can be much larger compared to conventional XPS. With HAXPES, the photo electron energy and thereby the IMFP and the probing depth is also increased and several examples with analysis of structures at > 100 nm depth have been reported [4,6]. Since lab based HAXPES is now commercially available it is being installed in many labs and its application in nanotechnology is expected to rapidly increase considerably.

Detailed tutorial videos of several of the examples discussed in the talk are available in [7].

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Surface composition of Sc and ScN by XPS

Stanislav Cichoň*, Joris More-Chevalier, Michal Novotný and Ján Lančok Institute of Physics, the Czech Academy of Sciences, Na Slovance 1999/2, Prague 18200 Czechia *e-mail: cichon@fzu.cz

ScN is an emerging medium width band gap semiconductor material for applications in the field of advanced electronic devices such as thermoelectrics, acoustic wave resonators, piezoelectrics and others [1-3]. It is a nitride with a cubic rocksalt structure and a very high melting point [4-6]. It is used either pure or in the form of ternary systems such as AlxSc1-xN [7]. ScN represents a borderline nitride between ionic nitrides and transition metal nitrides which is indeed reflected in its properties [8, 9]. ScN seems to be the only compound within the Sc-N binary system [10].

Chemical composition of ScN thin films can be easily elucidated by X-ray Photoelectron Spectroscopy (XPS). Many papers dedicated to the XPS of ScN can be found [11]. On the other hand, XPS knowledge base of Sc has been rather limited so far compared to other elements. In this study, we performed combined XPS analysis of Sc and ScN films endeavored to extract more information about chemistry of both. The films were prepared by sputtering deposition and characterized by several microscopy and spectroscopy techniques. After optimal deposition conditions were found, the resulting high quality samples were selected for the XPS analysis. What is important in this study is that both sample synthesis and characterization were performed under high purity conditions.

As received ScN surfaces are composed of ScN covered by a native Sc oxide / hydroxide and adventitious carbon contamination in the form of hydrocarbons, oxygen derivates of hydrocarbons and Sc carbonate. Regarding a clean ScN surface, accessing it (by sputter etching or annealing) poses difficulties due to the Sc reactivity. For an air aged ScN material, the proportion of non-nitride components increases in time as a result of the reaction with the atmosphere, but no qualitative changes are apparent. It remains an open question whether the ageing process can reach a kind of saturation, or the surface can passivate. The resistance towards degradation depends on the microstructure which is controlled by synthesis technology.

Comparing ScN surfaces to Sc surfaces, Sc surface is appreciably more reactive. The Sc surface composition is very similar to that of ScN except nitride bonds of course; a native oxide / hydroxide covers the metallic Sc beneath. Accessing a clean Sc surface is even more difficult. A cross comparison of ScN and Sc suggests that interpretation of chemical analysis does not have to include oxynitride phases which may be otherwise found at nitrides of other elements.

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Transformative Data Insights: Advanced Hybrid Nano-Metrology for High-Resolution Material Characterization

Sang-Joon Cho^{*}, Yunkyung Lee

Park Systems Corp, KANC 4F, Gwanggyo-ro 109 Suwon, South Korea Fax: +82-(31)-546-6806 E-mail address: msjcho@parksystems.com

Atomic Force Microscopy (AFM) is a powerful tool for nanoscale imaging, manipulation, and material property characterization, offering sub-nanometer resolution in three dimensions. AFM can simultaneously provide electrical, nanomechanical, and chemical information, yielding comprehensive data from a single instrument. However, numerous parameters, such as tip material, shape, and environmental conditions, can influence the data. The importance of AFM analysis is growing due to the need to investigate and characterize innovative nanomaterials. Recent advances in AFM technology, combined with other metrological techniques like White Light Interferometry (WLI), Photo-induced Force Microscopy (PiFM), and Imaging Spectroscopic Ellipsometry (ISE), expand its application area. Hybrid AFM technology enhances the ability to provide chemical composition information at the nanoscale, alongside physical properties and mechanical behavior. As complex hybrid measurement technologies are applied to high-resolution material research, data analysis and processing technologies must also advance.



Data-driven analysis of spectrum and image data

Satoka Aoyagi*

Faculty of Science and Technology, Seikei University, 3-3-1 Kichijoji-kitamachi, Musashino, Tokyo *aoyagi@st.seikei.ac.jp

More sophisticated surface analysis machines are being developed, providing more complex and larger data. Analysis of such complex data is needed to extract useful information from the rawdata of surface analysis. For example, time-of-flight secondary ion mass spectrometry (ToF-SIMS) provides detailed chemical structure information and images of molecular distribution with high spatial resolution, and therefore has been applied to a wide range of fields from metals and semiconductors to organic devices and biological samples. Although ToF-SIMS provides extremely rich information, it is often difficult to understand all the information from ToF-SIMS results and only part of the information is interpreted. Machine learning methods such as techniques based on multivariate analysis have been applied to the interpretation of complex ToF-SIMS data, and more recently flexible machine learning methods including deep learning are often applied[1]. Unsupervised learning methods such as principal component analysis (PCA) are useful for extracting important features from complex sample data sets[2]. On the other hand, supervised learning methods are useful for quantitative analysis and identification of unknown materials in a sample[2-5]. Although artificial neural network (ANN)-based methods, so-called deep learning, are flexible for characterizing many of the chemical and physical phenomena, the learning processes are generally difficult to understand. However, the learning processes are necessary for further analysis, e.g. important mass peaks related to a particular material are needed to obtain detailed images. Then narrow deep learning using an ANN system containing one hidden layer has been applied to quantitative analysis based on whole mass spectra[2,3]. In terms of the identification of unknown materials in a sample, Random Forest, a decision tree-based supervised learning method, has been applied to ToF-SIMS spectra of peptide and organic samples[4,5]. In addition, machine learning application to electron backscatter diffraction (EBSD) raw data, Kikuchi patterns, is also useful to extract the information on unknown crystal structures[6].

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X-ray Emission Spectroscopy Data Processing and Analysis Using Artificial Intelligence.

In-Hui Hwang^{1*}, Chengjun Sun², Shelly D. Kelly², Maria K. Y. Chan³, Ik-Seon Kwon¹, Jehan Kim¹, and Ki-Jeong Kim¹

¹Pohang Accelerator Laboratory, POSTECH, Pohang 37673, Republic of Korea ²X-ray Science Division, Argonne National Laboratory, Argonne, IL 60439, USA ³Center for Nanoscale Nanomaterials, Argonne National Laboratory, Argonne, IL 60439, USA

The dispersive configuration spectroscopy using a position sensitive detector (PSD) has been widely used to obtain high-resolution X-ray emission spectra (XES). This experimental design takes considerable time to calibrate and transform the data, making it difficult to identify spectral features during beamline experiments. In addition, the new synchrotron called Korea 4th generation synchrotron radiation (Korea-4GSR), generates beam flux with micro-focusing that will be 100 times higher than 3rd generation, achieving a level capable of generating data more than 10 Gbit/sec. Thus, a method to effectively analyze massive amounts of data set was required. To overcome this situation, we studied a methodology to process and analyze data in a short time based on artificial intelligence (Figure 1). Unsupervised machine learning is applied to data processing for determining region of interests to calibrate PSD pixel location, and genetic algorithm, which is based upon an evolutionary metaphor that reflects the process of natural selection where the fittest individuals or parameters are selected repeatedly, was adopted to optimize the parameters to match experimental data and theoretical data [1, 2].

Furthermore, we are developing a system that collect emission lines by automatically aligning analyzers based on reinforcement learning.



Figure 1. Schematic diagram of AI-based XES data processing and analysis

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Toward advanced interface visualization in multi-layer stacks: Big data and simulation approaches using angle-resolved XPS

Satoshi Toyoda^{*} and Masatake Machida

Scienta Omicron, inc., Omori Rainbow Building 5F 6-17-10 Minami-Oi, Shinagawa-ku, Tokyo140-0013, Japan *Satoshi.Toyoda@scientaomicron.com

Toward advanced interface visualization in multilayer stacks, we have developed depth-profiling software for angle-resolved XPS measurement systems, which can be applied to various materials (Fig.1).

Additionally, the software allows for the verification of simulations for *spatiotemporal* 4D visualization of interfacial reactions in multi-layered stacks, including in-plane distribution (Fig.2) [1].

In our approach, spectral intensity data, captured simultaneously in the energy and angular dimensions using a 2D detector, are stacked along the sequence dimension to create a three-dimensional spectral intensity cube. A significant challenge arises when handling the large memory workload required for peak-fitting analysis of terabyte-scale measurement data. The size of this big data can range from 100 GB to 10 Tb, which exceeds the memory capability of standard computers.

To address this issue, we improved the computational algorithm, allowing for selective data loading from the disk, rather than loading all data into memory. By ensuring that fitting parameters are processed without loading into









memory, we successfully reduced the memory requirement from 1 TB to approximately 1 MB, representing a 99.99993% reduction, when processing 3.5 billion spectra [2]. These enhancements enable the handling of Big data not only on specialized workstations but also on standard laptops.

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S4. Novel Techniques and Instrument

Chair: Young Min Kim (Sungkyunkwan University, Korea) Chales Clifford (National Physical Laboratory, UK)




AFM Standardisation: From Lab to ISO

Charles A. Clifford^{*}

National Physical Laboratory, Teddington, TW11 0LW, UK *charles.clifford@npl.co.uk

International standards represent the best practice, are made by consensus of all stakeholders internationally and allow compatibility and intercomparison of measurements. The first step is identifying a need, followed by method development, or research into solving a particular problem. The next step is to undertake international interlaboratory tests which are used to test, validate and improve the method, International standards in ISO then follow. In this talk I will discuss the route to standardization in atomic force microscopy (AFM) from idea in the laboratory to full international standard in ISO by providing examples at each stage in the process.

In the lab, the measurement of fibres and fibrils is a common measurement undertaken by both AFM and scanning electron microscopy (SEM). The analysis of these is generally via image analysis routines and the skeltonise function. However, it has been found that this generally underestimates fibre length measurement. I will describe an accurate automated measurement of the length of fibres/fibrils from microscopy images and compare to manual analysis [1].

Force-distance curves using a variety of AFM modes are routinely used to measure pull-off forces from surface for a wide variety of applications including the measurement of adhesion. In this talk I report on an international interlaboratory comparison using AFMs to measure adhesion force at the nanoscale [2]. These studies were undertaken under the auspices of VAMAS, an international pre-normative organization and their technical working area (TWA) 2 on surface chemical analysis.

In the last few years, a large effort has been made by NPL on developing graphene measurement [3,4] and terminology standards [5]. In the final part of my talk I will briefly describe the standards that have been developed.

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Electron Microscopic Understanding toward Highly-Performed Cathode

Si-Young Choi*

Department of Materials Science and Engineering, POSTECH, Pohang 37673, South Korea Division of Analytical Science and Technology, NINT-POSTECH, Pohang 37673, South Korea *youngchoi@postech.ac.kr

The growing demand for electric vehicles has driven the development of high-energy and stable cathode materials for lithium-ion batteries. Better performance of cathode oxides can be achieved by the morpohological control as well as the chemical control such as doping and coating. For example, contrary to the cathodes in a polycrystalline form that suffer from microcrack during cycling, single-crystal cathode materials are regarded to as a more stable cathode morpohology. However, their large particles pose a challenge by slowing down lithium diffusion, which can be stronly influenced by particle morphology. In addition, dopants and surface coating are effectively utilized to enhance the structural stability and the cycling performance. But their specific mechansims are still veiled.

This talk will address the morphological/chemical understanding in the layered cathode oxide and explore their subsequent effects on the structural stability and Li diffusion kinetics. We aim to provide valuable insights into the development of morphology in single crystal cathode materials to improve Li kinetics, as well as design strategies to mitigate degradation processes.



Structural Insights into Non-Crystalline ("Amorphous") Thin Silicone-Nitride Films

Daniel Khaykelson^{1*}, Lothar Houben¹, Boris Rybtchinski¹

¹Department of Molecular Chemistry and Materials Science, Weizmann Institute of Science, Rehovot Israel ²Department of Chemical Research Support, Weizmann Institute of Science, Rehovot, Israel *Daniel.kh@weizmann.ac.il

Recent advancements in x-ray crystallography and electron microscopy have achieved sub-nanometer and sub-angstrom resolution in resolving various materials' structures. These improvements, driven by better detectors, aberration correctors, and high-quality crystals, have primarily benefited crystalline materials due to their strong Bragg diffraction signals. However, amorphous solids like silicate glasses present challenges for sub-nanometer structural studies.

In this talk I will showcase work done on the medium-range-order (MRO) structure of amorphous silicon nitride, a critical material in science and industry. Traditional studies often relied on the radial distribution function (RDF), which averages structural features and can obscure detailed insights. By employing 4D-Scanning-Transmission-Electron-Microscopy (4D-STEM) with varying probe sized, we observed a transition from average scattering rings to speckled diffraction patterns in 5nm amorphous silicon-nitride films. This finding reveals a coherence length of 1nm, indicating a non-random distribution of atoms within this scale.

To enhance reciprocal resolution and structural analysis, energy-filtered data acquisition was utilized. This technique separates elastically scattered electrons, which retain their initial energy and contain structural information, from inelastically scattered electrons, which typically add noise. By combing both Energy-Filtered 4D-STEM with advanced analytical techniques, we are able to get more insight into the local structure of glassy silicon nitride, opening the door for future structure-property research.



Suspended microchannel resonators

John E Sader

Graduate Aerospace Laboratories and Department of Applied Physics California Institute of Technology Pasadena CA, USA

A suspended microchannel resonator (SMR) is a cantilever sensor with a microfluidic channel embedded in its interior. Introduction of an analyte, e.g., a nanoparticle, into this channel increases the inertial mass of the device, which can produce a measurable shift in its resonant frequencies. A primary advantage of SMRs over conventional cantilever sensors is maintenance of a (high) quality factor similar to that in vacuum, regardless of the fluid used. In this talk, I will discuss theoretical and experimental work we have performed focused on understanding the fluid-structure interaction of the SMR itself, and the use of this knowledge in the development of new measurement protocols.



Applications of New Hyper Spectral Map Method by Auger Electron Spectroscopy

Kenichi Tsutsumi^{1*}, Konomi Ikita¹, Fuyuki Nabeshima¹, Tatsuya Uchida¹, Kazushiro Yokouchi¹, Akihiro Tanaka¹, Toshiyuki Ohama¹, and Noboru Taguchi²

¹JEOL Ltd., 3-1-2 Musashino, Akishima, Tokyo 196-8558, Japan ²National Institute of Advanced Industrial Science and Technology (AIST), Ikeda, Osaka 563-8577, Japan *tsutsumi@jeol.co.jp

Auger electron spectroscopy is a famous surface analysis method at a minute area of 100 nm² with depth of less than 10 nm. It has a strong ability to acquire an elemental map on the top surface with the high-spatial resolution of several nanometers. However, it takes acquisition time of a few 10 minutes to obtain even elemental map with enough signal-to-noise ratio because an elemental peak intensity is generally small on bigger background in an Auger electron energy spectrum. Furthermore, an Auger operator has to set all region of intensities (ROIs) or correct peak/background energy positions corresponding to interested elements before starting any Auger map analysis. In order to overcome these problems, we developed a new hyper spectral map method for AES [1], which we called as "*Spectrum Image*" of Auger. This method can provide a special Auger map including a wide range electron energy spectrum with any energy resolution as data cube format. So, it is possible to extract spectra from any area and form an intensity map by postprocessing.

In this presentation, we will introduce how to acquire data by *Spectrum Image* method and show some applications to practical samples. For example, this method is available to visualize the Fermi level difference to detect peak shift of Si KLL at the p-n junction. In Fig.1, the sample was a cross-sectional sample of a p-n-p epitaxial planar transistor, which was polished mechanically to expose some p-n junction areas. The electron beam condition was 20 kV, 30 nA and *Spectrum Image* was acquired by the constant analyzing energy mode (XPS mode) with the pass energy of 10 eV. Fig.1 (a) shows the spectra extracted from the cube data at the p-typed and n-typed Si areas respectively, and Figs. 1(b) and (c) show the intensity maps calculated by these peak differences. In this result, the work function of the top surface was estimated the same at both p-type and n-type area because it was observed no peak shift of the oxide Si KLL peak.

On the other hand, it was confirmed only a Si KLL peak shift of about 0.6 eV among both area, which was considered the Fermi level difference of the p-type / n-type silicon in the bulk.



Fig. 1. Visualizing a pn junction area by Si KLL peak shift caused by Fermi level difference by *Spectrum Image.* (a) Si KLL spectra extracted from the p-type (b) and n-type area (c) respectively.

Noboru Taguchi, Tatsuya Uchida, Konomi Ikita, AkihiroTanaka, Nobuyuki Ikeo, Kazushiro Yokouchi and Kenichi Tsutsumi, Ultra microscopy, 233 (2022) 113450.



Machine learning-assisted electron spectroscopic imaging for chemical analysis of energy-related materials

Young-Min Kim*

Department of Energy Science, Sungkyunkwan University (SKKU), Suwon 16419, Republic of Korea *youngmk@skku.edu

In the quest to understand and manipulate functionalities of nanomaterials at the atomic level, the tools we use to visualize and characterize these structures play a pivotal role in fundamental discoveries and the optimal design of their properties. Of these, scanning transmission electron microscopy (STEM) with electron energy loss spectroscopy (EELS) stands out as an indispensable technique. With its ability to perform correlative acquisition at high resolution, scanning probe-based electron spectroscopic imaging (ESI) creates a three-dimensional dataset that contains numerous spectral data with a 1:1 correspondence to each pixel in a STEM image. The attribute of position-specific spectral data allows one to understand the locality of chemical and electronic structure alterations that govern the structure-chemistry-property relationships of nanomaterials. The process of spectral data to map the distribution of different electronic or charge states within the ESI dataset has been challenging, particularly when the position-specific spectral features are similar. To tackle this issue, we utilized a machine learning-based clustering approach to group spectra with similar fine features from the ESI dataset without prior knowledge. This data-driven clustering method enables us to effectively distinguish meaningful spectral components through data dimensionality reduction, thus helping us to map distinct fine spectral features spatially.

Using machine learning-empowered ESI, we show exemplar applications for two energy-related material systems: a conducting ionomer-carbon support composite electrode in proton exchange membrane fuel cells and a Li-distributed Si/SiO_x composite cathode in Li-ion batteries. Those material systems are challenged in discriminating near-edge spectral features of C K, Li K, and Si L edges because the conventional reference-based fitting cannot reliably perform such a task due to spectral similarities. By optimizing machine-learning workflow architecture for ESI clustering, we demonstrate that direct mapping of the different bonding states of those elements in the composites at a high spatial resolution is viable. This novel approach provides vital information in understanding the cyclic-induced degradation phenomena regarding chemical phase separation, charge state alteration, and defective structure evolution, thereby suggesting insights into the efficient engineering of high-performance and durable electrode materials.



Practical determination of the transmission function of a near ambient pressure hemispherical electron analyzer

Benedikt P. Klein¹, Beomgyun Jeong^{1*}, Jeongjin Kim², and Jouhahn Lee¹

1Korea Basic Science Institute, 169-148 Gwahak-ro Yuseong-gu, Daejeon 34133, Korea ²Pohang Accelerator Laboratory, POSTECH, 80 Jigok-ro 127beon-gil, Pohang 37673, Korea *bjeong@kbsi.re.kr

X-ray photoelectron spectroscopy (XPS) is an imminently important tool for the quantitative chemical surface analysis in a wide range of scientific and engineering fields. The measured intensities of the desired XPS peaks or subpeaks can be extracted from the recorded spectra via peak fitting. For a reliable quantification, however, several external parameters need to be considered with significant accuracy. Namely, these parameters are the X-ray intensity, the X-ray absorption cross section, the inelastic mean free path, and the transmission function of the electron analyzer. Among these parameters, the X-ray intensity can be kept fixed, while good estimates for the X-ray absorption cross section and the inelastic mean free path can be obtained from the literature. The transmission function is the relative probability for a photoelectron of a certain kinetic energy to pass the analyzer and reach the detector. Because the transmission function is an instrumental property of the used analyzer system and may even vary for different possible analyzer lens settings, it is good practice to determine the transmission function directly by measurements. This approach is of increased importance for specialized analyzer systems where complex electronic lens systems complement the hemispherical part of the analyzer, e.g. analyzers used for near ambient pressure (NAP) measurements with differential pumping system. For such modern analyzers, the simple relations and approximations used for estimating the transmission function of more basic analyzer systems break down and the direct measurement of the transmission function is crucial.

Herein, we compare different methods of determining the transmission function of the SPECS Phoibos 150 NAP hemispherical analyzer mounted at the 8A2 beamline at the Pohang Light Source. In particular, we determined the transmission function using gas phase CO as a reference material. Making use of the synchrotron light source, we employed two methods, (1) keeping the pass energy constant and varying the kinetic energy via changing the photon energy, and (2) keeping the photon energy and kinetic energy constant and varying the pass energy. The results of these gas phase measurements were compared to a more traditional approach of determining the transmission function using surface samples, and the simulated transmission function provided by the manufacturer.



Designing Energy Materials Guided by 3D Atomic-Resolution Tomography

Se-Ho Kim^{*} and Chang-Gi Lee

Department of Materials Science and Engineering, Korea University, Republic of Korea *corresponding author: sehonetkr@korea.ac.kr

At the current stage of the "decarbonization" movement, Li-ion batteries and H-related materials have emerged as promising technologies for replacing combustion engines and fossil fuels. However, a critical bottleneck in the further development of these energy materials and the associated system maturation is that the atomistic mechanisms behind the intricate reactions/evolutions during operation remain elusive. This knowledge gap is caused by a lack of probing methods that allow us to observe the underlying microscopic chemical, structural and mechanical phenomena directly at the near-atomic scale in real space and three dimensions.

As we have long been able to conjecture about our reality on material structure beyond our ability to observe, the latest development of atom probe tomography (APT) can deliver high spatial resolution three-dimensional compositional information of materials with equally sensitive to all elements including lithium/hydrogen[1]. It can provide insights into crucial material characteristics, and the acquired knowledge will help to optimize lithium/hydrogen materials[2].

The first part of my talk will be about what an atom probe is, and acquired data from cryogenic-APT on each particular case (cathode/anode and H in materials) will be presented[3]. This talk will further discuss how the technique can be applied in batteries and hydrogen applications and how it can advance understanding of structure-property relationships.

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S5. Applications I (Device and Materials)

Chair: Richard Morris (IMEC, Belgium)





Innovative Applications of Surface Analysis for 3D Semiconductor Structures

Wooyoung Jung^{*}, Hokeun Kim, Taeone Youn, Seongjun Jung, Wanhee Lee, Sungho Lee, Seunga Shin SK hynix Inc., 2091, Gyeongchung-daero, Bubal-eup, Icheon-si, Gyeonggi-do, Republic of Korea *wooyoung3.jung@sk.com

This study explores methods for analyzing the various properties of 3D semiconductor devices using 1D and 2D surface analysis techniques. These techniques include impurity analysis using Secondary Ion Mass Spectrometry (SIMS), crystallinity analysis using X-ray Diffraction (XRD), stress & strain analysis of silicon using Raman spectroscopy, and contamination analysis using Atomic Force Microscope-InfraRed spectroscopy (AFM-IR), among others [1]. These methods were applied to analyze various actual devices such as DRAM & NAND cells, and package structures (PKG)

The most critical aspect of applying surface analysis techniques to actual device structures is to create a flat surface centered around the desired analysis target within the chip structure. To achieve this, various preprocessing techniques such as dimpling, ion beam etching, polishing, and wet etching were utilized as appropriate.

As a result, it was possible to analyze the composition, impurities, crystallinity, stress & strain, and contamination in the cell & PKG structures of semiconductor devices. The analysis results were found to correlate well with the electrical characteristics and failure rates of the devices.

Analyzing 3D semiconductor devices using 1D and 2D surface analysis techniques leverages the specific strength of each instrument, such as the high detection limits of SIMS. Compared to traditional nm-scale analysis techniques such as TEM, EELS, and APT, this approach handles information at the scale of μ m to mm [1], offering high representativeness of chip characteristics. Additionally, it provides exceptional efficiency in terms of analysis cost and time.

This study demonstrates that surface analysis techniques are powerful tools for quickly and accurately analyzing the comprehensive properties of 3D semiconductor devices, continuing to make significant contributions to the development of next-generation semiconductors.

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Photoelectron Holographic Study of Atomic Site Occupancy of the Si Dopant in κ-Ga2O3(001)

Yoshiyuki Yamashita^{1,2*}, Yu-Hua Tsai^{1,2}, Yusuke Hashimoto³, Tomohito Matsushita³, and Piero Mazzolini⁴

NIMS,1 Kyusyu Univ.,2 NAIST,3 and IMEM-CNR,4 1-1 Namiki, Tsukuba, Ibaraki, 305-0044, Japan Yamashita.yoshiyuki@nims.go.jp

For Ga₂O₃, there are six crystal polymorphs: α -, β -, γ -, ε -, and κ -Ga₂O₃. Among them, β -Ga₂O₃ has received the most attention due to its highest thermal stability. Recently, the orthorhombic κ -Ga₂O₃ has gained attention due to its large spontaneous polarization and its ferroelectricity. For κ -Ga₂O₃, Si is used as the dopant to control the electrical properties. There are three inequivalent Ga atomic sites as the dopant sites in κ -Ga₂O₃; octahedral (Octa), pentahedral (Penta), and tetrahedral (Tetra). Therefore, in order to control the electrical properties, the atomic site occupancy of Si dopant in Si-doped κ -Ga₂O₃ should be clarified. In the present study, we investigated the atomic site occupancy of the Si dopants for Si-doped κ -Ga₂O₃ using photoelectron holography (PEH).

The Si-doped κ -Ga₂O₃ epitaxial layers were grown on a c-plane sapphire substrates prepared by the MOVPE method. The PEH measurements were performed at the BL25SU beamline of SPring-8.

Figure 1(a) shows the Ga 3*p* and Si 2*p* PES spectrum for the Si-doped κ -Ga₂O₃(001) measured at an incident photon energy of 911 eV. The corresponding PEH for Si 2*p* are shown in Fig. 1(b). Figure 1(c) shows the experimental and the simulated Si 2*p* PEHs for the Si-doped κ -Ga₂O₃(001). By comparing the experimental and the simulated PEHs, the ratios for the Tetra, Penta, and Octa Si_{Ga} sites are estimated to be 51.0%, 35.2%, and 13.8%, respectively.[1]



Figure 1. (a) Ga 3*p* and Si 2*p* PES spectrum for Si-doped κ -Ga₂O₃(001). (b) PEH of Si 2*p* for Si-doped κ -Ga₂O₃(001). (c) Experimental (yellow) Si 2*p* and the simulated (blue) PEHs for the Si-doped κ -Ga₂O₃(001).

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Interface Energy Level Offset in Organic Solar Cells Measured by UPS and IPES and Its Correlation with Voc and CT Energy

G. Lee¹, Y. Kim¹, M.-J. Maeng¹, K.-M. Lee¹, J.-A. Hong¹, K.-G. Lim², S. Cho³, and Y Park^{1,4,*}

¹Dept. of Physics, Kyung Hee University, 26 KyungHeeDae-ro, Seoul 02447, Republic of Korea

²Applied Measurement Science, University of Science and Technology, and Korea Research Institute of Standards and Science, Daejeon 34113, Republic of Korea

³Dept. of Semiconductor Physics and Energy Harvest Storage Research Center, University of Ulsan, Ulsan 44610, Republic of Korea ⁴Dept. of Information Display, Kyung Hee University, 26 Kyungheedae-ro, Seoul 02447, Republic of Korea *parky@khu.ac.kr

We have developed highly sensitive inverse photoemission spectroscopy (IPES) instrument for the LUMO level measurement if organic semiconductor materials. In combination with the existing ultraviolet photoemission spectroscopy (UPS) we can determine all the relevant energy levels (HOMO, LUMO, Fermi level and vacuum level) at surfaces and interfaces.

We determined the energy levels at both C60/pentacene and C60/CuPc model planar organic photovoltatic cells (OPV) interfaces so that the voltage losses that led to the observed Voc value can be evaluated. We also fabricated bilayer OPV devices in which the deposition sequence of each layer was alternated resulting in four different types of devices for two material combinations. We confirmed that there exists difference in interfacial energy offset between C60/pentacene and pentacene/C60 devices, which is also reflected in Voc values of respective devices. This is due to the difference in molecular orientation for pentacene depending on the deposition sequence. We could not observe any dependence of Voc on deposition sequence for C60 and CuPc devices nor could we measure any energy offset at the interface, where the molecular orientation is expected to be independent of deposition sequence. We further investigate the charge transfer (CT) exciton energies for all the devices by using sensitive external quantum efficiency (EQE) measurement. These combined measurements led us to identify the most important parameter in determining the Voc of these model bilayer OPVs.

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Correlative XPS Multi-technique sample analysis

Adam Bushell^{*}, Tim Nunney, Paul Mack, Robin Simpson, Simon Bacon Thermo Fisher Scientific, 1 The Felbridge Centre, East Grinstead, RH19 1XP, UK *adam.bushell@thermofisher.com

XPS has long been established as an analytical technique for gaining information on the elemental composition and chemical bonding states of material surfaces. This information is especially important when tuning parameters of materials to perform specific functions e.g. for a specific surface electrical conductivity, or if the amount of material on a surface needs to be carefully controlled. While XPS gives this valuable surface chemical information, often what is desired is to combine that with material morphology and/or electrical performance to gain further insight into the process or material being developed.

Modern XPS spectrometers now often come with a range of additional analytical techniques on the same chamber which can greatly enhance sample XPS measurements and assist in the interpretation of XPS data. In addition, it is also possible to correlate measurements between XPS and other analytical tools, via registration of sample position between those tools. This presentation will demonstrate both on-tool and off-tool correlation of analysis techniques on a range of samples, including 2D materials and perovskites, to show how a more complete picture can be built up at a single analysis position.



Atom probe tomography: Application and challenges within the semiconductor field

Richard J.H. Morris

imec, Kapeldreef 75, Leuven 3001, Belgium. richard.morris@imec.be

The origins of atom probe tomography (APT) can be dated back to 1935 when Erwin Müller first developed the field emission electron microscope (FEEM). This was then superseded by the field ion microscope (FIM) in 1955 and resulted in the first visualisation of individual atoms from the surface of tungsten. In 1967 the 1D atom probe was realised by using a time-of-flight mass analyser combined with electric field pulsing to reveal the chemical identification of these atoms. As technology continued to improve, a natural progression towards the 3D atom probe (3DAP) was finally achieved in 1988. Although the addition of a laser was shown in the 1980s to enable atom probe of semiconductors and insulators, it was not until 2005 before the first commercial laser assisted APT tool came onto the market. [1]

In this talk, we will focus on the rapidly growing semiconductor material field for laser assisted APT analysis. With the continued scaling of state-of-the-art semiconductor devices and the transition from planar to 3D structures e.g., FinFETs, CFETS [2], many of the conventional metrology techniques (secondary ion mass spectrometry, X-ray diffraction, Rutherford backscattering etc.) used to determine the chemistry and/or elemental distributions are either struggling or becoming redundant. Given that APT offers sub-nm 3D resolution across all elements [3], it has become an extremely promising technique for filling the emerging void in our characterisation resources. We will begin by giving an overview of the APT measurement setup, sample preparation, data collection and reconstruction to obtain a 3D analysis. Moreover, examples demonstrating the ongoing effort into the quantification and its benchmarking, the need for reproducibility, and extracting atomic scale information, will be presented. As with all characterisation techniques, limitations and challenges exist, especially when they are still in their infancy like APT. Therefore, we will also highlight some of the known issues e.g., elemental biases, tip asymmetry etc. along with some of the ongoing efforts to overcome these. To conclude, we will present several device structure measurements and analyses, illustrating the capabilities of APT for both current and future semiconductor metrology applications.

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Nano Imaging of Ultrafast Exciton Dynamics in 2-Dimensional Materials with s-SNOM

<u>Hwi Je Woo^{1*}</u>, Mingu Kang^{1,2}, Eun Seong Lee¹, Junghoon Jahng^{1*}

¹Korea Research Institute of Standards and Science, 2University of Science and Technology ²Hyperspectral Nano-imaging Lab, KRISS (267 Gajeong-ro, Yuseong-gu, Daejeon 34113 Korea) *phyjjh@kriss.re.kr

This study focuses on the elucidation of ultrafast excitonic dynamics in two-dimensional (2D) materials, particularly transition metal dichalcogenides (TMD), using scattering-type Scanning Near-field Optical Microscopy (s-SNOM). Understanding exciton behavior - such as generation, recombination, and transport processes - at ultrafast time scales is crucial for advancing next-generation optoelectronic devices.

Utilizing s-SNOM, the research achieved nanometer spatial resolution and temporal precision on the order of a few picoseconds, allowing for the direct observation of exciton dynamics with unprecedented detail.[1] The method involved synchronizing ultrafast laser pulses with the imaging capabilities of s-SNOM, enabling the capture of transient exciton states in real-time.

The results reveal complex patterns in exciton dynamics, including their spatial distribution and diffusion, as well as the significant impact of material heterogeneities, such as defects and grain boundaries, on exciton behavior. Notably, variations in exciton lifetimes were observed in defect regions of TMD, highlighting the critical role of these imperfections in modulating exciton dynamics.

This study emphasizes the importance of advanced nano-imaging techniques like s-SNOM in enhancing our understanding of ultrafast processes in 2D materials. The insights gained contribute to the foundational knowledge necessary for engineering 2D materials with tailored optoelectronic properties, which are essential for the development of innovative applications in solar energy conversion, light-emitting diodes, and photodetectors.

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Investigation of 3D atomic distributions in functional materials through atom probe tomography

Chanwon Jung*

Department of Materials Science and Engineering, Pukyong National University, 45 Yongso-ro, Nam-gu, 48513 Busan, Republic of Korea *c.jung@pknu.ac.kr

Since the functional properties of materials are significantly influenced by their nanostructures, it is essential to thoroughly investigate these nanostructures to understand the structure-property relationship. For instance, segregation at grain boundaries can affect carrier transport by altering boundary characteristics[1], chemical fluctuations in the nanoscale can modify carrier mobility by filtering low-energy carriers[2], and interfaces between nano-precipitates and the matrix can influence carrier transport properties[3]. Atom probe tomography (APT) is a powerful analytical tool, offering three-dimensional (3D) elemental distribution and thus precise local chemical composition can be revealed[4]. With sub-nanometer spatial resolution and parts-per-million (ppm) level chemical sensitivity[5], APT has been applied to reveal 3D elemental distributions in various materials, including alloys, semiconductors, and biomaterials, clarifying the linkage between nanostructures and properties[6]. In this presentation, I will outline the principles of APT and showcase its applications in analyzing functional materials, particularly focusing on thermoelectric materials.

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Advancements and Challenges in Surface Metrology and Inspection for the 3D Integration Era

Dongchul Ihm*, Minjung Shin, Seok Park, Jongmin Park, and Eunpa Kim

SAMSUNG Electronics Co., LTD., 1-1, Samsungjeonja-ro, Hwaseong-si, Gyeonggi-do, Republic of Korea *dongchul.lim@samsung.com

As the era of artificial intelligence (AI) unfolds, the demand for high-performance semiconductors has become imperative. This necessity drives the adoption of 3D integration processes, which offer enhanced performance and efficiency. The 3D integration process is characterized by advanced bonding techniques, such as hybrid Cu bonding, leading to challenges like the small pitch of Cu pads and high wafer warpage due to the high memory density.[1-3] Surface metrology and inspection techniques are critical in addressing these challenges, ensuring the reliability and performance of 3D integrated devices.

This work explores the latest trends in the 3D integration process, focusing on advancements in bonding metrology and inspection technology and the associated challenges happened before and after bonding. The small pitch of Cu pads requires precise alignment and bonding height control, while high warpage and void at the bonding interface can lead to bonding misalignment and reduced yield, respectively. Advanced metrology and inspection techniques, including atomic force microscopy (AFM), interferometry, IR overlay, IR inspection and acoustic microscopy, are essential for detecting and mitigating these issues.

Furthermore, this study provides a comprehensive overview of current metrology solutions and highlights ongoing research aimed at overcoming limitations in sensitivity and throughput. Innovations in high throughput and resolution of bonding metrology and inspection methods are discussed, emphasizing their role in supporting the continued advancement of 3D integration. Key insights into the future directions of surface and interface metrology and inspection technologies such as multi probe AFM with significantly improved their measurement speed are also presented, underscoring their importance in the semiconductor industry's evolution.

By addressing the challenges and leveraging advancements in surface metrology and inspection, the semiconductor industry can continue to meet the growing demands of the 3D integration era, ensuring the development of reliable, high-performance, and high-density devices.

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Characterization of colloidal Pd nanoparticles using Atom Probe Tomography

Pyuck-Pa Choi^{1*}, Kyuseon Jang¹, and Seho Kim²

¹Department of Materials Science and Engineering, Korea Advanced Institute of Science and Technology, Daejeon, Korea ²Department of Materials Science and Engineering, Korea University, Seoul, Korea *p.choi@kaist.ac.kr

In this work, we present a novel approach for preparing atom probe tomography (APT) specimens from Pd electrocatalyst nanoparticles of less than 10 nm in size [1]. This method is based on electrophoresis of nanoparticles on a substrate followed by electroplating of a metallic layer. Using transmission electron microscopy (TEM) we could observe that particle shape and size were well preserved after these two process steps. We could routinely prepare APT specimens from the deposited nanoparticle/metal films using focused-ion-beam milling (FIB). Using APT we were not only able to map the elemental distribution within the nanoparticles but also the distribution of surfactants i. e. stabilizing and shape-controlling agents, used in the synthesis of the nanoparticles [2].

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S6. Applications II (Energy)

Chair: Masahiro Terashima (ULVAC PHI, Japan) Hyun-Wook Lee (Ulsan National Institute of Science and Technology, Korea)





Using high-throughput XPS analysis in determining Na-Fe-Mn-O cathode materials chemistry

Chris Blomfield^{1*}, Chris Moffitt², Shipeng Jia³, and Jonathan Counsell¹

¹Kratos Analytical Ltd, Wharfside, Manchester, UK ²Kratos Analytical Inc, Nanuet, New York, USA ³Department of Chemistry, McGill University, Montreal, Canada *chris.blomfield@kratos.co.uk

Due to the abundance of sodium, Na-ion batteries are of increasing interest as an alternative to the ubiquitous Li-ion battery, particularly for large-scale application of grid energy storage. However, the Na-ion battery performance has not been able to match that of Li-ion batteries, with promising ternary Na-Fe-Mn-O materials limited by poor stability in air and unsatisfactory long-term cycling.

A high-throughput approach was used to systematically screen the entire ternary-oxide system using a number of materials characterization techniques. The constructed phase diagram showed solid-solution regions for 3 layered oxide phases P2, P3 and O3. This chemometric approach allowed identification of over 50 single-phase materials of potential interest for use as battery cathode material.

High-throughput XPS was used on aged samples to determine stability in air. Surface segregation and enrichment of Na was observed with the formation of Na carbonate identified as a degradation product detrimental to cathode performance. To further understand sample chemistry, a simplified and robust analysis of complex Fe and Mn spectra was used to determine oxidation states.

This XPS study reinforced the conclusion that the sample stability with both carbon dioxide and moisture is very sensitive to composition and structure. Importantly specific phases P3 and Mn-rich P2 were shown to exhibit the best stability in air.

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Investigation on XPS Charge Neutralization Method for Carbon-Based Battery Materials.

Takahiro Suzuki^{1*}, Kana Kamoto¹, Ayumi lijima¹, Kazuyoshi Tsukamoto¹, and Shunsuke Oishi¹

Cataler Corp., Characterizaion Dept., Fundamental Research & Development Div. 1905-10 Shimonobe, Iwata, Shizuoka, 438-0112, Japan *takahiro-suzuki@cataler.co.jp

In the XPS analysis of developed carbon-based battery materials, a stable C 1s spectrum could not be obtained with a general sample holding method[1]. We consider that differential charging was the cause because of the non-uniformity of the sample. As charge correction using C 1s was difficult in the case of carbon materials, we investigated new sample holding method and charge correction using standards simultaneously. As a result, we developed a new method in which the sample was coated to the surface of a ZrO_2 disk pellet for XPS measurement.

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Novel Strategies for the characterization of the next-generation energy storage materials by ToF-SIMS: from an in-situ exploration to an operando measurement

Tanguy Terlier*

SIMS laboratory, Shared Equipment Authority, Rice University, Houston, TX 77005, USA *tanguy.terlier@rice.edu

Recently, advances in instrumentation and sample preparation have permitted a rapid development for characterizing a wide range of applications such as next-generation energy storage materials. Developing new materials is one of the most crucial topics for emerging technologies. However, the complexity of these materials in their structures makes them particularly challenging for numerous characterization and analytical techniques. Exploring chemical composition and the potential chemical reactions such as degradation, diffusion, or doping is crucial to understand advanced materials and to transfer the new technologies to the industry. Among the most suitable characterization tool, time-of-flight secondary ion mass spectrometry (ToF-SIMS) is a very sensitive surface analytical technique providing detailed elemental and molecular information about the surface, thin layers, interfaces, and full three-dimensional analysis of the samples.

Thanks to the advances in ToF-SIMS characterization, understanding of the chemical composition and the different components in the complex structures, permit a deeper exploration and a better knowledge in the next-generation energy storage materials such as batteries, perovskites, and 2D materials.

Firstly, we will discuss the sample preparation and our specific setup for transferring the specimens from the inert atmosphere in the glovebox to the ultra-high vacuum chamber of our instrument. We will illustrate the possibility of studying the reversibility of the chemical composition between pristine, charged, and discharged batteries using surface mass spectrometry by ToF-SIMS. Then we will compare three methods of cross-sectioning used to identify the interfacial species in a composite cathode. We will introduce how in operando ToF-SIMS can be a novel approach for probing in situ the chemical evolution of the devices.

Secondly, we will show a study of an in-depth distribution of the 3D/2D heterostructures for perovskite solar cells where we have been able to identify individually the 3D and 2D heterostructures along with the depth of the film. Then, we will illustrate the characterization of interdiffusion in quasi-2D perovskite light-emitting diodes as a function of the organic ligand layer inserted into the perovskite crystals.

Finally, we will demonstrate how the retrospective analysis using ToF-SIMS can be very powerful and useful for exploring any single feature in 2D materials. Typically, ToF-SIMS acquisition is recording a full mass range spectrum per pixel (or voxel), which permits to isolate and to decorrelate specific regions of interest for resolving interfaces, diffusion, and doping in thin 2D structures. We will present how to treat a 3D volume image of a multilayer perovskite device for extracting useful information.



Observation of the Nucleation and Growth of Lithium Metal Dodecahedra in Anode-free Lithium Batteries

Hyun-Wook Lee*

Ulsan National Institute of Science and Technology, 50 UNIST-gil, Ulsan 44919, Republic of Korea *hyunwooklee@unist.ac.kr

The diffusion-limited mass transport in electrolytes has been considered the origin of Li dendritic growth. When the formation of metallic Li is initiated by the charge transfer on a Cu current collector, the local distribution of Li ions within a liquid electrolyte deviates from its equilibrium, causing a concentration gradient of Li ions. At the point where the concentration of Li+ goes to zero, a local steep concentration gradient of Li ions in the electrolytes eventually triggers dendritic Li growth, which is commonly discussed in terms of the Sand's equation. Although many previous studies have attempted to reduce this concentration gradient of Li ions in the electrolyte including highly concentrated electrolytes, modified electrodes with lithiophilic property, and metallic alloying with heteroatoms, these studies have mainly focused on Li adsorption and ignored the surface migration of Li atoms that can occur directly after Li adsorption.

In this work, we demonstrate that Li plating is a collective motion of Li adatoms that is affected by the crystallographic orientation of the Cu substrate and that Li adatoms can be redistributed by interacting with individual Cu grains via surface migration. By comparing centimeter-sized single-crystal Cu(111) and Cu(410) foils, we show that Cu(111) foil inhibits dendritic growth of metallic Li, likely due to the near-zero migration barrier of Li adatoms according to our modeling. We propose that understanding and controlling the Li adatom surface-migration behavior can open a new avenue for achieving high-performance anode-free Li batteries.

^[1] Min-Ho Kim, Dong Yeon Kim, Yunqing Li, Juyoung Kim, Min Hyeok Kim, Jeongwoo Seo, Benjamin V. Cunning, Taewon Kim, Sang-Wook Park, Rodney S. Ruoff^{*}, Dong-Hwa Seo^{*}, Sunghwan Jin^{*}, Hyun-Wook Lee^{*}, Energy & Environmental Science, online published.



Surface Engineering and Regulation of a Photoelectrode for Solar Rechargeable Zn-Air Batteries

Hasmat Khan, and Se-Hun Kwon*

School of Materials Science and Engineering, Pusan National University, Busan 46241, Republic of Korea Institute of Materials Technology, Pusan National University, Busan 46241, Republic of Korea *Correspondence: sehun@pusan.ac.kr (S.-H. Kwon)

Utilization of solar energy in battery system is an attractive approach. In this regard, solar rechargeable zinc-air batteries (SRZBs) demonstrate potential as future next-generation batteries because of their high safety, resource-abundant, and high theoretical energy density[1]. In SRZB, a bifunctional photoelectrode with light-induced water oxidation reaction (WOR) and oxygen reduction reaction (ORR) is the key component for the overall battery performance[2].

Herein, a surface and interface engineered photoelectrode have been strategically fabricated to promote light-induced WOR and ORR performance for reducing charging potential and enhancing output potential of the battery, respectively. The metal oxide semiconductor based-photoelectrode (α -Fe₂O₃/Fe₂TiO₅/Pt) with a type-II heterojunction band alignment, comprising n-type α -Fe₂O₃ nanorod core, a thin pseudobrookite phase of Fe₂TiO₅ shell, and embedded Pt NPs over the Fe₂TiO₅ shell was fabricated by the combination of wet-chemical and ALD techniques. The main advantages of this photoelectrode are: (i) a type-II heterojunction band alignment with a suitable band gap energy, which ensures broad light absorption in the visible wavelength region, and stimulates light induced-WOR/ORR activity; (ii) improved light absorption in the heterojunction photoelectrode facilitates the photogenerated charge separation efficiency, decreases overpotential for WOR kinetics, and improves battery performance [1]; (iii) both α -Fe₂O₃ and Fe₂TiO₅ are highly stable in alkaline aqueous electrolyte, leading to the excellent electrochemical/photoelectrochemical durability of the SRZB during charging/discharging cycles; and (iv) the Pt NPs on Fe₂TiO₅ layer accumulate photogenerated electrons that facilitate ORR kinetics of the photoelectrode. The fabricated α -Fe₂O₃/Fe₂TiO₅/Pt photoelectrode exhibited photo-enhanced charging/ discharging abilities with a voltage gap of only 0.3 V under 1 sun illumination, and maintained a good cycling stability of the SRZB over 130 cycles for 50 h at 0.1 mA/cm². This work provides the way to design an efficient and robust bifunctional photoelectrode for SRZB.

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The Solidification Effect of Using Benzenesulfonyl Fluoride Assistants for Liquid Electrolyte in Lithium-Sulfur Batteries

Hyejun Kim, Daon Lee, Young-uk Kim, and Junyoung Mun*

School of Advanced Materials Science and Engineering, Sungkyunkwan University, 2066 Seobu-ro, Suwon 16419, Republic of Korea * e-mail: munjy@skku.edu

Lithium-Sulfur batteries are considered one of the next-generation batteries due to their high energy density (2600 Wh kg⁻¹) and theoretical capacity (1675 mAh g⁻¹).¹ However, Li-S batteries operate through solid-liquid-solid phase conversion during in the charge-discharge process. The conversion reaction of S8 + $16Li^+ + 16e^- \rightarrow 8 Li_2S$ includes a series of intermediates such as Li_2S_8 , Li_2S_6 , Li_2S_4 and Li_2S_2 . In the Lithium polysulfide (LiPSs) series, solid-phase materials like Li_2S present a significant challenge in Li-S batteries. The dissolved liquid form of LiPSs in the electrolyte tends to migrate to the anode and deposit on its surface, causing the known "shuttle effect".² To solve the shuttle effect, an electrolyte modification approach can be used to control LiPSs dissolution and migration to the anode. Excessive electrolyte conditions can lead to the generation of by-products such as poly-DOL and poly-DME. Conversely, lean electrolyte conditions are not viable due to their low ionic conductivity and the limited solubility of LiPSs.³ Therefore, selecting a suitable electrolyte is crucial for controlling the dissolution of LiPSs under specific conditions.

In this research, Benzenesulfonyl fluoride (BF) are used to decomposition of LiPSs in a suitable electrolyte condition. As an electrolyte additive, BF achieves higher capacity compared to the conventional DOL/DME electrolyte. The reactivity of BF with LiPSs has been verified through FT-IR measurements and UV spectrum. Subsequently, the morphologies of the cathode and anode electrodes were observed after the charge/discharge process.

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Chemical state and energy band structure analysis for interface modification in All-Solid-State Battery materials.

Masahiro Terashima*

ULVAC-PHI Inc., 2500 Hagisono, Chigasaki, Kanagawa, 253-8522, Japan *masahiro_terashima@ulvac.com

All solid-state batteries (ASSBs) are gaining attention as the next generation of batteries, expected to improve safety and energy density. The electrolyte in ASSBs commonly uses sulfide-based materials with high ion conductivity, while the anode and cathode often incorporate Li metal and NCM-based materials (Ni, Co, and Mn) known for their high energy density. However, the combination of these materials can lead to increased internal resistance and reduced ion conductivity due to solid-solid reactions at the interface, resulting in a deterioration of cycling performance. To address these challenges, protective coatings such as LiNbO₃ or Li₃PO₄ are generally applied to the anode and cathode surfaces [1]. Despite numerous reports indicating the improvements in the battery performance of ASSBs, the mechanism underlying these enhancements by surface coating is not fully understood. In this study, ultraviolet photoelectron spectroscopy (UPS) and low energy inverse photoelectron spectroscopy (LEIPS) techniques were employed to examine the energy band diagrams of Li metal, $Li_{10}GeP_2S_{12}$ (LGPS), a sulfide-based solid electrolyte, and NCM (Figure 1), providing insights into predicting reactions occurring at the solid-solid interface. The energy band diagrams enable the prediction of oxidation/reduction reactions at the interface before cycle tests and facilitate discussion on the effects of interface modification, providing crucial guidelines for battery design.



Figure 1. The energy band diagrams of Li metal, LGPS, and NCM811.

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Unveiling the Longevity Mechanism of Si/Graphite Composite Anodes in Sulfide-based All Solid-State Batteries: Interplay of Nanostructure Evolution and Interface Stability

Hyun-Woo Gong^{1,2}, Hye-Young Cho¹, Tae-Kyeong Kim¹, Ji-Min Lim¹, Hae-Ryoung Kim¹, Hong-Kyu Kim¹, Jae-Pyoung Ahn^{1,2*}

¹Advanced Analysis and Data Center, Korea Institute of Science and Technology, Seoul 02792, Republic of Korea ²Division of Nano & Information Technology, KIST School, University of Science and Technology, Seoul 02792, Republic of Korea *jpahn@kist.re.kr

All solid-state batteries (ASSBs) based on sulfide electrolytes are gaining attention as next-generation energy storage devices due to their high safety and energy density. Silicon (Si) is a promising anode material for ASSBs due to its high theoretical capacity (3579 mAh g⁻¹), but the significant volume expansion (~300%) during charge and discharge cycles presents a major challenge for maintaining performance. Recent studies have demonstrated the superior performance of micro-sized pure Si, but inconsistent cycle life characteristics make it difficult to understand the degradation mechanisms of Si anodes. To address this, a-Si-coated graphite (Si/Gr) composite with a nanometer-thick Si layer has been proposed, but the performance and degradation mechanisms in ASSBs remain unclear.

In this study, we investigated the impact of Si's morphological characteristics on the cycle life stability of sulfide-based ASSBs and analyzed the degradation mechanisms of Si/Gr composite anodes. Half-cells were fabricated using Si/Gr composites (~10 μ m spherical particles with ~50 nm Si coating) as working electrodes and lithium metal as counter electrodes, and cycled 50 times to evaluate cycle life characteristics. The microstructural and chemical changes in the electrodes were examined using various analytical techniques such as μ XRD, SEM/EDS, XPS, TEM/EDS/EELS.

The initial delithiation capacity of the Si/Gr composite was approximately 820 mAh g^{-1} , which is significantly higher than that of pure Gr (340 mAh g^{-1}). However, after 50 cycles, the capacity retention of the Si/Gr composite dropped to 82%, compared to 97% for pure Gr, indicating faster degradation. This more rapid degradation of Si/Gr compared to pure Gr is attributed to the interactions between Si and Gr within the composite, which had a greater impact than the interfacial reactions with the solid electrolyte. Specifically, the Si coating within the composite gradually decreased the crystallinity of Gr during cycling, leading to a reduction in lithium storage capacity. Additionally, this process induced morphological changes in the Si/Gr particles and the formation of Li₂O as part of the solid electrolyte interphase (SEI). In contrast, Si/Gr composites with a thinner Si coating (580 mAh g^{-1}) demonstrated similar high cycle retention to pure Gr, with no significant degradation phenomena observed. On the other hand, cells using micron-sized pure Si as the anode material exhibited a rapid capacity drop to 0% within just 10 cycles. This was due to the formation of lateral cracks during lithiation, which blocked lithium ion pathways. These cracks also led to the formation of excessive SEI with insulating

properties, causing a sharp decline in capacity.

In conclusion, the degradation rate of Si/Gr particles was influenced by the thickness of the Si coating. Thickly coated Si/Gr particles provided higher capacity compared to pure Gr but exhibited a faster degradation rate. In contrast, thinly coated Si/Gr maintained relatively high capacity while demonstrating a slow degradation rate comparable to pure Gr. Specifically, when thin Si coatings were applied, the anode could accommodate localized volume changes, thereby slowing the degradation rate and satisfying both high capacity and high charge-discharge cycle requirements.

This study elucidates the degradation mechanisms of Si-C composites in sulfide-based ASSBs and suggests optimization strategies for Si-based anode materials. These findings provide crucial insights for the development of high-performance all-solid-state batteries with improved long-term reliability using Si-based anodes. The results are expected to contribute significantly to the advancement of all-solid-state battery technology with enhanced long-term stability and performance.



Single-Atom Platinum Catalyst for CO Oxidation on Multi-Component Vanadia/Titania Support

Hongjin Park, Eunji Kang, Minkyeong Kim, and Hyun You Kim*

Department of Materials Science and Engineering, Chungnam National University, Daejeon 34134, Republic of Korea *kimhy@cnu.ac.kr

Single atoms catalysts(SACs) are regarded as the breakthrough for the effective usage of noble metals. However, SAs have a critical disadvantage when developing and being applied to industrial systems, which is that they are extremely unstable under operating temperatures, indicating that the SAs are inevitable in aggregation into nanoclusters or nanoparticles. Herein, to handle this issue, we focus on stabilizing platinum single atoms at the interfacial site of multi-component oxide support by using the hybrid oxide support consisting of early transition metal oxides, which are vanadia and titania. Interestingly, the vanadia (VO_x), a key component of our catalysts system, exhibits multiple oxidation states (+2, +3, +4, +5), as its size is artificially controlled. Such characteristics allow vanadium oxide to provide reactive oxygen, which can lower the temperature required for oxidation reactions. With this advantage, vanadium-based catalysts are widely used in various oxidation reactions. The structure of vanadium oxide varies with V-loading (monomeric, polymeric, and crystalline V₂O₅). We characterized our catalyst using Raman spectroscopy, in-situ infrared spectroscopy, transmission electron microscopy, and X-ray photoelectron spectroscopy. Catalytic activity was measured using mass spectrometry and gas chromatography. Based on our results, we firmly believe that the interface engineering of multi-component oxide supports the stabilization of platinum single atoms, which is tentatively likely to extend to other novel metal catalysts.



Ru-Based High Entropy Oxide as Acid Stable Electrocatalyst for Oxygen Evolution Reaction

Alireza Razazzadeh, Hasmat Khan, and Se-Hun Kwon^{*}

School of Materials Science and Engineering, Pusan National University, Busan 46241, Republic of Korea Institute of Materials Technology, Pusan National University, Busan 46241, Republic of Korea *Correspondence: sehun@pusan.ac.kr (S.-H. Kwon)

Proton exchange membrane electrolyzers (PEMWEs) have been recognized as promising technology for generating pure hydrogen. Despite the merits of low ohmic resistance, high conversion efficiency, high current density, utilizing PEMWEs faces barriers like as high cost of IrO₂ as the state-of-the-art acid stable electrocatalyst. Recently, high entropy oxide drew the attention of the researchers due to outstanding activity and durability as different electrocatalyst. In the mentioned new types of materials, coexistence of more than 5 metallic elements could create multi cites for reactions [1, 2].

This study rationally designs a novel and low-cost high entropy oxide based on volcano plots for oxygen evolution reactions to satisfy both activity and durability. Sol-gel method as a common method for synthesizing multi component oxides was applied to synthesize Ru-Ti-Sn-Mn-Cr-O high entropy oxide. Different characterization methods such as X-ray diffraction, and transmission electron microscope were conducted to study the microstructure and elemental distribution of the synthesized high entropy oxides. Further studies have shown that decreasing tin was effective in formation of single-phase solid solution in form of rutile structure. Even distribution was observed which was a further confirmation of solid solution formation. Applying sol-gel method contributed to form a porous structure which was beneficial to enhancing the mass transport and overall catalytic activity. At the same time the activity and stability increased by decreasing tin content (from 0.75 to 0.5). The optimized high entropy oxide with the average particle size of 12 nm illustrated astonishing durability (over than 12 hours) as an anode for acidic water splitting which was superior that commercial RuO₂ as a reference. Sush enhancement was attributed to porous structure and the unique properties of the high entropy oxide like stabilizing the solid solution and severe distortion. Such observation paved a logical strategy to develop acid stable electrocatalyst with the help of high entropy materials.

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9th International Symposium on Practical Surface Analysis

Capri Room

S7. Applications III (Bio and Organics)

Chair: Tanguy Terlier (Rice University, USA) Jaekyung Hyun (Sungkyunkwan Universit, Korea)





Unravelling Pleomorphic Immature Poxvirus Structure Using Cryo-Electron Microscopy

Jaekyung Hyun^{*}, Yeontae Jang, Seungmi Kim

School of Pharmacy, Sungkyunkwan University, 2066 Seobu-ro, Jangan-gu, Suwon-si, Gyeonggi-do 16419, Korea *jhyu002@skku.edu

Poxviruses are a group of large, dsDNA viruses that are widely known for variola virus, a causative agent for the dreadful disease smallpox [1]. Assembly of immature poxvirus is driven by the self-assembly of multiple copies of scaffolding protein on the viral membrane, resulting in the formation of a capsid-like shell [2]. Although pleomorphic, the scaffold determines the overall shapes and sizes of the virus particles and is therefore critical for subsequent virus maturation. To understand the molecular mechanism that governs the assembly, we produced assembly products in vitro using scaffold protein D13 from vaccinia virus (VACV), a prototypal poxvirus, followed by structural investigation using various cryo-electron microscopy (cryo-EM) approaches.

The cryo-EM revealed that D13 assembles into two distinct structures; the scaffold-like particles (SLP) that resemble authentic virus particles and the short rodlets with twisted lateral arrangements. In SLP, D13 trimers assemble via electrostatic interactions and intertrimeric torsion induce mild and continuous curvature that renders spherical morphology of the virion with approximately 300nm in diameter. By contrast, rodlets are composed of two apposed rings of six D13 trimers that are tethered with twist. We found that conformational variation of short N-terminal α -helix plays critical roles in both assembly initiation and the regulation of scaffold formation and suggest that the two assembly products represent preand pro-assembly of virion scaffold in which the N-terminal helix is intricately involved in the morphological changes.

Given that the scaffolding proteins are widely conserved across various poxvirus genera, we propose that they are potential targets for antiviral treatments in case of unexpected outbreaks of smallpox-like diseases as in the case of recent Mpox infections.

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Mass imaging analyses for practically utilized polymers and bio materials

J. Sameshima^{*}, T. Suda, T. Shibamori, H. Seki, K. Matsuda

3-2-11, Sonoyama, Otsu, Shiga, Japan *junihiro.sameshima.q8@trc.toray

Secondary Ion Mass Spectrometry (SIMS) has been one of the indispensable tools for dopant analysis in semiconductor fields with the exclusive advantage of the high sensitivity. Still then, SIMS would be also available for polymers or related materials. NanoSIMS, which is one types of dynamic SIMS, has been utilized in biology, cosmology, geoscience field [1-4]. It has, moreover, a potential to insight materials used in a wide range of industry although the finding would be just an elemental information and does not reach organic analysis. Time-of-flight SIMS (TOF-SIMS) has become an essential method with the high sensitivity and high mass resolution abilities especially as surface organic analyses. This feature certainly matches cause analysis owing to the qualitative ability, and available in order to research unintentional component in various targets in both R&D or manufacture processes. In this study, various applications with these tools for organic or related materials widely employed as a practical usage are represented. Data obtained by other analytical techniques such as Transmission Electron Microscopy (TEM) or Scanning Electron Microscopy (SEM) etc. are also indicated along with SIMS since these microscope images would make these findings clear and reliable by combining with them.

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Arrays of spherical cap particles: Fabrication of substrates for cell cultures by dewetting of thin polymer films

Karolina Głowacka¹, Katarzyna Medyńska^{1,2}, Katarzyna Wiktorska², Maciej Chotkowski¹, Maciej Mazur^{1*}

¹Department of Chemistry, University of Warsaw, Pasteura 1, 02-093 Warsaw, Poland

²Department of Physics and Biophysics, Institute of Biology, Warsaw University of Life Sciences - SGGW, Nowoursynowska 166, 02-787 Warsaw, Poland

*mmazur@chem.uw.edu.pl

Dewetting phenomenon is the disintegration of a thin layer deposited on a solid substrate, often requiring an external stimulus to initiate. In current work, we harnessed the dewetting of thin polymer layers on solid substrates to fabricate arrays of spherical cap-shaped particles.

The fabrication process involved several stages. Initially, a polymer layer was spin-coated onto a flat substrate. The coated substrate was then immersed in a polar solvent and heated above the polymer's melting point, inducing dewetting that resulted in polymer droplets randomly distributed across the substrate. Subsequent cooling solidified these droplets into spherical cap particles adhered to the substrate surface. This versatile method enables the fabrication of non-spherical particles from various materials, including polycaprolactone, polylactide and PLGA. Moreover, the particles can be modified through incorporation of inorganic nanoparticles and small organic molecules.

The prepared structures were characterized employing a comprehensive suite of surface analysis techniques, encompassing microscopic methods (AFM, SEM, TEM) and spectroscopic methods (Raman, FTIR, XPS, TOF-SIMS). These analyses determined the particle size, shape, and surface number density.

The arrays of spherical cap particles serve as effective substrates for cell culture. Notably, when the polymer particles incorporate compounds or nanoparticles with cytotoxic properties, they present a compelling platform for cancer research. In this work cancer cells were cultured on substrates with arrays of biodegradable polymer particles (polycaprolactone, polylactide) with incorporated cytostatic agents (doxorubicin and/or selenium nanoparticles). *In vitro* MTT assays revealed reduced cancer cell viability in the presence of particles containing anticancer agents, highlighting their promising potential for novel cancer therapies.

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Multiplexing analysis using microarray by ToF-SIMS: a high throughput exploration tool for rapid chemical screening.

Tanguy Terlier^{1,2*}

¹SIMS laboratory, Shared Equipment Authority, Rice University, Houston, TX 77005, USA ²Woodside-Rice Decarbonization Accelerator, Nexus, Office of Innovation, Rice University, Houston, TX 77005, USA * tanguy.terlier@rice.edu

Multiplexing analysis is a type of assay that permits to characterize complex samples in a single run analysis. Here, we used a computer-controlled CO_2 laser cutter for machining glass plates to pattern multiples 10-microns depth microwell. Among the most suitable characterization tool for producing multiplexing analysis, time-of-flight secondary ion mass spectrometry is a powerful surface analytical technique for providing detailed elemental and molecular information about the surface, thin layers, interfaces, and full 3D analysis of the samples.

Thanks to integrated large imaging capability by scanning an area of few mm2, ToF-SIMS characterization permits a deeper exploration and a better knowledge of the organic and biological materials with complex chemical structures. ToF-SIMS produces hyperspectral images where each individual pixel contains a full mass-range spectrum. Spot areas can be selected by generating a region of interest area to treat each individually each sample. The glass plate permits to create a library of 120 individual samples. After identification of the characteristic fragment ions, multivariate analysis is used to establish the correlation between the molecular ions and to classify the relationship between the samples.

Beyond the combination of the hyperspectral images with MVA techniques, we can elucidate the chemical composition of a large set of specimens to address complex analytical challenges or chemical reactions. The operation consists of performing a rapid single-scan ToF-SIMS analysis of the plate and then classifying the dataset for database-matching or quantification of the composition. In an initial study, a small number of monomers were characterized and then we used the dataset to discriminate the molecular signature as function of the functional groups. The method has been extended to several lipids to establish a library of characteristic fragments for further understanding of lipid deposition profiles from foreign body responses. A second study has consisted of identifying the surface composition of antibody-conjugated gold nanoparticles. Our final example will focus on developing methods for inhibiting asphaltene deposition.

To conclude, we will demonstrate through various case studies how multiplexing analysis using microarray plate for fast analysis by ToF-SIMS can offer a rapid solution for building databases and establishing reference libraries of fragmented ions. In addition, this approach allows the classification and the correlation of chemical profiles from complex compounds, and potentially the quantification of mixture by dosing species ions from ToF-SIMS data.



Time-of-Flight Secondary Ion Mass Spectrometry Imaging of Biological Samples

Heejin Lim

Center for Scientific Instrumentation, Korea Basic Science Institute (KBSI), 169-148 Gawhak-ro, Daejeon 34133, Korea hjlim0111@kbsi.re.kr

Advanced analytical techniques for multidimensional chemical imaging of biomolecules such as proteins, lipids, and metabolites in cell membranes at a subcellular resolution are in high demand to study their distributions and complex interactions, which are crucial for understanding molecular mechanisms in health and disease [1]. Time-of-flight secondary ion mass spectrometry (ToF-SIMS) is a surface analytical technique that uses energetic ion beams for surface composition, chemical imaging, and depth-profile analyses. The continued development of ion sources, such as liquid metal ion sources (LMIS) and gas cluster ion beams (GCIB), has reduced the unwanted fragmentations of molecules, enabling ToF-SIMS to analyze and image small molecules like lipids and metabolites in cells and tissues more effectively [2]. Recently, ToF-SIMS has been future developed for multiplex protein imaging using metal-tagged antibodies [3,4]. Here I will show methods for mass spectrometry imaging of wet/live cell membranes with ToF-SIMS. Additionally, I will introduce a technique for simultaneously imaging metal-tagged proteins and label-free lipids in cell membranes at a subcellular resolution.

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9th International Symposium on Practical Surface Analysis

Grand Ballroom I

S8. Electron Spectroscopy

Chair: Jouhahn Lee (Korea Basic Science Institute, Korea)





Electronic Structure of 2D Halide Perovskites: Insights from Photoelectron Spectroscopy Measurement Techniques

Kitae Kim^{1,2}, Donghee Kang¹, Sylke Blumstengel^{3,4}, Nicolas Zorn Morales^{3,4}, J. W. List-Kratochvil^{3,4}, Sang Wan Cho⁵, Hyunbok Lee⁶, Soohyung Park², Yeonjin Yi^{1*}

¹Department of Physics, Yonsei University, Seoul, Korea

²Advanced Analysis & Data Center, Korea Institute of Science and Technology, Korea

³Institut fur Physik & IRIS Adlershof, Humboldt-Universitat zu Berlin, Germany

⁴Institut fur Chemie, Humboldt-Universitat zu Berlin, Germany

⁵Department of Physics, Yonsei University, Wonju-si, Korea

⁶Department of Physics, Kangwon National University, Korea

*yeonjin@yonsei.ac.kr

Two-dimensional (2D) Ruddlesden-Popper (RP) perovskites exhibit promising potential for various optoelectronic applications. However, their optoelectronic properties are often hindered by their vulnerable to photodegradation, which results in the formation of metallic Pb (Pb⁰) defects. This study elucidates the passivation mechanism of these Pb⁰ defects in phenylethylammonium lead iodide (PEA₂PbI₄) using the strong molecular acceptor 2, 2'- (perfluoronaphthalene-2, 6-diylidene) dimalononitrile (F6-TCNNQ). In situ X-ray photoelectron spectroscopy reveals that F6-TCNNQ effectively eliminates light-induced Pb⁰ states, facilitating the recovery of photoluminescence in degraded PEA₂PbI₄ samples and significantly enhancing the photostability of pristine material. Atomic force microscopy and scanning electron microscopy analyses indicate that F6-TCNNQ preferentially protects the terrace edges of PEA₂PbI₄, which are vulnerable to initial degradation. In situ ultraviolet photoelectron spectroscopy measurements confirm substantial electron transfer from Pb⁰ to F6-TCNNQ, resulting in the oxidation of Pb⁰ to Pb²⁺. Additionally, the staggered energy level alignment between PEA₂PbI₄ and F6-TCNNQ prevents detrimental charge transfer, preserving the pristine electronic structure of the perovskite. These findings offer new insights into defect passivation strategies for 2D RP perovskites and provide a design pathway towards the fabrication of highly stable optoelectronic devices.

Kitae Kim, Donghee Kang, Sylke Blumstengel, Nicolas Zorn Morales, J. W. List-Kratochvil, Sang Wan Cho, Hyunbok Lee, Soohyung Park, Yeonjin Yi, Appl. Phys. Rev. 10, 041411 (2023)



Comprehensive Analysis of Electronic Structure in PdSe₂

Kyung-Tae Ko

Korea Basic Science Institute, 169-148, Gwahak-ro, Yuseong-gu, Daejeon 34133, Korea

Transition metal dichalcogenide systems has been a steady research topic in condensed matter physics as well as applied material science. In the early transition metal dichalcogenides, the various electronic natures - charge density wave, superconductivity, valley spin-orbital structure, and topological electronic structure - have been studied within the itinerant electron point of view. Besides, in the late transition metal dichalcogenide, the d electrons are more localized while the p states get closer and the pd hybridization begins to play an important role [1.2].

PdSe₂ is a very unique dichalcogenide because of not only its orthorhombic puckered crystal structure [3] but also the detailed electronic structure itself [4]. We performed spectroscopic analyses (ARPES and XAS-LD) and theoretical studies and elucidated the detailed nature of the electronic structure of PdSe₂. The zigzag stacking of the Se₂ dimer results in an orthorhombic puckered structure, and its unit cell expansion leaves a trace of orbital-dependent band folding effect. The valence top band consists of the Pd $3z^2$ -r² orbital, which exhibits the most dispersive band along the k_z-direction. The change of band gap in the exfoliated samples explained within the quasi-1D chain nature of the valence top band and its bifurcation. In localized electron point of view, the molecular orbital formation of Se₂ and the pd hybridization are essential to explain the insulating state. The strong metal-ligand charge transfer was observed, which makes an electron of Pd⁺ into (Se₂)⁻ molecular orbital, and the ground state is dominated by the $|d^{8}L^{1}>$ configuration in which each molecular orbital is occupied with two electrons and PdSe₂ becomes a band insulator.

In this talk, I would like to demonstrate how comprehensive spectroscopic approaches could reveal the detailed electronic structure and emphasize that the efforts of synchrotron-based spectroscopy are crucial to delivering a clear understanding of electronic nature for advanced material science.

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Probing the Surface Electronic Structure and Reaction Intermediate using Synchrotron-Based AP-XPS

Jeongjin Kim^{*}

Pohang Accelerator Laboratory, POSTECH (Pohang, Gyeongbuk 37673, Republic of Korea) *jeongjkim@postech.ac.kr

Molecular interactions on metal or metal-oxide surfaces are considered an important early step in most industrial chemical reactions to produce value-added chemicals. For several decades, surface science tools have been dedicated to characterizing the correlation between surface structures and adsorbate species on surfaces; as a result, the elegant characterization techniques have accomplished probing the critical evidence for various kinds of physisorption and chemisorption fingerprints and products at active sites [1,2].

However, the ultra-high vacuum (UHV)-based characterizations have inevitable technical limitations to detecting reaction intermediates because the chemically active species could exclusively exist under working conditions in most industrial reaction pathways [3]. To overcome this issue, sorts of differential-pumping technology is necessarily required to transcend the pressure gap between UHV and environmental conditions. Among the popular surface science techniques, ambient pressure X-ray photoelectron spectroscopy (AP-XPS) is a useful tool for revealing chemical binding species at the gas-solid or liquid-solid interfaces [4]. By employing AP-XPS observations, our knowledge can be extended to understand unusual physical phenomena caused by molecular diffusion and adsorbate-induced surface reconstruction [5].

In this talk, I will discuss chemical reaction pathways on Pt- or Pd-based surface alloys probed with synchrotron-based AP-XPS technique under reaction conditions. Adsorbate CO or CO₂ gas molecules could evolve unexpected surface restructuring on bimetallic structures at ambient pressures, and the activated surfaces interact with surrounding molecules for efficient energy conversions. For example, Pd-incorporated indium oxide surfaces could effectively produce methoxy-related intermediates toward methanol conversion at mild temperatures (< 400 K) during CO₂ activation. Those *in situ* surface observations at elevated pressures and temperatures provide us with essential information to figure out correlated reaction pathways, and those observations may open the door to a new horizon in the nanoscopic world.

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Recent advances in soft and tender X-ray photoemission spectroscopies at the Pohang Accelerator Laboratory

Siwoo Noh^{1,2}, Jeongjin Kim², Seong Hee Park¹, and Ki-jeong Kim^{2*}

¹Department of Accelerator Science, Korea University, Sejong 30019, Republic of Korea ²Pohang Accelerator Laboratory, POSTECH, Pohang, Gyeongbuk 37673, Republic of Korea *kjkim@postech.ac.kr

Recent *in situ/operando* surface science studies using synchrotron-based ambient pressure X-ray photoemission spectroscopy (AP-XPS) at the 8A2 beamline at the Pohang Light Source II show intriguing physicochemical phenomena at the gas-solid or liquid-solid interfaces. It implies that energy conversion processes occur via complicated reaction pathways, and we could get critical clues to identify physical and chemical relationships at the interface based on the careful spectroscopic characterization results. In this talk, we will discuss our recent *in situ/operando* model studies probed with AP-XPS, demonstrating the adsorbate-induced surface reconstruction on model surfaces under O₂(g) or CO₂(g) environments at elevated temperatures. Our AP-XPS results indicate that the oxygen or dissociated CO from CO₂ adsorbates could alter surface geometries and electronic structures. In addition, those spectroscopic observations are exclusively observed above a few mTorr pressures due to the pressure gap effect. Secondly, we will focus on the role of buried surfaces in a view of interface science. For example, the next generation AP-XPS, the "tender" X-ray source-based photoemission spectroscopy technique enables exploring the nanoscopic world beyond the surface using the new bright X-ray source developed by the Korea-4GSR project. We would like to briefly introduce our recent status of 4GSR beamline sciences to construct a novel soft-tender X-ray photoemission beamline in Ochang.



Figure 1. Schematics of the 4GSR soft X-ray NanoProbe beamline layout.

9th International Symposium on Practical Surface Analysis

Grand Ballroom I

S9. Electron Microscopy

Chair: Sangmin An (Jeonbuk National University, Korea)





Understanding dislocation dynamics in advanced steels via transmission electron microscopy

Sung-Dae Kim*

Department of Materials Science and Engineering, Pukyong National University, 45, Yongso-Ro, Nam-Gu, Busan 48513, Republic of Korea *sdkim@pknu.ac.kr

Aluminum-containing austenitic high-Mn steels (Fe-Mn-Al-C steels) have been widely revisited as one of the most promising subgroup of the high-Mn steels because of their attractive mechanical properties as well as low specific weight. Addition of 1 wt% Al reduces 1.5% of specific weight, rendering the alloys to be so-called 'light-weight steels' and an encouraging candidate for automotive applications. Deformed microstructure of the Fe-Mn-Al-C can be characterized by the pronounced planar dislocation glide. The origin of the unique deformed structure has been controversially discussed, and the majority of researcher attributes origin of the unexpected finding to the ordered phase in the alloys. That is, the ordered phases dispersed in the austenite matrix hinder dislocation movement, whereas if the ordered phases are sheared by some leading dislocations then the trailing dislocations are easy to glide on the same slip plane ("glide plane softening"). Many researchers agreed the validity of the "glide plane softening" effect, although, there are significant distinctions in the interpretations of the strain hardening process in the alloys. The present study aims to elucidate the deformation mechanism of the Al-added austenitic high-Mn steels by means of transmission electron microscopy (TEM). Especially, we conduct *in-situ* mechanical straining TEM experiments to show the dynamic evolution of the deformed microstructure including the dislocations gliding behavior. We seek to visualize the pronounced planar glide of the dislocations and the process of the mutual intersection of dislocations in the slip bands. In comparison with the previous *post-mortem* analysis on the deformation microstructure of the lightweight high-Mn steels, this study provides more evident clues towards understanding the high strain hardening capacity of the alloys by observing plastic deformation process in real time.



대기 중 단일 입자의 모양 및 성분 분석

박지원, 김기현, 김동희, 김성민, 김정택, 최지원, 송영철^{*} *한국화학연구원 화학분석센터 *ycsong@krict.ac.kr*

대기 입자는 Sea salts, Mineral dust와 같은 자연 발생 물질과 매연, black carbon 등 인간 활동에 의해 발 생하는 물질로 나뉘게 된다. 에어로졸은 태양복사 에너지를 흡수 또는 산란시킴으로써 환경에 직접적인 영향을 미치거나 혹은 CCN(Cloud condensation nuclei)으로 작용하게 되어 간접적인 영향을 준다. 에어로 졸이 환경에 미치는 영향을 예측하려면 입자의 화학적 특성을 파악하는 것이 필수적이다. 본 연구에서는 초미세먼지 단일 입자의 모양과 성분을 SEM/EDS를 통해 분석하여 대기 입자의 발생원, 반응성, 거동 등 에 관한 연구를 진행하였다.

연구에 필요한 대기 입자 포집은 3단 임펙터(cascade impactor)를 사용하였으며, 2.5 ~ 10 μm, 1.0 ~ 2.5 μm, < 1.0 μm 의 미세먼지를 포집할 수 있다. 이 중 2단에 포집된 초미세먼지 입자를 분석에 사용하였으며 초미세먼지 입자의 크기와 성분은 Field Emission Scanning Electron Microscope (FE-SEM)와 Energy Dispersive X-ray Spectrometer (EDS)로 측정하였다.

이번 연구에서 대기 입자의 주성분을 바탕으로 총 180 개의 대기 입자를 분석하였고, 4가지 종류의 화합 물로 분류하였다. 연구 결과 C, N, O, S로 구성된 유기 입자와 NO_x와 SO_x와 반응한 단일 입자, 토양 기원의 단일 입자가 기원일 것으로 추정되었다.



그림 1. SEM/EDS로 분석한 대기 중 단일 입자

^[1] IPCC 2021

^[2] H. J. Eom et al, Atmos. Chem. Phys., **16**(2016), p.13823



Gate-dependent interactions between Fe atoms on graphene

Jungin Yeo, Gahee Lee, Sangjun jeon*

Department of Physics, Chung-Ang University Seoul 06974, Republic of Korea *E-mail: jsangjun@cau.ac.kr

The electrical, optical, thermal, and magnetic properties of metallic materials are influenced by the size and shape of the Fermi surface. However, adjusting the Fermi level in conventional materials is challenging due to the high density of states at the charge-neutral state. Recent studies have shown that a few layers of two-dimensional materials can undergo various phase transitions when an external electric field is applied, thanks to reduced charge screening and fewer states in low-dimensional materials. In graphene, the Dirac behavior of electrons allows the Fermi wavelength to be tuned from zero to several nanometers. This makes graphene a versatile substrate for mediating the coupling strength of atoms adsorbed on it. In this study, we investigate the strength of adatoms and the substrate, as well as the indirect interaction between adatoms on graphene by controlling the charge level of graphene. Using charge-tunable scanning tunneling microscopy (STM), we resolve the hybridization of magnetic adatoms with the Dirac system and observe changes in magnetic ground states at the atomic scale. S9-4

In situ and *operando* transmission electron microscopy study of one-dimensional InAs-based compound semiconductor nanowires

Young Heon KIM*

Graduate School of Analytical Science and Technology (GRAST), Chungnam National University, 99 Daehak-ro(St), Yuseong-gu, Daejeon 34134, Republic of Korea *v.h.kim@cnu.ac.kr

InAs-based compound semiconductor nanowires have attracted great attention due to their exceptional electrical and optoelectrical properties, such as high room-temperature mobility and narrow bandgap engineering. Specifically, a tunable InAsP system is of potential interest for both electrical and optoelectronic devices. Advances in *in situ* and *operando* transmission electron microscopy (TEM) technologies, for example, heating and biasing, have enabled researchers to observe changes in the atomic and electronic structures of various materials in real time. By adopting appropriate *in situ* and/or *operando* TEM techniques, it is possible to explore novel atomistic behaviors and measure the physical properties during morphological and microstructural evolutions. In addition, because nanometer-scale materials can be observed by TEM without specific specimen preparation, the experimental artifacts may be minimized during observation and measurement.

In this talk, I introduce the atomistic evolution of InAs nanowires with and without an aluminum oxide shell during *in situ* heating with respect to the polarity, based on a high-resolution scanning transmission electron microscopy (STEM) measurements. It was possible to directly observe the morphological change and atomistic behaviour of InAs nanowirs depending on the presence of a shell. Finally, I present the electromechanical properties of ternary InAsP nanowires; a single nanowire-based device was fabricated to investigate these properties.

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Recent advancements in elasto-visco-plastic self-consistent model and its application to various polycrystal metals

Youngung Jeong

School of Materials Science and Engineering, Changwon National University

An elasto-visco-plastic self-consistent based on an incremental formulation (Δ EVPSC) has been recently developed [1] and interfaced with a commercial finite element solver [2]. The versatility of the Δ EVPSC model has been demonstrated by applying it to various problems, cluding the springback of single phase mild steel and high strength dual-phase steel, as well as interpreting the evolution of internal lattice strain of a commercially-pure Ti alloy. Additionally, thermo-mechanical behavior of various cermets and a polycrystal uranium has been successfully analyzed by the Δ EVPSC model. In this talk, the Δ EVPSC model is briefly reviewed, and recent advancements are highlighted. A few examples are discussed where crystallographic orientaion distribution obtained via electron back-scattered diffraction is used to characterize the initial and deformed states of polycrystalline metals simulated.

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Real-Time Investigation of Corrosion Behaviors in Zn-Mg-Al Alloys Using Liquid-Phase TEM

Jungjae Park^{*}, Sung Kang

Analysis and Assessment Research Group, Research Institute of Industrial Science and Technology (RIST), 67 Cheongam-ro, Nam-gu, Pohang, Gyeongsangbuk-do, Republic of Korea (37673) *jungjae10@rist.re.kr

Zn-Mg-Al alloy coated steel sheets are highly regarded for their excellent corrosion resistance, making them ideal for challenging marine, coastal, and industrial applications. These coated steel sheets are extensively used in construction, infrastructure, automotive, and renewable energy sectors due to their robustness and ability to withstand severe environments. The exceptional corrosion resistance of this alloy is mainly attributed to its intricate microstructure of Zn-Mg-Al compounds and the formation of stable, dense corrosion products like Layered Double Hydroxides (LDH). Despite this, the connection between microstructural features and the development of corrosion products remains somewhat unclear due to the complex nature of the microstructures and the corrosion mechanisms involved. In this study, we utilized in-situ liquid-phase transmission electron microscopy (TEM) to observe the real-time corrosion behaviors of the Zn-Mg-Al alloy in a saline environment. Our findings shed light on the mechanisms underpinning the high corrosion resistance of Zn-Mg-Al alloy coatings and offer valuable insights into the interactions between alloying elements and microstructural evolution, which contribute to the alloy's superior corrosion resistance.

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Grand Ballroom I

S10. Ion Beam Technology

Chair: Taeeun Hong (Korea Basic Science Institute, Korea)





Status and Utilization of Tandem Accelerator-Based Ion Beam Analysis System of KAERI

Kye-Ryung Kim^{*}, Yong-Sub Cho, Han-Sung Kim, Hyeok-Jung Kwon, Young-Gi Song, and Jae-Ha Kim

Korea Atomic Energy Research Institute, 181 Mirae-ro, Gyeoncheun-eup, Gyeongju, 38180, Korea *corresponding.kimkr@kaeri.re.kr

Ion beam analysis is an advanced non-destructive precision analysis technology that has been mainly used in the field of semiconductor material research and development, and demand is continuously increasing. Typical ion beam analysis techniques include PIXE (Proton Induced X-ray Emission), RBS (Rutherford Backscattering Spectroscopy), ERD (Elastic Recoil Detection), ToF (Tiom-of-Flight)-ERD, PIGE (Proton Induced Gamma-ray Emission), and NRA (Nuclear Reaction Analysis). Each of these analysis techniques has its own strengths and has its main application field according to their characteristics, and when these analysis techniques are applied complementarily, a better understanding of the material is possible.

The Korea Atomic Energy Research Institute has 1.7 MV and 3 MV Tandem accelerators and has built and operated ion beam analysis systems such as PIXE, RBS, and ERD based on the 1.7 MV Tandem accelerator, and plans to build additional ion beam analysis devices such as ToF-ERD and PIGE in the near future. Recently, a dedicated beamline has been built to respond to the demand for analysis of cultural heritage.

In this presentation, we would like to present the current status and plan of the development and use of Tandem accelerator-based ion beam analysis device by the Korea Atomic Energy Research Institute, and in particular, we would like to address the recent establishment of an external beam PIXE beamline dedicated to cultural heritage.



가스클러스터 이온빔개발 및 X-ray광학계 표면가공 활용 (Development of Gas Cluster Ion Beam and Application to the Surface Processing in X-ray mirror)

최명철^{1*}, 홍아람¹, 현상원¹, Mourad Idir², Tianyi Wang², Dae Wook Kim³

¹ 한국기초과학지원연구원 연구장비개발부 (34133 대전시 유성구 과학로 169-148) ²Brookhaven National Lab., NSLS- II, Optics & Metrology (Upton, NY 11973-5000, US) ³University of Arizona, Large Optics Fabrication and Testing Group (Tucson, Arizona 85721-0094, US) *cmc@kbsi.re.kr

TOF-SIMS에서 3차원 질량 이미징 분석에 중요한 기능을 담당하는 가스 클러스터 이온 빔(GCIB)의 국 내 개발을 소개합니다. 그리고 GCIB의 특성을 활용한 광학시스템 표면 처리에 대한 새로운 접근 방식을 제시합니다.

고정밀 X선 광학 시스템을 제작하기 위한 기존 이온 빔 성형(IBF) 방법은 고정밀 표면 처리를 제공했습 니다. 그러나 시료표면의 빔보다 작은 고주파 영역에서 표면구조의 수정 및 거칠기를 줄일 수 없다는 한계 가 있었습니다. [1]

이 문제를 해결하기 위해 IBF보다 더 높은 가속전압을 사용하는 GCIB를 사용한 새로운 마무리 방법을 제안합니다. GCIB는 기존 원자 빔과 다른 클러스터 빔으로 표면 에칭이 더 매끄러운 것으로 알려져 있습니다.

본 연구에서는 Si-웨이퍼에 GCIB를 사용하여 가공된 표면의 특성을 보여줍니다.



그림 1. 20 kV로 가속된 GCIB에 의한 Si-wafer의 표면 가공면의 공간 주파수 특성에서 High frequency영역의 변화

Tianyi Wang, Lei Huang, Yi Zhu, Stefano Giorgio, Philip Boccabella, Nathalie Bouet, Mourad Idir, Nanomanufacturing and Metrology, 6(20), 2023



Compositional and Interfacial Analysis of Ag incorporated CIGS Solar Cell using SIMS, AES and APT

Yun Jung Jang^{1,3}, Jung-Hyeon Yoon¹, Ji Yeong Lee¹, Jeung-Hyun Jeong², Donghwan Kim³, and Yeonhee Lee^{1*}

¹Advanced Analysis Data Center, Korea Institute of Science and Technology ²Advanced Photovoltaics Research Center, Korea Institute of Science and Technology ³Department of Material Science and Engineering, Korea University *vhlee@kist.re.kr

CIGS (Cu(In,Ga)Se2) solar cell is considered to be a flexible solar cell because its property of high absorption coefficient permits the sufficient absorption of light through the 1 μ m thickness of absorber layer. The polyimide (PI) substrate is needed for the flexible CIGS solar cell, however, PI cannot afford to bear the high temperature of 550°C, that is used ordinarily for thermal treatment during the deposition process of CIGS solar cell.[1] Ga distribution is not favorable at the low temperature, which decrease the photovoltaic conversion. Alternatively, the Ag doping in CIGS absorber layer can reduce the melting point and enhance the crystallinity of the thin film at a low temperature. Because the band gap is also increased slightly with adding of Ag, the (Ag, Cu)(In, Ga)Se₂ absorber layer can be adjustable for the band-gap.[2]

In this study, we investigate the compositional effect of Ag in the CIGS solar cell using a combination of surface analytical techniques such as secondary ion mass spectrometry (SIMS), auger electron spectroscopy (AES) and atom probe tomography (APT). The major constituents using SIMS and AES were quantified based on the concentrations obtained using electron probe micro analyzer (EPMA), then band gap as a function of depth was determined using the quantified Ga and In. We found out the uniformity of the Ga gradient and difference in quantities of Na and K impurities as incorporation of Ag in the region of absorber layer in SIMS and AES results. The interface and grain boundary (GB) regions were analyzed using APT, which indicates the segregation of Ag components at the near-surface of CIGS and the formation of MoSeX layers. This comprehensive analysis has provided valuable insights into the composition for the absorber layer of solar cell as incorporation of Ag

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Advantages of non-destructive depth profile analysis using TOF-MEIS over destructive method

Kyungsu Park, Soo-Bang Kim, Won Ja Min*

HB solution, Techno 8ro 33, Yuseong-gu Daejeon, Republic o Korea, 34028 *wj.min@hb-solution.co.kr

Depth profile analysis using sputtering is commonly used in the field of surface analysis. Secondary Ion Mass Spectrometry (SIMS) detects secondary ions generated from a sample after sputtering. X-ray photoelectron spectroscopy (XPS) or Auger Electron Spectroscopy (AES) performs the depth profiling by repeating sputtering and measurement for the sample that the thickness to be measured is thicker than the probing depth. However, the composition on the surface changes at about 2 to 10 nm due to the difference in sputtering yield by element and the mixing of the sample when sputtering. Therefore, the measurement data is not the original state. As an alternative, there is a non-destructive depth profiling technique.

Non-destructive depth profiling (NDDP) refers to techniques that allow the characterization of a material's composition or structure as a function of depth without physically removing layers of the material, in contrast to destructive methods like sputtering. These non-destructive techniques are recommended for analyzing samples where maintaining the material's integrity is crucial. One of them is MEIS (Medium Energy Ion Scattering), which is a surface analysis technique that allows non-destructive quantitative depth profiling of ultra-thin films with single-atom resolution.

In the presentation, we look into the reason why MEIS is quantitative in depth-profiling in principle and observed the deformation of the specimen due to sputtering by performing MEIS analysis before and after sputtering of each specimen. The samples used for measurement were IGZO, TiNTaN(5) multi-layer samples, etc. Based on the observation results of specimens before and after sputtering, MEIS measurement is strongly recommended to obtain the intact compositional depth distribution of the sample without sputtering damage.

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Grand Ballroom I

S11. Photon Beam Technology

Chair: Kwangseuk Kyhm (Pusan National University, Korea) Un Jeong Kim (Dongguk University, Korea)





Metrology and Inspection Tool for Low Dimensional Materials

Un Jeong Kim

Department of physics, Dongguk university, Seoul 04620, Republic of Korea *ujjanekim@dongguk.edi

Nanomaterials and its nanostructured array can introduce interesting optoelectronic properties. Nano material itself exhibits outstanding physical properties such as direct electronic band gap, large light matter interaction, polymorphism, and so on. Moreover, nanomaterials possesses high surface to volume ratio, or all surface morphology. Thus, it is very sensitive to the ambient environment resulting in strain and doping. Such susceptibility to the environment can be conversely considered as an advantage from an engineering perspective as a means to control the work function of a material which allows us to demonstrate unique optoelectronic devices. On the other hand, investigating the physical properties of nanomaterials before integrating it into devices is very critical. In this talk, Raman spectroscopy and phase shifting interferometery can be industrial metrology and inspection tool for low dimensional semiconductor. This provides initial condition of the materials efficiently which will improve the quality of device fabrication process. My goal for research is developing on-destructive metrology and Inspection(MI) tool for multi-layered electronic and optoelectronic devices.

Un Jeong Kim, et. al. Hyperspectral Imaging of Complex Dielectric Functions in 2d Materials, Nano Today, V55, 102170 (2024)

^[2] Yoojoong Han, et. al. under review in Small.



Analysis of Tellurium/Indium Zinc Tin Oxide Heterostructures and Their Device Applications

Sooji Nam^{1,2*}, Jung Hoon Han¹, Dong Yeob Shin³, Kwun-Bum Chung³, Sung Haeng Cho¹

¹Electronics and Telecommunications Research Institute (ETRI), ²University of Science and Technology, ³Dongguk University ¹Flexible Electronic Device Research Division, ETRI (218 Gajeong-ro, Yuseong-gu, Daejeon 34129 Korea) *sjnam15@etri.re.kr

Amorphous oxide semiconductor (AOS) thin-film transistors (TFTs) are ideal for display panels and sensors due to their high mobility, low leakage current, and low-temperature processability.[1] However, issues such as threshold voltage (V_T) shifts and poor stability persist.

In this study, a new approach is proposed to control the V_T of indium-zinc-tin-oxide (IZTO) TFTs using a heterojunction structure with p-type Tellurium (Te). The Te layer acts as a charge-trapping layer, while IZTO serves as the charge-carrier transporting layer.[2] By adjusting the thickness of the p-type Te layer, V_T can be modulated up to +20 V. We systematically investigate the structural, optical, and electrical properties of Te/IZTO films using X-ray photoelectron spectroscopy, UV-Vis spectroscopy, spectroscopic ellipsometry, X-ray diffraction, and transmission electron microscopy analyses. The energy-band structure analysis of the Te/IZTO heterojunction reveals how the Te film thickness affects charge-carrier transport and V_T shift.



Figure 1. (a) Device schematic and TEM images, (b) electrical characteristics, (c) extinction coefficients and valence-band spectra, and (d) energy band structures of Te/IZTO films.

[1] K. Nomura, et al., Nature 432 (2004) 488

^[2] J. H. Han, et al., ACS Applied Materials & Interfaces 16 (2024) 31254



Bottom-up synthesis of 2D materials for future electronics

Seok Joon Yun

Department of Semiconductor Physics and Engineering, University of Ulsan, 93 Daehak-ro, Nam-gu Ulsan 44610, Korea

Two-dimensional (2D) semiconductors have been intensively studied for their potential to overcome the limitations of current Si semiconductor technology. The semiconductor industry requires the large-scale synthesis of high-quality 2D materials for various applications. Equally critical is the ability to engineer the physical properties of these 2D materials and seamlessly integrate them into electronic devices. To achieve these goals, a bottom-up synthesis approach, such as chemical vapor deposition (CVD), is essential. CVD, as a versatile bottom-up synthesis technique, provides precise control over the growth process and enables fine-tuning of material properties to meet specific requirements. In this talk, I will present an overview of research on the synthesis and modification of 2D materials using chemical vapor deposition, with the aim of advancing the realization of 2D material applications.

- I. Engineering the physical properties of 2D materials through substitutional reactions allows for the effective modification of carrier type, carrier density, and bandgap.
- II. Developing a facile platform for layer-by-layer growth of 2D vertical heterostructures using CVD, where activating the basal surface of 2D materials is key to achieving layer-by-layer growth.
- III. Investigating the growth mechanism and controlled synthesis of 2D materials using in-situ diagnostics, providing feedback for AI-assisted autonomous bottom-up synthesis.



Molecular-level structural understanding of temperature induced phase transitions in bromine functionalized metal organic framework.

Yoon Mi Choi^{1*}, Jintaek Gong², Hyeon Ju Noh¹

¹Chemical Analysis Center, Korea Research Institute of Chemical Technology (KRICT), 141 Gajeong-Ro, Yuseong-Gu, Daejeon 34114, Korea

²Department of Chemistry Education, Sunchon National University, Sunchon 57922, Republic of Korea *ymchoi@krict.re.kr

This study presents the first empirical structural report on a bromine-functionalized DMOF (DMOF-Br₂) across various temperature ranges (80 K - 400 K), alongside comparable analyses of its parent DMOF. Using thermogravimetric analysis (TGA), differential scanning calorimetry (DSC), and Raman spectroscopy, we investigate the temperature-induced phase transitions of these structures in relation to their crystalline configurations through X-ray crystallography. Accompanying the dramatic change in unit cell volume (18000 Å³ to 1150 Å³), the study showed a phase transition from the I4₁/acd space group to the P4mm space group of the tetragonal crystal system within the transition temperature range. Furthermore, X-ray crystallography revealed that the Br-functionalized ligand (DBrTPA) exhibited four possible spatial arrangements at high temperatures. This was induced by the lack of interaction between the solvent and the Br atom on the ligand, leading to a disordered structure. Tracking these structural changes and understanding the crystalline DMOF-Br₂ structure are expected to provide molecular-level insights into the mechanisms underlying its practical applications



Ultrafast spectroscopy and Microscopy on Nanomaterials

Kwangseuk Kyhm^{*}

Department of Optics & Mechatronics, Pusan National University Geumjung-Gu, Busan, 46241, Republic of Korea * kskyhm@pusan.ac.kr

Femtosecond laser is used to study various nanomaterials. Utilizing the transient optical nonlinearities of a laser pulse, time-resolved spectroscopy uncovers ultrafast phenomena in terms of carrier and exciton dynamics, and nonlinear optical microscopy provides a high- resolution image.

Beginning with cross-correlation measurement of femtosecond pulses, various time-resolved spectroscopy techniques will be introduced, where I will mainly focus on center-of-mass exciton confinement, excitonic dipole-dipole interaction, and Auger process in droplet quantum dots [1,2]. For coupled quantum dot molecule and quantum ring, magneto-optical microscopy and photon-correlation techniques were also utilized to measure quantum coherence [3,4].

For nonlinear optical microscopy, two-photon excitation fluorescence (2PEF) and second harmonic generation (SHG) microscopy will be introduced. In our case, these techniques were utilized to reveal the internal dentinal structures. Tubular structures were obtained through optical image analysis and a fluorescence bleaching of the ingredient collagen was also observed.

^[1] H. Kim et al. Light: Science & Applications, 9(100) 2022.

^[2] H. Kim et al. Nano Letters, 16(1) 27 (2016)

^[3] H. Kim et al. Nano Letters, 18(10) 6188 (2018)

^[4] Vladimir M. Fomin, Physics of Quantum Ring, Springer p231 (2021)



Label-free Spectroscopic Detection of Biomolecules for Diagnosing Alzheimer's Disease

Chaejeong Heo^{1,2*}

¹Brainics Lab, Institute of Quantum biophysics (IQB), Department of Biophysics ²Center for Integrated Nanostructure Physics (CINAP), Institute for Basic Science (IBS), Sungkyunkwan University, Suwon, Republic of Korea *corresponding. cjheo@skku.edu

Alzheimer's pathology is correlated with structural conformation change of aggregated amyloid beta (A β) proteins. We identified the progressive aggregation stages of the A β protein growth in a buffer solution using by the near-field THz spectroscopy and the newly defined biophysical marker (DQ) based on real-time THz optical conductance. Frequency-dependent conductance for A β aggregates was obtained by measuring the differential transmittance of the time-domain spectroscopy in the THz range with a molar concentration of monomer, oligomer, and fibrillar forms. We also found the new phase transitions within three aggregation steps by label-free continuous A β dynamics monitoring during macro scale fibrils from monomers under physiological conditions. [1]

Furthermore, we elucidated this basic mechanism by studying how the charge transfer behavior of the surface of three-state-proteins is different on the graphene surface. We probe the charge transfer of $A\beta$ proteins at different aggregation stages adsorbed on monolayer graphene (Gr) using Raman spectroscopy. The shifts in Raman parameters showed that the small $A\beta$ monomers withdraw electrons, whereas fibrils donate electrons to Gr. Oligomers undergo transient charge states near the neutrality point. This finding provides insight into the electronic properties of $A\beta$ s that could be essential to identifying the onset of toxic fibril forms and developing a straightforward, label-free diagnosis using Gr. [2]

C. Heo et al., "THz Conductance Measurement for Fibrilization of Amyloid Beta Protein". ACS Nano (2020) 14(6):6548-6558

^[2] W. Cha[†] and C. Heo^{†*} et al., "Probing Interfacial Charge Transfer between Amyloid-β and Graphene during Amyloid Fibrillization Using Raman Spectroscopy." ACS Nano (2023)17, 5, 4834-4842



Photoelectron Spectroscopic Study of the Interfacial Electronic Structures of Metal-Ion Containing Polyelectrolytes on ITO Substrates

Jin Hee Lee, Yeasin Khan, Seunghwan Kim, Ae Jin Choi, Bright Walker, Soohyung Park, and Jung Hwa Seo^{*}

Department of Physics, University of Seoul, Seoul 02504, Republic of Korea Department of Chemistry, Kyung Hee University, Seoul 02447, Republic of Korea Advanced Analysis Center, Korea Institute of Science and Technology, Seoul 02792, Republic of Korea * seojh@uos.ac.kr

Research in the field of organic electronics has witnessed dramatic improvements in device performance over the past several decades through an ever-improving understanding of electron and hole movement and the development of new interfacial materials. In this study, a type of interfacial material that relies on ionic charges comprising metal:poly(styrenesulfonate) (PSS) polyelectrolytes are synthesized and investigated as structural analogs of the ubiquitously used poly(3,4-ethylenedioxythiophene:polystyre nesulfonate) (PEDOT:PSS) hole transport layer, in order to investigate correlations between metal cation ions and the cationic PEDOT component. The metal ions selected for this study include Li, Mg, V, Mn, Co, Ni, Cu, Zn, Pd, Ag, Cs, and Pb ions. To analyze the interfacial energy level alignment, electronic band structure, and band bending at the Indium tin oxide (ITO)/metal:PSS interface, X-ray photoelectron spectroscopy (XPS) and ultraviolet photoelectron spectroscopy (UPS) are employed. Alkali (earth) and post-transition metals show deep highest occupied molecular orbital (HOMO) levels and low work function (WF) due to Fermi level balance, implying poor hole transport. Remarkably, Cu:PSS displays a unique electronic structure, suggesting potential as a hole transport layer with increased WF and low hole injection barrier. Period 5 transition metals mirror PEDOT:PSS trends, and Ag:PSS holds the potential to form effective ohmic contacts.



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S12. Nano Scientific Symposium Korea (NSSK)

Chair: Sang-Joon Cho (Park Systems, Korea)





Improved sensitivity of atomic force microscopy images by machine learning

Yunseok Kim*

School of Advanced Materials Science and Engineering, Sungkyunkwan University (SKKU), Suwon 16419, Republic of Korea *yunseokkim@skku.edu

Atomic force microscopy (AFM) becomes a quasi-essential tool for exploring microstructural, physical, and chemical properties of materials at the nanoscale. In particular, as the research focus on the sizes or dimensions has shifted from bulk to nanosized materials, the AFM techniques with better signal are continuously developing. Nonetheless, the interpretation of the AFM data is still insufficient to fully understand materials properties due to technically limited signal. Recently, machine learning based analysis has received considerable attention because it allows overcoming the current technical drawbacks. The improved sensitivity of AFM techniques could allow better interpretation of the AFM data and, eventually, allow better understanding of material properties. In this presentation, I will discuss about application of machine learning for improving sensitivity of AFM images. In particular, I will focus on the application of deep learning to the piezoresponse force microscopy, which can be used to observe piezoelectric, ferroelectric, and electrochemical properties, for improving sensitivity and spatial resolution.



Unconventional micro-/nanofabrication via high temperature annealing

Jungchul Lee^{*} and Taeyeong Kim

Department of Mechanical Engineering, Korea Advanced Institute of Science and Technology 291 Daehak-ro, Yuseong-gu, Daejeon, South Korea *jungchullee@kaist.ac.kr

In integrated circuits (IC) and micro-/nanoelectromechanical systems (MEMS/NEMS), annealing is commonly employed to relieve stress, relocate or activate dopants and heal implant damage for semiconductor materials and to activate the interfacial reaction of metal contacts. It's interesting to note that for pre-structured semiconductor materials, annealing can cause shape evolution, or morphological change, towards the minimization of surface energy. Consequently, standard etching and post-annealing procedures can be used to create unique semiconductor micro-/nanostructures. Here, we introduce membrane-cavity and pedestal sphere structures, which are the end product of annealing semiconductor materials at high temperature, and discusses the technical uses of them.



Ultra-sensitive and Nanoscale Imaging of Individual Biomarkers in a Single Neuronal Cell Using Force-Based AFM

Ikbum Park^{1*}, Hyun Jin Kim², Joung-Hun Kim^{2*}

¹Korea Research Institute of Chemical Technology (KRICT), 2Pohang University of Science and Technology (POSTECH) ²Technical Support Center for Chemical Industry, KRICT (45 Jongga-ro, Jung-gu, Ulsan, 44412, Korea) *ibpark@krict.re.kr

Atomic force microscopy (AFM) has been used to study molecular interactions of ligand-receptor, DNA-DNA, and antigen-antibody at the single-molecule level. AFM nanoscale imaging enables to detect cell structures in solution and at high resolution. In addition, Force-based AFM has been used for the quantitative analysis of biomarkers. In this approach, the target molecules are captured on the surface on which target-binding molecules are immobilized, and the captured targets are recognized by an AFM tip-immobilized molecule that binds to the captured targets. By recording the specific rupture curves in a given area, the individual target molecules can be visualized. This method does not require labeling and modification, and promise superb sensitivity down to the single copy without amplification.

We reported visualization and quantification of biomarkers (e.g. miRNA, LIMK1 protein, PSA, HCV-RNA) captured on biochip surface and single cell[1-5]. To locate individual molecules, high resolution force mapping should be employed. It is expected that the results provide a sound platform for further development of AFM as an interesting and powerful tool for molecular diagnostics.

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^[2] I. Park, H. J. Kim, Y. Kim, H. S. Hwang, H. Kasai, J.-H. Kim, J. W. Park. Proc. Natl. Acad. Sci. USA, 116 (2019), 9616.

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^[4] J-S. Lim, H. J. Kim, I. Park, S. Woo, J.-H. Kim, J. W. Park. Nano Lett. 22, (2022) 3865.

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The nanoscale lattice deformations in two-dimensional materials

Dong Hyeon Kim¹, Chanwoo Lee², Mun Seok Jeong^{1*}

¹Hanyang University, ²Sungkyunkwan University ¹Department of Physics, Hanyang University (222, Wangsimni-ro, Seongdong-gu, Seoul 04763 Korea) mjeong@hanyang.ac.kr*

Since the first discovery and application of two-dimensional materials as 2D transistors due to their extraordinary electrical and optical properties, the lattice deformations such as vacancies, substitutions, and strained regions have been widely researched to prevent and overcome the deterioration of the device performance. Moreover, the importance of defects is re-examined with two representative aspects: defect-induced performance degradation and defect engineering for new applications.

Tip-enhanced Raman spectroscopy (TERS) is the most suitable non-destructive method to investigate the nanoscale lattice deformations of two-dimensional materials with correlative information (topological and physicochemical). Using TERS, we have explored new lattice vibrations come from the transition metal and chalcogen vacancies, atomic substitutions/reconstructions at the interfaces of 2D heterostructures, and the changes of atomic spacing by inherent strain. [1-3]

Overall, our study highlights the importance of advanced nanoscale characterization to investigate and understand the lattice deformations for new challenges with low-dimensional materials.



Figure1. Tip-enhanced Raman spectroscopy for two-dimensional physical properties

^[1] C. Lee, et al., ACS Nano 12 (2018) 9982-9990

^[2] C. Lee, et al., npj 2D Materials and Applications 6 (2022) 67

^[3] D. H. Kim, et al., Nanophotonics 12 (2024) 1069-1077



Advances and challenges in dynamic photo-induced force microscopy

Junghoon Jahng^{*}

Material Property Metrology Group, Korea Research Institute of Standards and Science, Daejeon, 34113, South Korea *phyjjh@kriss.re.kr

Photo-induced force microscopy (PiFM) is a scanning probe technique celebrated for its capability to achieve high-resolution spectroscopic imaging at the nanoscale. This method exploits the amplification of tip motion by photo-induced forces, which arise from interactions with the local medium, ranging from induced dipole effects to thermal expansion. These force responses demonstrate complex behaviors linked to both far-field and near-field phenomena, depending on their spectroscopic origins. In this talk, a detailed overview of past research, emphasizing the technical challenges involved is provided. We present perspectives on photo-induced dipole and thermal forces, while also exploring the dynamic PiFM modes relevant to each case. This talk is intended for those new to the field, offering a balanced introduction that spans from theoretical principles to practical applications, covering both fundamental and advanced topics.

^{[1] &}quot;Photo-induced force microscopy (PiFM)-principles and implementations", Chemical Society Reviews 51 (11), 4208-4222

^{[2] &}quot;Linear and nonlinear optical spectroscopy at the nanoscale with photoinduced force microscopy", Accounts of chemical research 48 (10), 2671-2679



Charge trapping memory based on 2D materials heterostructures

Young-Jun Yu*

Department of Physics, Chungnam National University *yjyu@cnu.ac.kr

Van der Waals (vdW) heterostructures using two dimensional (2D) atomic crystals have been attracted intensely for high performance as well as low-power memory applications. Furthermore, floating-gate (FG) memory devices based on 2D heterostructures exhibit stability with dielectric barriers such as hexagonal boron nitride (hBN) between semiconductors and various charge storage layers. However, the reported operation voltage and energy consumption for hBN barriers cannot be reduced below several tens of volts. In this presentation, I will introduce ultrahigh energy efficiency of 2D material heterostructure-based memory devices for approaching to the biological synaptic energy level with employing ultrathin charge-trap layer underneath 2D semiconductor channel measured by scanning Kelvin probe microscopy.



The Present and Future of Scanning Probe Technology for Advanced Semiconductor Device Manufacturing

Eunpa Kim^{*}, Yesol Song, Yongjin Kwon, Jongmin Park, Minjung Shin, Dongchul Ihm

¹SAMSUNG ELECTRONICS Co., Ltd., Semiconductor R&D Center 1, Samsungjeonja-ro, Hwaseong-si, Gyeonggi-do 18448 Korea *eunpa.kim@samsung.com

Since its introduction to the semiconductor industry in the '90s, scanning probe technology has seen increasing utilization and significance. Specifically, during the research and development phase of semiconductors, inline automated atomic force microscopy (AFM) equipment is extensively employed for both comprehensive analysis and providing rapid feedback within processes.[1] Although the current footprint of scanning probe microscopy (SPM) technology within semiconductor process metrology remains relatively modest, its impact and relevance are progressively escalating. SPM has become the de facto standard for nanometer-scale surface analysis such as roughness, step height, and depth measurement. There are no comparable technologies that match its precision. Historically, it has been integrated into etching, deposition, lithography, and chemical mechanical planarization (CMP) processes. Recently, significant demand is anticipated in bonding and advanced packaging sectors. To achieve the stringent planarity requirements post-CMP in bonding processes and manage the step heights within patterns, including copper (Cu) pads, dishing, erosion, and edge roll-off (ERO) management, there will be a considerable increase in the number of AFM and profiler-utilized processes, as well as the volume of wafers requiring measurement.[2,3] Furthermore, with ongoing scaling, the demand for high-resolution metrology will escalate, along with the increased adoption of various SPM modes capable of measuring electrical, mechanical, and magnetic properties.

M. Lee *et.al.*, Proc. SPIE 7272, Metrology, Inspection, and Process Control for Microlithography XXIII, 72722R (23 March 2009); https://doi.org/10.1117/12.813389

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^[3] S. -A. Chew et al., "700nm pitch Cu/SiCN wafer-to-wafer hybrid bonding," 2022 IEEE 24th Electronics Packaging Technology Conference (EPTC), Singapore, Singapore, 2022, pp. 334-337, doi: 10.1109/EPTC56328.2022.10013108.



Atomic force microscope-based analysis of the nanoscale materials and fabrication of the microscale probes

Sangmin An^{1,2*}

¹Jeonbuk National University ¹Department of Physics, Research Institute of Materials and Energy Sciences, Jeonbuk National University (567 Baekje-daero, Jeonju 54896, Republic of Korea) ²K-tip Corporation (567 Baekje-daero, Jeonju 54896, Republic of Korea) * san@jbnu.ac.kr

The Atomic Force Microscope (AFM) has emerged as a crucial tool for investigating the intrinsic properties of low-dimensional materials, such as zero-dimensional (0D) [1] and two-dimensional (2D) [2] nanomaterials. With its exceptional capability for high-resolution topographical imaging, AFM provides invaluable insights into the structure and behavior of these materials. This research offers an overview of recent advancements in advanced AFM techniques, focusing on their application to low-dimensional materials, including both 0D and 2D systems, while also exploring their relevance in 3D printing technologies.

A novel approach that integrates a nanopipette with a quartz tuning fork-based AFM [3] is introduced, enhancing the versatility and precision of AFM in these areas of study. Additionally, this work reviews the current state of microscale cantilever fabrication, emphasizing the significant progress made in this field. By providing a comprehensive analysis of these advanced AFM techniques and their applications, this research highlights cutting-edge developments and lays the groundwork for future discoveries and innovations.

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^[3] C. Kim et al., Nano-Micro Lett. 14 (2022) 13



Quartz tuning fork-based microviscometry for selecting high-quality sperm from semen

Manhee Lee^{*}

Department of Physics, Research Institute for Nanoscale Science & Technology, Chungbuk National University, Cheongju 28644, Chungbuk, Korea *mlee@cbnu.ac.kr

The viscometry of minute liquid amounts is crucial for biomedical diagnosis and engineering. However, interfacial effects complicate measurements and analysis, especially for nanoliter samples. Here, we present a quartz tuning fork-based microviscometry technique that determines the viscosity of single sessile drops at the nanoliter scale. We circumvent the interfacial effects by measuring the negative-valued shear elasticity, originating purely from the retarded fluidic response inside the drop. This method provides an exact formula for viscosity determination from the shear elasticity.

We applied this viscometry technique to create sperm sorting media with appropriate viscosity, enabling the selection of high-quality sperm in conjunction with microfluidic techniques. We show that highly motile sperm can be separated in a viscous medium, where the sperm actively diffuses throughout the medium depending on their motility. We separate motile sperm from semen and identify bovine blastocysts through in vitro fertilization of matured oocytes. Our quartz tuning fork-based microviscometry technique has potential applications in clinical diagnosis and treatment.



Figure 1. (a) Schematic representation of the quartz tuning fork-based micro-viscometer and (b) Trajectories of all objects including sperm and debris in each medium: M199 (PVP 0%), PVP 0.75%, and PVP 1.5%.

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Tip displacement detection technology AFM using Quadrature Phase Differential Interferometry.

Tae Sung Lee*

Oxford Instruments Aylum Research, D 45, 5F 10 Chungmin-ro, Seoul 05840, Korea *Taesung.Lee@Oxinst.com

Conventional common AFMs have measured the angular deflection of the cantilever's reflected laser. Dubbed various names such as "optical beam detection," "optical beam deflection," "optical lever detection," and "beam bounce detection," the system is intuitive to and convenient to use for the angle change of the laser, but has many problems that affect the deflection angle systematically, its easy exposure to such variables, and its lack of accuracy and precision due to the limitations of noise levels. This leads to measurement errors and uncertainties.

Here, AFM using an orthogonal phase difference interferometer directly measures the displacement of the tip to compensate for the shortcomings of AFM using the existing OBD system, eliminating errors and uncertainties, and improving accuracy and precision. AFM using an orthogonal phase difference interferometer will innovate the existing AFM and redefine what can be done with AFM.

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9th International Symposium on Practical Surface Analysis

POSTER I



Particle dispersibility evaluation: An approach to quantifying impressions

Ogata Shuji^{*}, Kuroiwa Kazuya, Maeda Tomoya and Kanno Yuta

Nissan Chemical Corporation, Chiba, Japan ogatas@nissanchem.co.jp

Electron microscopes such as SEM (Scanning Electron Microscope) and TEM (Transmission Electron Microscope) were commonly used to observe nanometer-order particles. The spatial distribution of countless particles could be observed by electron microscope images. The purpose of this study was to quantify and order the dispersion of nanoparticles by observing their spatial distribution using electron microscope.

We used two samples for the evaluation. The first sample was inorganic nanoparticles in solution. We know that when the same inorganic particles were dissolved in different solvents, the state of the solution was different, so we used Cryo-TEM to observe the inorganic particles in solution. [1] TEM observation of the frozen samples allowed us to observe the samples in the water-containing state and to observe differences in the spatial distribution of particles between samples with different solvents. The second sample was inorganic nanoparticles in resin. We thought that adding particles with different compositions to resin causes different dispersion of the particles in the resin. After processing the resin using FIB-SEM and performing cross-sectional SEM observations, we were able to observe differences in the spatial distribution of particles.

The electron microscope observation of the two samples above showed differences in particle dispersion, but the evaluation was based on visual impressions and was not precise enough to rank the samples. In this study, image analysis was conducted using the following method to quantify and rank the dispersion. First, we identified the particles from the obtained electron microscope image. Based on the identified positions of the particles, we conducted Voronoi tessellation in the observation area. (Voronoi tessellation; A method of partitioning regions by drawing boundaries where the distance to each point was equal). [2] We calculated the distribution of area values for the regions segmented by the Voronoi tessellation, and quantified dispersion by calculating the width at half-maximum (FWHM) of the distribution. We thought that a sample with better dispersion would have more uniform segments, resulting in a sharper distribution and a smaller FWHM. We quantified the dispersion using this method and showed the usefulness of this method.

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Development of evaluation method for ligand conjugation of Fe3O4 and AuNPs using mass images and statistical analysis

Hyun Kyong Shon, Tae Geol Lee^{*}, and Jin Gyeong Son^{*}

Nano-bio measurement group, Korea Research Institute of Standards and Science (KRISS), Daejeon 34113, Korea *tglee@kriss.re.kr, yeskyong@kriss.re.kr

Nanoparticles are being used in biological applications such as for delivery, molecular imaging, enzyme nanoreactors, and sensing. For these applications, nanoparticles must be coated with an appropriate ligand suited to the purpose. Surface modification of nanoparticles typically involves several steps. During a ligand exchange process, researchers want to introduce only the target ligand onto the surface of nanoparticles. However, if access ligands are not completely removed during this process in solution, the biological application of nanoparticles can be problematic. Therefore, assessing whether the desired ligands is attached to the surface of nanoparticles and whether free ligands existed in the solution is critical to the biological application. Shon et al. previously develop the method to assess the presence of ligands on the surface of nanoparticles and the absence of free ligands coated on nanoparticles and other free ligands in solution [1]. In current work, we present a method to evaluate the simultaneous present of ligands coated on nanoparticles and other free ligands in solution. For the experiment, polyethylene glycol (PEG) was introduced to the surface of gold citrated nanoparticles (KRISS CRM) with a diameter of 30 nm and Fe3O4 particles with nitrilotriacetic acid (Ni-NTA) with a diameter of 1 μ m. We then centrifuged the samples from 1 to 4 times to remove the PEG ligands and then added octadecylamine (ODA) ligands as free ligands to each sample. We used a nanoliter dispenser for reproducible sampling. We obtained images corresponding to particles and ligands using ToF-SIMS, created a scatter plot with these two images, and calculated the correlation coefficient from the scatter plot.

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Porous Carbon Interlayer Derived from Traditional Korean Paper for Li–S Batteries

Yunju Choi^{*}, Hyungil Jang, Jong-Pil Kim, Jaeyeong Lee, Euh Duck Jeong, Jong-Seong Bae^{*}

Busan Center, Korea Basic Science Institute (KBSI), Busan 46742, Republic of Korea *Correspondence: jsbae@kbsi.re.kr

A carbonized interlayer effectively helps to improve the electrochemical performance of lithium-sulfur (Li-S) batteries. In this study, a simple and inexpensive carbon intermediate layer was fabricated using a traditional Korean paper called "Hanji". This carbon interlayer has a fibrous porous structure, with a specific surface area of 91.82 m² g⁻¹ and a BJH adsorption average pore diameter of 26.63 nm. The prepared carbon interlayer was utilized as an intermediary layer in Li-S batteries to decrease the charge-transfer resistance and capture dissolved lithium polysulfides. The porous fiber-shaped carbon interlayer suppressed the migration of polysulfides produced during the electrochemical process. The carbon interlayer facilitates the adsorption of soluble lithium polysulfides, allowing for their re-utilization in subsequent cycles. Additionally, the carbon interlayer significantly reduces the polarization of the cell. This simple strategy results in a significant improvement in cycle performance. Consequently, the discharge capacity at 0.5 C after 150 cycles was confirmed to have improved by more than twofold, reaching 230 mAh g⁻¹ for cells without the interlayer and 583 mAh g⁻¹ for cells with the interlayer. This study demonstrates a simple method for improving the capacity of Li-S batteries by integrating a functional carbon interlayer.

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Evaluation of CSR-based Tool-to-tool matching of LEAP 6000XR in Samsung Electronics

Hosun Jun^{*}, Seungyang Heo, Bokyoung Kim, Seungju Park, Jihyun Lee, and Joongjung Kim

Samsung Electronics, 114 Samseong-ro, Pyeongtaek-si 17786, Korea *hosun.jun@samsung.com

Atom Probe Tomography (APT) is an analysis technique widely adapted in analysis of nanoscale structural-compositional analysis of variety of materials, owing to its ppm-level chemical sensitivity and sub-nm spatial resolution. Laser pulse-assisted APT have enabled analysis of dielectric or insulating materials, leading to the further adaptation of the technique to wider variety of materials.

Previous works on laser pulse-assisted APT analyses have reported that laser pulse energy affects various properties of the resulting data, such as mass resolving power (MRP)[1], stoichiometry[2], and crystallographic spacing[3]. Therefore, it is crucial to monitor and control the laser pulse energy to perform reproducible analysis.

In addition, the increasing demand on high-throughput APT analysis has recently led to development of parallel set-up of multiple APT systems in field of semiconductor industry. Accordingly, a demand for standardized tool to measure, calibrate and match the laser pulse energy between APT devices has arisen.

In this study, the performance of Charge state ratio (CSR)-based Tool-to-tool matching (TTTM) procedure for LEAP 6000XR developed by CAMECA is reviewed. Reference specimen with known composition was analyzed under various laser pulse energy values, using two LEAP 6000XR APT systems implemented in Samsung Electronics. Comparison of resulting concentrations from each APT systems were made to evaluate the reproducibility and reliability of the data after TTTM process.

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Exploring Beyond Linear Relations in Catalyst Performance

Kihyun Shin*

Department of Materials Science and Engineering, Hanbat National University, Daejeon 34158, Republic of Korea *kihyun@hanbat.ac.kr

Recent studies in electrochemical reaction simulations have revealed the construction of Volcano plots and 2D contour plots based on a strong linear scaling relation between the adsorption energies of intermediate species. This linear scaling relation provides researchers with a straightforward descriptor to predict catalyst performance and enables the visualization of large datasets of catalyst performance on simple contour plots. However, to maximize catalyst performance, it is crucial to identify outliers that do not follow the linear scaling relation. Particularly in the oxygen reduction reaction (ORR), a strong linear scaling relation between OH and OOH adsorption energies sets clear limits on catalyst activity. Overcoming these limits requires understanding how outliers arise and how researchers can control them. In this presentation, we will explore the fundamental assumptions and theories of electrochemical catalyst simulations and examine how Volcano plots and 2D contour plots are formed based on the linear scaling relation. Additionally, we will investigate the impact of ensemble, electronic, and strain effects on adsorption energies and explore various possibilities for generating outliers that deviate from the linear scaling relation.

Understanding CO Oxidation at Au9/MO_x Interfaces: Reaction Mechanisms and Catalytic Efficiency through DFT

Jongseok Kim, Hyuk Choi, Ju Hyeok Lee, Eunji Kang, Jieun Yun, Yejung Choi, Hongjin Park, Minkyeong Kim and Hyun You Kim^{*}

Department of Materials Science and Engineering, Chungnam National University, Daejeon 34134, Republic of Korea *kimhy@cnu.ac.kr

Understanding the catalytic reaction mechanisms and identifying the reactive species under actual reaction conditions are crucial initial steps in catalyst research. Historically, size-dependent activity and the interfacial effect between metal and support have been reported tremendously. Following these studies, the reaction center is the interface of metal NPs and oxide support. Oxide-supported Au-based heterogeneous catalysts have received significant attention due to their effectiveness in CO oxidation at low temperatures. However, activating O2 on Au nanocatalysts remains a challenge, as only small Au nanoparticles exhibit this ability. Here, we used density functional theory (DFT) calculations to study the mechanism of CO oxidation-catalyzed CeO₂, TiO₂, and Al₂O₃-supported Au nanoparticles under reaction conditions. We found that the diverse reaction mechanism exhibited for kinds of oxide supports. The CeO₂-supported Au9 NPs catalyze CO through the MvK mechanism without additional activation of O2 regardless of the facet of CeO₂ (111) and (100), respectively. In contrast, the activation of O₂ occur on TiO₂ and Al₂O₃. In case of Au NPs on TiO₂, the reaction mechanism of CO oxidation is followed by utilizing pre-activated O_2 as well as the lattice oxygen of TiO_2 . The Al₂O₃, regarded as inert oxide, the lattice oxygen cannot participate in oxidation, but the pre-activated O₂ on Lewis acid site (Al3+) can catalyze CO. Our study delivers comprehensive understating about the detail of interfacial effect as following the oxide supports, enabling rational design of heterogeneous catalysts.

Quantitative Analysis of Cu⁰, Cu⁺ and Cu²⁺ Compounds with Multiple Core-level XPS Spectra Decomposition Method

Hiroshi Okumura^{1*}, Hiroshi Shinotsuka³, Ryo Murakami³, Kenji Nagata³, Sho Okamoto², Masamitsu Sato², Satoshi Oshima¹, Masaaki Mita¹, Aoi Nii¹, Nobuyasu Nita¹, Hideki Yoshikawa³

¹Innovation Center, Mitsubishi Materials Co. Ltd., 1002-14 Mukohyama, Naka, Ibaraki 311-0102, Japan

²Innovation Center Omiya Branch, Mitsubishi Materials Co. Ltd., 1-600 kitabukuro, Omiya, Saitama 330-8508, Japan

³National Institute for Materials Science, 1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan

*okumurah@mmc.co.jp

Quantitative analysis of copper surface chemistry is crucial for understanding bonding with other materials. X-ray photoelectron spectroscopy (XPS) can differentiate Cu^0 , Cu^+ , and Cu^{2+} compounds based on peak positions of photoelectron and Auger electron peaks. However, quantitative analysis has been challenging due to small chemical shift differences and difficulty in peak separation for photoelectron peaks, as well as human interpretation and reproducibility issues for Auger electron peaks. Recently, Murakami et al. developed a technique to simultaneously analyze multiple photoelectron peaks [1]. Applying this technique, we established a comprehensive and automated method to evaluate the chemical state of copper compounds. This result is expected to be applicable to transition metal materials other than copper.

First, depth profiling analysis was performed on naturally oxidized oxygen-free copper plates to investigate the near-surface chemical state using XPS with a mono-Al-K α X-ray and Ar⁺ ion sputtering (2 kV) at a pass energy of 23.5 eV. The resulting narrow spectra included Cu 2p_{3/2} photoelectron and Cu L₃M₄₅M₄₅ Auger peaks. Then, narrow spectra for pure-Cu, CuO, and Cu₂O were obtained by measuring samples of pure copper plate, CuO powder, and Cu₂O powder, respectively. For Cu(OH)₂, narrow spectra were obtained by referring to literature [3]. These narrow spectra were reconstructed by optimizing Voigt function parameters using the exchange Monte Carlo method, resulting in reference spectra. Genetic algorithm analysis [1, 2] with the reference spectra was performed on the measured narrow spectra of the oxygen-free copper plate.

Spectra without sputtering showed peaks from $Cu(OH)_2$ and Cu_2O , with contribution ratios of 33.5% and 66.5% for photoelectron peaks. Spectra with sputtering for 1 min, showed peaks from metal-Cu, Cu_2O , and $Cu(OH)_2$, with contribution ratios of 49.8%, 48.9%, and 1.3% respectively. Details will be presented later.

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계면 분석을 통한 InGaZnO 산화물 TFT 소자 Hysteresis 원인 연구

<u>고민지</u>, 박현우^{*}, 노원빈, 김종민, 박혜경, 박상무, 최영석

LG Display 표면분석팀, LG Display, 경기도 파주시 엘지로 245, 대한민국 *hyunwooo.park@lgdisplay.com

Organic Light-Emitting Diode (OLED) 산업에서 InGaZnO (IGZO) 물질은 높은 이동도, 낮은 누설전류 특성으로 인해 저전력/고효율 산화물 Thin Film Transistor (TFT) 소자를 위한 차세대 물질로써 널리 사용 되고 있다. TFT에서 IGZO 채널 층은 증착 조건, 열처리, 외부 Stress 등의 다양한 제조 공정으로 인해 막 내 조성, 결정성 등이 변화할 수 있으며 이는 소자의 이동도, Off-current, 신뢰성과 같은 전기적 특성 저하에 큰 영향을 준다. 특히, 공정 요인에 의한 IGZO 채널 층 및 Gate insulator (GI)-IGZO-Buffer layer 계면에 형 성된 Defect states는 장기적인 소자 Transfer 특성에도 치명적인 영향을 줄 수 있어 고성능/고품질 디스플 레이 개발을 위해 제어해야 할 요소 중 하나이다.

본 연구에서 우리는 표면 및 계면 분석을 통해 IGZO 계면의 Oxygen 조성 변화와 소자 특성 간 상관성 및 메커니즘을 규명하였다. Hysteresis 특성을 보이는 소자의 GI/ACT/Buffer 층의 ToF-SIMS 분석을 통해 Active layer 내 과잉 산소 및 Active-GI-Buffer 계면 부로의 산소 확산을 확인하였다. 과잉 산소에 따른 소 자 영향성 확인을 위해 AC transconductance 측정을 진행하였으며 계면 부에서 확인된 결함 밀도 증가가 Oxygen-related trap sites를 형성하여 소자 열화 유발 요인으로 작용하는 것으로 확인되었다.

4 characteristics and film physical properties for good performance SiNx encapsulation films

Jung Min Bae^{*}, Sera Kwon, Jae Won Lee, Jihye Yoo, Hye Kyoung Park, Sang-Moo Park, Young Seok Choi

> LG Display Production Technology Center, LG Display (245 LG-ro, Paju-si, 10845, Korea) *jungmin.bae@lgdisplay.com

OLED (Organic Light-Emitting Diode)는 자체 발광, 얇은 두께, 유연성으로 인해 현재 양산 가능한 최고 디스플레이 기술로 꼽히고있다. 하지만 OLED의 핵심인 유기 발광층은 수분과 산소에 의해 쉽게 열화 (Degradation)되어 제품 수명 및 불량에 대한 이슈를 지속적으로 발생시키고 있다. OLED 패널을 외부 수 분과 산소로부터 차단하는 공정을 봉지 (Encapsulation)라고 하며, Flexible Display를 위해 유기 발광층 위 에 박막 공정을 통해 일체형으로 제막하는 공정을 박막봉지 (Thin Film Encapsulation)라고 부른다. 봉지 박막은 무기막/유기막 다층 구조를 가지며 무기막으로 Silicon nitride (SiNx)가 사용되는데, 증착 공정 중 열에 의한 유기 발광층의 변성을 피하기 위해 저온 공정이 요구되고, 따라서 Si3N4에 가까운 High Quality 박막이 아닌 Si-rich하며 H를 다량 포함하고 있는 Defective한 SiNx 박막이 사용된다.

좋은 성능의 SiNx 봉지 박막이란, 상하부막과의 잔류응력이 낮아 휨이 없어야 하고, 유기 발광층에서의 광추출 효율은 높고, 투습은 극미량 수준이어야 하며, 사용 시간에 따른 박막의 변화가 최소화되어야 한다. 이를 측정 가능한 4가지 특성인 (1) 잔류 응력, (2) 굴절률, (3) 투습 특성, (4) 경시 변화 특성으로 표현 할 수 있다.

SiNx 봉지 박막은 PECVD (Plasma Enhanced Chemical Vapor Deposition) 방법으로 증착되며, 원하는 특성의 박막 증착을 위해 각 Gas의 유량, Power, 압력 등의 조건을 제어하는데, 이러한 공정 조건의 제어는 박막의 특성을 직접적으로 결정하는 것이 아닌 박막의 구성과 상태를 먼저 바꾸고, 바뀐 구성과 상태로 인 해 막의 특성이 바뀐다. 따라서 공정 조건으로 원하는 특성을 제어하기 위해서는 박막의 구성과 상태를 대 변하는 물성과의 관계를 알아야 한다.

본 연구에서는 2가지 물성인 Nitrogen : Silicon (N/Si)조성 과 박막 내 Defect으로 판단되는 결합하지 않는 전자 수를 통해 SiNx 봉지 박막의 4가지 특성과의 상관관계를 도출해보았다.

Analysis of impurities on the substrate surface using FT-IR microscopy

Dongchan Lee, Chaelim Lee, Yunju La, and Changwoo Byun*

Advanced Institute of Convergence Technology (AICT), 145 Gwanggyo-ro, Yeongtong-gu, Suwon-si, Gyeonggi-do 16229, Suwon, Republic of Korea *corresponding. byuncw@snu.ac.kr

In the semiconductor industry, Fourier-Transform Infrared Spectroscopy (FT-IR) is a widely used technique to detect and quantify substrate components and process-related impurities. In particular, FT-IR microscopy provides high-resolution optical images and comprehensive chemical information via focal plane array (FPA) detector. Chemical images of the mapped sample surface can be created in less than 1 minute with a spatial resolution of 5 μ m/pixel

Here we report the FT-IR analysis of chemical mapping and IR spectra to identify the contaminant particles on Fine metal mask (FMM) substrate and Integrated circuit (IC) chip pad. The presence of organic or polymeric impurities was identified using visible images and FPA chemical imaging. We also used FT-IR in conjunction with X-ray Photoelectron Spectroscopy (XPS) to verify the chemical composition ratio of thin films.

Atomic force microscope-guided 3D printed carbon nanotube nanowires with in situ Raman spectroscopy

Yeonju Bae^{1†}, Hojin Jang^{2†}, Taesun Yun², Jongwoo Kim^{3*}, and Sangmin An^{1,2*}

¹Department of Energy-AI Convergence Engineering, Jeonbuk National University, Jeonju 54896, Republic of Korea

²Department of Physics, Institute of Photonics and Information Technology, Jeonbuk National University, Jeonju 54896, Republic of Korea

³Department of Physics, Chungnam Natioinal University, Daejeon 34134, Republic of Korea *jongwoo.kim@cnu.ac.kr, san@jbnu.ac.kr [†]These authors contributed equally.

Carbon nanotubes (CNTs) have attracted significant attention in various fields due to their outstanding electrical, thermal, and mechanical properties. One of the methods to utilize CNTs is the integration with 3D printing technology. 3D printing has been increasingly adopted in scientific and industrial fields as it can fabricate complex structures in a single process. In this study, a 3D printing experiment was conducted with the control of a water meniscus using a nanopipette filled with a CNT solution as a nozzle and a quartz tuning fork (QTF) as a single sensor. That is, by combining the quartz tuning fork atomic force microscope (QTF-AFM) system and the 3D printing system, printing was carried out on a nanoscale basis, and accurate placement of CNT nanowires was possible through precise force control. In addition, the CNT nanowires thus produced were analyzed by in situ Raman spectroscopy. The results of this study are expected to provide useful information for the development of CNT nanowire-based electronic devices and sensors. Particularly, the integration of 3D printing technology and in situ Raman spectroscopy analysis can contribute to the optimization of the CNT nanowire fabrication process.

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Characteristics of Magnesium-Ion-Implanted Gallium Nitride for Power Semiconductor Applications

Taehun Jang¹, Mirang Byeon^{1,2}, Minji Kang¹, Tae Eun Hong^{1*}, Sang-Geul Lee³, Sang-Gil Lee⁴, Ji Hyun Lee⁴, and Won Ja Min⁵

¹Busan Center, Korea Basic Science Institute, Busan 46742, South Korea ²Department of Materials Engineering, Pusan National University, Busan 52828, South Korea ³Daegu Center, Korea Basic Science Institute, Daegu 41566, South Korea ⁴Research Center for Materials Analysis, Korea Basic Science Institute, Daejeon 34133, South Korea ⁵Business Development Team, HB Solution, Daejeon 34028, South Korea

*Correspondence: tehong@kbsi.re.kr

Gallium nitride (GaN) is widely used in high power, high frequency, and high temperature devices for high-performance power semiconductor devices owing to its superior properties such as large bandgap, high electrical breakdown field, high electron mobility and relatively high thermal conductivity [1,2]. To enhance the electrical properties of GaN power semiconductors, doping with impurities is crucial. In GaN-based electronic devices, a p-type layer is formed through impurity doping during epitaxial growth [3]. Currently, magnesium (Mg) is extensively used as a p-type dopant in GaN power semiconductors. For the advancement and optimization of next-generation GaN power semiconductors, precise analysis of the distribution and concentration of various dopants is absolutely essential.

In this study, we focused on developing a reference sample for the precise analysis of Mg dopants, which are crucial in GaN power semiconductors. We investigated the structure and surface properties of ion-implanted GaN films with magnesium ions, without undergoing annealing heat treatment. The ion-implanted GaN films were analyzed using transmission electron microscopy (TEM), X-ray diffraction (XRD), atomic force microscopy (AFM), medium energy ion scattering (MEIS), and secondary ion mass spectrometry (SIMS). We will present the detailed experimental results of the Mg ion-implanted GaN films and discuss the potential use of the developed material as a reference sample for SIMS analysis of p-type dopants in GaN power semiconductors.

Keywords: Gallium Nitride (GaN), Power Semiconductor, Magnesium Dopant, Reference Sample, Secondary Ion Mass Spectrometry (SIMS)

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Characterization of Individual Airborne Particles Using Complementary Analytical Methods with Combined SEM/EDS, Fluorescence Microscope, and O-PTIR

Ji-Won Park¹, Han-Jin Yoo², Kyoung-Eun Lee¹, Myung-Joo Kim¹, Young-Chul Song^{1*}

¹Korea Research Institute of Chemical Technology, 141 Gajeongro, Yuseong, Daejeon 34114, Korea ²Inha University, 100 Inharo, Michuholgu, Incheon 22212, Korea *ycsong@krict.re.kr

Atmospheric particles are classified into those originating from natural sources, and those from anthropogenic activities. To predict the environmental impact of these aerosol particles, it is essential to understand their physicochemical properties.

In this study, aerosol particles were collected from the atmosphere and classified using various surface analysis instruments (fluorescence microscope (FM), Raman spectroscopy, O-PTIR, SEM/EDS) to determine their physicochemical properties. SEM/EDS was used to analyze the main components, size, and shape of the particles. FM was used to identify naturally fluorescent particles. Raman spectroscopy and O-PTIR were employed to identify the chemical functional groups of each particle. By combining multiple surface analysis methods, the reliability of determining aerosol particles was enhanced, and various forms of particles could be analyzed. Additionally, the physicochemical properties of the particles could be comprehensively understood. This approach is expected to help identify the origin of atmospheric particles and further predict their behavior under different environmental conditions.



Figure 1. Images of airborne particle analyzed by SEM/EDS, O-PTIR, Raman and FM.

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Hydrogen-Inclusive Compositional Analysis of SiOCH Thin Films

Sung-Jin Chang^{1*}, Wonja Min², Kyungsu Park², Haejoon Hahm², Sungwoo Lee³, Sanghak Yeo³, and Kwanwoo Lee³

¹National Nanofab Center, 291 Daehak-ro Yuseong-gu, Daejeon 34141, Korea ²HB Solution, 33 Techno8-ro Yuseong-gu, Daejeon 34028, Korea ³TES, 2374-36 Jungbudae-ro Yangji-myun Cheoin-gu, Gyeonggi-do 17162, Korea *sjchang@nnfc.re.kr

In the semiconductor industry, Low-k materials refer to substances with lower dielectric constants compared to the commonly used silicon dioxide (SiO₂). These materials are used as insulators or insulating films between interconnects in semiconductor devices. As semiconductor devices continue to shrink in size, there is ongoing development of Low-k materials that not only have lower dielectric constants to reduce signal delay caused by the insulation between interconnects but also maintain excellent mechanical properties.

Organic and inorganic hybrid-type carbon incorporated silicon oxide (SiOCH) thn films are emerging as promising next-generation low dielectric materials for interlayer insulation [1,2]. Active Research and development of materials and process technologies are underway to develop SiOCH thin films with characteristics suitable for next-generation semiconductor devices. For systematic development, it is crucial to accurately analyze the film characteristics, including composition, structure, and electrical/mechanical properties. However, quantitatively analyzing the hydrogen content in SiOCH thin films remains challenging because X-ray photoelectron spectroscopy (XPS) cannot detect hydrogen and the preparation of standard samples for quantitative hydrogen analysis in secondary ion mass spectrometry (SIMS) remains a difficult issue.

In this work, we present the results of compositional analysis, including hydrogen, of SiOCH films deposited on silicon substrate using plasma-enhanced chemical vapor deposition. Various analytical methods such as medium energy ion scattering analysis, XPS, SIMS, and Fourier-transform infrared spectroscopy were employed. We discuss the significance of the results obtained through various analytical techniques.

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Hydrogen Diffusion Model in Austenite Steel Containing Martensite Structure

Hiromi Kato¹, Akiko N. Itakura², Naoya Miyauchi², Daisuke Hayashi¹, and Satoka Aoyagi^{1*}

¹Faculty of Science and Technology, Seikei University, Musashino, Tokyo 180-8633 Japan ²National Institute for Materials Science, 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan *aoyagi@st.seikei.ac.jp

Hydrogen embrittlement, caused by hydrogen permeation into metals, is one of the most important problems in the development of metallic materials because it causes cracking and deterioration of the material. However, the mechanism of hydrogen embrittlement has not been clarified because direct observation of hydrogen is difficult. There are many unclear points about the behavior of hydrogen. Therefore, an operando hydrogen microscope (OHM) [1] was developed to observe hydrogen on metal surfaces. The relationship between crystal structures and hydrogen permeation has been investigated by the image fusion of the electron backscatter diffraction (EBSD) and the OHM images [2,3]. We have reported hydrogen diffusion in the previous study [4], which was based on the hydrogen diffusion in one dimension from the bottom to the surface. The relationship between the hydrogen distribution at the surface and the crystal structures inside the steel sample containing face-centered cubic (fcc) and body-centered cubic (bcc) structures was suggested by simulating hydrogen diffusion in the vertical direction from the bottom to the surface of the metal sample [4]. It had not been considered hydrogen diffusion in the horizontal direction on surfaces in contact with different conditions, such as grain boundaries, strains, and polycrystals with different crystal structures and orientations. In this study, the time course of hydrogen distribution was simulated by considering hydrogen diffusion in the horizontal direction in addition to the vertical direction based on Fick's second law of diffusion. Several interfaces between different crystal structures were selected to simulate hydrogen diffusion in vertical and horizontal directions. The time evolution images of hydrogen distribution on the steel surface simulated in this study were compared with those observed using the operando hydrogen microscope [4].

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Influence of Electron Beam Acceleration Voltage on Critical Dimension Measurements in Semiconductor Metal Lines Using Scanning Electron Microscopy

Taek-Soo Shin*, Jae-Jun Yoon, and Seung-Boo Jung

Department of Semiconductor and Display Engineering, Sungkyunkwan University, Suwon, Korea Samsung Electronics Co., Ltd, Hwaseong, Korea *sbjung@skku.edu

In this study, we propose appropriate measuring conditions and data processing methods for accurately measuring critical dimensions at heterogeneous junction interfaces in semiconductor metal line processes using Scanning Electron Microscopy (SEM). General semiconductor structure analysis is typically conducted using SEM and Transmission Electron Microscopy (TEM). However, due to the principles of SEM image generation, variations in critical dimension measurements can occur. SEM measurements are significantly influenced by electron beam conditions, sample surface morphology, and sample composition. These factors lead to changes in the interaction volume, complicating the accurate measurement of critical dimensions.

The primary focus of this study is the influence of electron beam acceleration voltage on the changes in critical dimensions of semiconductor metal line structures. To verify the impact of acceleration voltage on critical dimension measurements in semiconductor metal line structures forming W/SiO₂ heterogeneous junction interfaces, we investigated the changes in image signal intensity profiles at acceleration voltages ranging from 5 kV to 20 kV. Furthermore, the changes in critical dimensions due to varying acceleration voltages were phenomenologically organized by comparing and analyzing Monte Carlo simulation results with actual SEM images.

Based on the results of this study, we aim to enhance the reliability and accuracy of SEM metrology for advanced semiconductor processes involving semiconductor metal line structures with diverse and fine pitches.

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Analysis of Palladium Diffusion from ENEPIG Surface Finish into Solder Joint

JaeJun Yoon¹, Minji Lee², Taek-Soo Shin³, and Seung-Boo Jung^{1,2*}

¹Department of Semiconductor Convergence Engineering, Sungkyunkwan university, Suwon, Korea ²School of Advanced Materials Science & Engineering, Sungkyunkwan University, Suwon, Korea ³Samsung Electronics Co., Ltd, Hwaseong, Korea *sbjung@skku.edu

ENEPIG (Electroless Nickel Electroless Palladium Immersion Gold) surface finish comprises nickel, gold, and palladium layers. Each element prevents various issues and ensures high reliability. Unlike OSP and ENIG finishes, ENEPIG includes a palladium layer, which acts as a diffusion barrier between the nickel and gold layers, preventing gold from diffusing into the nickel. Additionally, palladium stabilizes electrical connections, reducing contact resistance, and plays a crucial role in mechanical, electrical, and thermal reliability tests.

In this study, we compare and analyze the characteristics of ENEPIG surface finish by varying the thickness of the palladium (Pd) layer. The Pd layers were set at thicknesses of 0.05μ m, 0.1μ m, and 0.15μ m. SAC 305 solder balls were used to form ball grid array (BGA) solder joints with SAC 305 solder paste. The resulting intermetallic compounds (IMCs) were analyzed using Scanning Electron Microscope (SEM), Transmission Electron Microscope (TEM), and Electron Probe MicroAnalyzer (EPMA). SEM analysis confirmed that the shape and size of the IMCs varied with the thickness of the Pd layer. Furthermore, we investigated the dissolution of Pd into the solder joint during the formation process. TEM was utilized to analyze the small amounts of dissolved Pd, and TEM-EDS was used to determine the composition of the metal layers and IMCs in the ENEPIG surface finish samples. This analysis revealed that the amount of dissolved Pd within the solder joint differed according to the thickness of the Pd layer. Consequently, we confirmed that the Pd layer thickness affects the shape and size of the IMCs. EPMA was utilized to compare the composition and concentration of Pd and other elements within the IMCs.

In-situ characterization of interface layer between ZnO overlayer and Al metal by XPS and HAXPES

Ayuto Kawamura, and Hisao Makino*

Kochi University of Technology, 185 Miyanokuchi, Tosayamada, Kami, Kochi 782-8502, Japan *makino.hisao@kochi-tech.ac.jp

Zinc oxides is attractive materials for several sensing applications, like as ultraviolet light, hydrogen and alcohol gas, and so on. Because of lack of inversion center in wurtzite ZnO structure, there is polar axis in c-axis direction with spontaneous and piezoelectric polarizations. The crystallographic polarity of ZnO cause very different properties not only in single crystals or nanostructures, but also in polycrystalline thin films. It is important to control polarity of ZnO thin films. It was found that ZnO thin films directly deposited on glass substrates shows O-polarity. We proposed extremely thin Al layer on glass substrates to deposit Zn-polar ZnO films on glass substrates. In this study, we characterized the interfacial layer between Al thin films and ZnO overlayer deposited by a magnetron sputtering method using in-situ XPS measurement.

30-nm-thick Al thin films were deposited on alkaline free glass substrates by RF-superimposed DC magnetron sputtering at room temperature. 250-nm-thick ZnO films was deposited on glass substrates at the substrate temperature of 200°C by RF magnetron sputtering with and without the Al bottom layer. The ZnO deposited on Al showed Zn-polarity, while the ZnO film deposited without the Al layer showed O-polarity. The chemical states of Al thin and buried interface were measured by a custom made XPS system equipped with Al K α . line (1486.6 eV) and Cr K α . line (5414.8 eV) as excitation x-ray sources. The film can be measured without exposure to air after the deposition by transferring through high vacuum chambers. For charge compensation, an Ar ion gun and a low energy electron gun were used.

The surface of the deposited Al film was slightly oxidized more likely due to oxygen remained inside the deposition chamber after the deposition. The Al film was heated up at the substrate temperature of 200° C, then cooled down to room temperature in the deposition chamber. The surface of Al film was measured again by XPS. The Al 2*p* region of XPS spectra showed only metallic Al peak, the oxide peak was nearly negligible. It can be considered that the Al layer could be thermally cleaned. On the Al surface, 20-nm-thick ZnO film was deposited by the RF magnetron sputtering at 200°C. After cooling down to room temperature, the layered films were measured by the XPS and HAXPES. We could not observe Al 2p spectra by XPS using Al K*a*. line. However, we observed Al 2p and Al 1s spectra by HAXPES. The Al 1s spectra consists of two peaks corresponding to metallic Al and oxide. The Al oxide interfacial layer could be formed during the deposition of ZnO. The oxidization process at the first stage of growth of ZnO may be influence the determination of polarity of ZnO over layer.

Development of a Humidity Sensor Based on CaCu3Ti4O12/NaCl Using the Aerosol Deposition Method

Yuan-bo Zhang, Jun-Woo Lee, Jong-Min Oh*

Department of Electronic Materials Engineering, Kwangwoon University, Seoul 139-701, Republic of Korea * jmOH@kw.ac.kr

The ambient humidity profoundly affects human life, industry, agriculture, food storage, and perceptual comfort. Monitoring and controlling environmental humidity is crucial. Therefore, the development of high-performance and highly sensitive humidity sensors is imperative. This study introduces, for the first time, the utilization of the natural properties of NaCl ions and their strong reaction with water, as well as the polarity response of water, in the preparation of CCTO (CaCu₃Ti₄O₁₂))/NaCl humidity sensors. In the treatment of NaCl, we employed four different methods: grinding and ball milling for 4 hours, 24 hours, and 48 hours, respectively. The obtained powders were combined with CCTO to form composite powders. Benefiting from NaCl's assistance, we achieved outstanding sensitivity and excellent linearity. Notably, this is an amazing result in the case of CCTO /NaCl humidity-sensitive sensors, achieved through a simple post-annealing process of the aerosol-deposited films at room temperature. Here, we utilized environmentally friendly and cost-effective NaCl, surpassing other expensive doping treatments. Reaffirming the feasibility of aerosol deposition in humidity sensor applications and highlighting CCTO as a promising candidate material for innovative humidity sensors.

Keywords: CaCu₃Ti₄O₁₂/NaCl; Aerosol Deposition (AD); Humidity sensor; Sensitivity; Post-Annealing



Atomic Layer Deposition of Ru-Ir Thin Films for Advanced Interconnects

Yeong-Seo Cho, Se-Yun Kim, Ji-Hye Baek, Kyeong-Moon Lee, and Se-Hun Kwon*

School of Materials Science and Engineering, Pusan National University, Busan 46241, Korea *sehun@pusan.ac.kr

Copper (Cu) has been predominantly used as an interconnect material in semiconductor Back-End-of-Line (BEOL) processes. However, it faces significant challenges due to a drastic increase in resistivity when the line width decreases below 10 nm. To address this issue, it is essential to develop new interconnect materials with a low Figure of Merit (FoM; $\rho_0 \lambda$) and high cohesive energy compared to Cu that minimize electron scattering and reduce line resistance. Currently, single-metal candidates such as Ru, Co, and Mo has been extensively studied using atomic layer deposition (ALD) techniques as potential alternatives to Cu due to their favorable FoM characteristics and cohesive energies. However, the ALD of these single metals has shown limited improvements in resistivity compared to Cu.

Herein, therefore, we propose an alternative ALD binary alloy, Ru-Ir, as a new advanced interconnect material based on its FoM ($\rho_0 \lambda$) characteristics, which is capable of achieving lower resistivity than Cu at line widths below 10 nm. Since both Ru and Ir possess lower FoM values compared to Cu and share the same valence, they are expected to minimize the increase in resistivity when forming an alloy. Additionally, the Ru-Ir binary alloy has a wide solid solubility range, allowing effective control of the mean free path. To investigate this new advanced interconnect material, we systemically examined the effect of compositions and thickness on the electrical resistivity of ALD Ru-Ir binary alloy thin films. And, it was carefully compared with those of Cu interconnect material. In this presentation, the detailed optimization of ALD Ru-Ir binary alloy interconnects will be discussed with a appropriate theoretical explanations, aiming to address the resistivity increase issue of Cu at interconnect width less than 10 nm, and ultimately to develop a metallization material that outperforms Cu in future interconnect applications.

Development of a Humidity Sensor Based on CaCu3Ti4O12/NaCl Using the Aerosol Deposition Method

Yuan-bo Zhang, Jun-Woo Lee, Jong-Min Oh*

Department of Electronic Materials Engineering, Kwangwoon University, Seoul 139-701, Republic of Korea *jmOH@kw.ac.kr

The ambient humidity profoundly affects human life, industry, agriculture, food storage, and perceptual comfort. Monitoring and controlling environmental humidity is crucial. Therefore, the development of high-performance and highly sensitive humidity sensors is imperative. This study introduces, for the first time, the utilization of the natural properties of NaCl ions and their strong reaction with water, as well as the polarity response of water, in the preparation of CCTO (CaCu₃Ti₄O₁₂))/NaCl humidity sensors. In the treatment of NaCl, we employed four different methods: grinding and ball milling for 4 hours, 24 hours, and 48 hours, respectively. The obtained powders were combined with CCTO to form composite powders. Benefiting from NaCl's assistance, we achieved outstanding sensitivity and excellent linearity. Notably, this is an amazing result in the case of CCTO /NaCl humidity-sensitive sensors, achieved through a simple post-annealing process of the aerosol-deposited films at room temperature. Here, we utilized environmentally friendly and cost-effective NaCl, surpassing other expensive doping treatments. Reaffirming the feasibility of aerosol deposition in humidity sensors applications and highlighting CCTO as a promising candidate material for innovative humidity sensors.

Keywords: CaCu₃Ti₄O₁₂/NaCl; Aerosol Deposition (AD); Humidity sensor; Sensitivity; Post-Annealing

Indium-Gallium-Zinc-Oxide Based Negative Capacitance Field Effect Transistors for Low Power Consumption

Ji Hyeon Min, Kyong Jae Kim, You Seung Rim, and Hyun-Suk Kim*

Pildong-ro 1-gil, Jung-gu, Seoul, 04620, Republic of Korea *khs3297@dongguk.edu

With the advent of various technologies such as self-driving cars and artificial intelligence, research is actively being conducted on devices that can efficiently process large amounts of data with low power consumption. Negative Capacitance Field-Effect Transistor(NCFET)s operate at lower voltages than conventional transistors, reducing power consumption and enabling high-speed switching, and can improve performance by increasing the response speed of the device.

HfO₂-based ferroelectric thin films can maintain strong ferroelectricity even at the nanoscale, which allowing for samller and denser, and higher-capacity memory devices. In addition, it is a suitable material for CMOS processes due to its Si compatibility and chemical non-toxicity. However, ferroelectrics undergo rapid polarization switching and there is a point where they exist in an unstable state. To stabilize it, a high-k dielectric layer with excellent surface adhesion, high capacitance, and thermal and chemical stability is added to the ferroelectric layer. This heterostructure stabilizes the ferroelectric layer and enables low-power operation of the transistor.

The active layer of TFT is a critical part that determines the overall performance and efficiency of the device, and directly affects the electrical characteristics and performance optimization in NCFET. Amorphous oxide semiconductors(AOS) have garnered significant attention due to their relatively high mobility, low fabrication temperature, and large-area uniformity. In particular, Indium-Gallium-Zinc-Oxide (IGZO)-based TFTs can effectively reduce standby power consumption due to their extremely low off-current characteristics. Based on these properties, they are suitable for application in low-power consumption devices, especially when combined with their negative capacitance characteristics.

In this study, an oxide semiconductor-based NCFET was fabricated using a HZO($Hf_{0.5}Zr_{0.5}O_2$)/Al₂O₃ stack as a gate insulator. The HZO thin films deposited by PEALD exhibited ferroelectric properties through the PMA process, and IGZO, which has the advantages of high mobility and low off-current characteristics, was applied as a channel. The proposed NCFET achieved low off-current and SS characteristics by combining oxide semiconductor and ferroelectric materials. These results suggest promising applications in advanced devices such as low-power electronic devices, the Internet of Things, and memory devices.

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Fluorescence and electrochemical dual-mode detection of norepinephrine with a portable smartphone assay using nitrogen-doped Ti_3C_2 MXene quantum dots via instant microwave-assisted synthesis

Murugesan Chandran, Gayathri Chellasamy, Mekala Veerapandian, Barkavi Dhanasekaran, Saravanan Govindaraju^{*}, Kyusik Yun^{*}

Department of Bionanotechnology, Gachon University, Gyeonggi-do 13120, Republic of Korea *E-mail: ykyusik@gachon.ac.kr (K.Yun.), biovijaysaran@gmail.com (S.G.)

The physicochemical features of next-generation 2D materials, namely transition metal carbides and nitrides (MXenes), have drawn greater attention. In this study, we used a simple and fast microwave-assisted approach to synthesis highly intence fluorescent materials known as nitrogen-doped MXene quantum dots (N-MQDs). Using techniques including atomic force microscopy, high-resolution transmission electron microscopy, UV-visible, fluorescence, Fourier transform infrared, X-ray diffraction, Raman studies, zeta potential, and contact angle, it was determined that these N-MQDs were spherical, fluorescent, and extremely sensitive materials. For the fluorescence and electrochemical sensing of the neurotransmitter norepinephrine (NE-0.1 to 500 µM), N-MQDs were employed as dual probes. The sensing strategy was based on the inner filter effect acquired by the N-MQDs, leading to fluorescence quenching at 400 nm and a new emission peak at 500 nm with color changes and the NE to NE quinone conversion in an electrochemical reaction. The limit of detection (LOD) values in human serum samples were 40 and 33 nM, respectively, as determined by fluorescence and electrochemical measurement. We created a sensor array incorporated into a smartphone to measure the relative red/green/blue (RGB) values at various concentrations of NE for a point-of-care study. The synthetic fluorescent probe is a potentially useful tool for biofluid NE detection. It was ideal for the early diagnosis of neurological disorders and shown a high degree of selectivity toward NE.

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Plasma Enhanced Atomic Layer Deposition for High-Performance Scaled Indium Oxide Thin Film Transistors

Jaewon Park, Seong Cheol Jang, Hyun-Suk Kim*

Dept.of Energy and Materials Engineering, Dongguk University, 30 Pildong-ro 1(St), Jung-gu, Seoul 04620, Korea *E-mail: khs3297@dongguk.edu

Oxide semiconductors have risen as promising materials for electronic devices, due to their electrical, optical, and structural characteristics. With attributes like high mobility, visible spectrum transparency, and minimal leakage current, these materials are well-suited for serving as the active layer in the thin-film transistors (TFTs). Among the oxide semiconductors, In-rich oxide semiconductors have been extensively studied due to their high mobility. The thickness of the In₂O₃ layer plays a crucial role in determining the electronic transport properties, significantly influencing the electrical characteristics of TFTs. Therefore, the comparative analysis of the electrical characteristics of TFTs employing In₂O₃ layers of varying thicknesses was necessary.

In this study, the thickness of the In_2O_3 layer was finely controlled from 5 nm to 1 nm. Using In_2O_3 as the channel layer in TFTs offers high conductivity, transparency, chemical stability, and cost-effectiveness. Thanks to the layer-by-layer self-limiting growth mechanism of ALD process, ultra-thin high-quality channel layer can be deposited at the low process temperature of 150 °C. PEALD can result in higher-quality films because the plasma can assist in the removal of impurities and does not use the reactants containing hydrogen. Due to these advantages, the PEALD process is a promising process applicable to highly integrated circuits and 3D structural devices. The properties of the In_2O_3 thin-film including thickness, chemical structure and electrical properties were measured by various analysis method including XPS, Hall-effect measurement, ellipsometry and TEM. These findings show the necessity for precise control over In_2O_3 thickness in both the fabrication and application of TFTs, providing valuable insights for enhancing their performance across various electronic devices.

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Highly Conductive and Stretchable AgNW/PEDOT:PSS Heater via Laser Patterning Process for Soft Heater

Jeong Eun Byun, Jung Woo Lee*

Pusan National University, 2, Busan Daehak-ro 63beon-gil, Busan, Korea *corresponding.author@jungwoolee@pusan.ac.kr

With growing interest in health, the healthcare industry, particularly in heat-based therapies, is rapidly expanding. However, traditional heat delivery devices made from rigid materials face significant limitations due to their bulk size, low flexibility, and discomfort during use. These drawbacks limit their effectiveness in localized thermal therapies and drug delivery applications.

In this study, we suggest a stretchable and skin-mountable heater fabricated using a composite film consisting of silver nanowires (AgNWs) embedded within a PEDOT:PSS matrix. The conductive composite structure applies the "Conductive Bridge Effect," which compensates for conductivity degradation under strain, enhancing both mechanical stability and electrical performance. This film is formed by a cost-effective solution process conducted under ambient conditions. Additionally, mechanical stability is further improved by introducing various stretchable patterns via a laser patterning process. It enables the simple and rapid production of large-area patterns compared to conventional patterning processes such as photolithography.

The fabricated stretchable heater shows high electrical conductivity and excellent heating performance, even under mechanical deformation. These characteristics make it a promising candidate for advanced healthcare applications, particularly in precise and customizable thermal therapies. Furthermore, this work demonstrates the feasibility of next-generation heat supply devices in drug delivery systems.

Control of Microstructure and Micropatterning of Carbon-based Functional Materials for Soft Electronics

Jung Woo Lee*

Department of Materials Science and Engineering, Pusan National University, 2, Busandaehak-ro 63beon-gil, Geumjeong-gu, Busan, 46241, Republic of Korea *jungwoolee@pusan.ac.kr

Wearable biosensor is the most emerging field that can monitor physiological signals from the human body. Although the current biosensor demonstrates high fidelity and stability, there are still high demands to replace expensive materials and reduce complicated and time-consuming procedures. Laser-based direct micro-patterning is a promising technology owing to its fast, scalable, and cost-effective processing. In addition, large-sized reduced graphene oxide (LrGO) facilitates electron transfer through its large basal plane, leading to high electrical-conductivity as well as low cost, long-term usability/stability, and excellent biocompatibility. In this study, femtosecond (FS) laser-directed micro-patterning was adopted to realize several types of biosensors, providing various advantages, such as high-speed (~500 mm s⁻¹), high-resolution (~50 µm), and large-area processing (>8 in.). Moreover, the development of LrGO facilitated a solution-based process and the coating of the LrGO on the FS laser-directed micro-pattern could result in skin-mountable biosensors, so-called laser-directed micro-patterning for skin-mountable graphene sensors (LMGSs), with simplified steps. The LMGSs monitored important biological information such as skin temperature, skin hydration, and electrophysiological signals with electrocardiogram, electromyogram, and electrooculogram at the clinical level. This strategy could be established for not only the wearable biosensors but also the interconnect of stretchable electronics or inductive coils for wireless communication.

Analysis of Pore within SiOCH Films on Si Substrate

Sung-Jin Chang^{1*}, Hoil Cha¹, Hyeongmin Jin², Jinman Kim², Sungwoo Lee³, Sanghak Yeo³, Kwanwoo Lee³

> ¹National Nanofab Center, 291 Daehak-ro Yuseong-gu, Daejeon 34141, Korea ²Chungnam National Univeristy, 99 Daehak-ro Yuseong-gu, Daejeon 34134, Korea ³TES, 2374-36 Jungbudae-ro Yangji-myun Cheoin-gu, Gyeonggi-do 17162, Korea *sjchang@nnfc.re.kr

Low-k materials refer to materials with low dielectric constants. They are specifically used as insulators or insulating films between interconnects in semiconductor devices. As semiconductor device sizes continue to shrink, there is ongoing development of Low-k materials that have even lower dielectric constants while maintaining excellent mechanical properties. This is to reduce signal delay caused by the Low-k materials filling the spaces between interconnects.

One approach to lowering the dielectric constant of Low-k materials involves creating pores within the material. Understanding the characteristics of these internal pores is crucial for achieving structures with low dielectric constants and superior mechanical properties, but it remains a challenging issue. Small-Angle X-ray Scattering (SAXS) analysis is a very useful technique for obtaining information about nanometer-scale pores and pore densities [1,2]. However, X-rays cannot penetrate silicon, which poses a limitation. Therefore, to use SAXS for understanding the pore characteristics of Low-k films deposited on silicon substrates, it is critical to prepare samples in a suitable form for analysis.

In this work, we present the sample preparation process for SAXS analysis to examine the pore characteristics of SiOCH films deposited on silicon substrates using plasma-enhanced chemical vapor deposition. We also show the results of pores within SiOCH films using SAXS analysis technique.

Acknowledgement

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Correlation Between Micropatterned Strain Domains in Graphene on Copper Substrates and Facet Structures

Joonhee Moon^{*} and Jaesung Park^{*}

¹Research Center for Materials Analysis, Korea Basic Science Institute, Korea ²Convergence Research Center for a tangible world in Meta-verse based on Touch standards Korea Research Institute of Standards and Science, Daejeon 34113, Republic of Korea *junnymoon@kbsi.re.kr

Metallic catalysts have become key materials for graphene synthesis, as the choice of substrate plays a crucial role in determining graphene's properties. Among these catalysts, copper (Cu) stands out as a particularly effective substrate for promoting monolayer graphene growth. However, the growth process can introduce strain and structural deformations, impacting graphene's electronic properties and device performance. In this study, we report the first observation of micropatterned strain domains in graphene grown on Cu substrates using chemical vapor deposition. Distinct strain-induced shifts and broadening in the Raman peaks by employing Raman spectroscopy and atomic force microscopy are revealed, demonstrating the unique structural characteristics within the patterned domains. Moreover, a strong correlation between the strain patterns in graphene and the facet structures of the Cu surface is established. Our results reveal intriguing variations in strain within the patterned domains and along the line boundaries, providing valuable insights into the complex interactions between graphene and the Cu substrate. These observed strain patterns and their spatial relationship with the Cu facet structures offer essential guidance for designing graphene-based devices with customized strain engineering.

Enhanced Capacitance Density and Leakage Current Performance of BaTiO₃/BaTiO₃-Ag Double-Layer Structure

Jwa-Bin Jeon, Jun-Woo Lee, Sang-Mo Koo, Weon Ho Shin, Jong-Min Oh*

Department of Electronic Materials Engineering, Kwangwoon University, Seoul 139-701, Republic of Korea

Recently, improved electronic component performance is required for high performance, multifunction, miniaturization and stable power supply due to the development of AI semiconductor devices. Ferroelectric materials are being used to enhance the dielectric properties of capacitors which are passive components that take up a lot of space in electronic components. However, there are limits to improving dielectric properties with BaTiO₃, a single ferroelectric material. Accordingly, research on improving dielectric constant with metal fillers through percolation theory is actively being conducted. Many studies have significantly improved the dielectric constant, but the performance of dielectric loss and leakage current needs to be improved. In this study, a composite film was fabricated with Ag, a metal filler, based on BaTiO₃, a ferroelectric material. Then, a buffer layer was fabricated using same base material, BaTiO₃, and a double-layer structure was fabricated as a composite film through an aerosol deposition process. Measurements and comparisons with the properties of earlier research were made of the film's microstructure, crystal structure and enhanced dielectric and electrical properties.

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Surface Engineering of Ti₂N MXene Quantum Dots for Nano Thermometry

Afrizal L. Fadli, Anir S. Sharbirin, Annas S. Ariffin, and Jeongyong Kim*

Department of Energy Science, Sungkyunkwan University, Suwon 16419, Korea *Email: j.kim@skku.edu

Nano thermometry quantum dots (QDs) with high sensitivity have gained attention for optoelectronic and biomedical applications [1,2]. Most quantum dots have drawback of low photoluminescence (PL) or harmfulness due to contained heavy metals [3]. Ti₂N based MXene MQDs are promising candidates for PL-based nano thermometry. This is because Ti₂N MQDs offer non-toxicity and excellent biocompatibility, being suitable for biological applications [4,5]. However, nitride MQDs like Ti₂N based MQDs can be easily oxidized during hydrothermal synthesis process, damaging their intrinsic properties. This could lead to a low PL quantum yield (QY) which is crucial for the PL-based nano thermometry. In this work, we introduce ethylenediamine (EDA) with the general formula of $C_2H_8N_2$ to protect the nitride MQDs from oxidation during synthesis. Furthermore, EDA can increase the proportion of nitrogen through some-NH participating in hydrothermal reactions [6]. Our result showed the addition of EDA can increase the PLQY of MQDs and the sensitivity of thermometry was improved. Details will be discussed.

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Application of Neural Network Algorithms of Semiconducting Metal Oxide (SMO) gas sensors to Gas Sensing Discrimination Tasks

Huisu Shin, Jeong-Won Cho, Wooseop Lee, Dongwook Seo, Heesu Hwang, and Jin-Ha Hwang*

Department of Materials Science and Engineering, Hongik University, Seoul 04066, KOREA *jhwang@hongik.ac.kr

Neural network algorithms were applied to discriminate among volatile organic compounds (VOCs) such as benzene, xylene, toluene, formaldehyde, and ethanol using a sensor array constructed of semiconducting metal oxide (SMO) gas sensors. The SMO gas sensor array was chosen as a basic platform. The synergistic integration of SMO sensors into machine learning employed unsupervised learning and supervised learning methodologies, in terms of a function of the gas sensor data type/amount, neural network algorithms, sensor combinations, and environmental factors. Neural network-based approach could significantly improve the gas detection/discrimination against VOCs by exploiting numeric-based deep neural networks (DNNs) and 1-dimensional convolutional neural networks (1D CNNs) for gas detection and discrimination. The applicability of numeric- and image-based data formats to gas sensing strategy will be discussed along with the concurrent limitations in terms of practical applications encountered in home and industrial sites.

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Hydrophobic Surface Modification of MgO for Application as Heat-Dissipating Filler in Electric Vehicle Batteries

Seyoung Park, Jinyoung Lee, Eunseo Lee, Yueun Jun, YouJin Park and Sungwook Mhin*

Department of Advanced Materials Engineering, Kyonggi University, Suwon 16227, Korea *E-mail: swmhin@kgu.ac.kr

With the growth in electric vehicles worldwide, thermal management interfaces (TMIs) have become increasingly important for preventing fire accidents and enhancing battery safety. TMIs refer to materials designed to efficiently transfer and dissipate heat generated by batteries, which requires high thermal conductivity. Among various types of fillers for TMIs, Al₂O₃ has been commonly utilized, but its high density and low thermal conductivity make it less appropriate for TMIs. As a promising alternative for Al₂O₃, MgO has been actively studied due to its commercial applicability, relatively low density, and high thermal conductivity, which can be expected to replace Al₂O₃ and significantly improve TMIs performance. However, the hydrophilicity of MgO can lead to degradation through reactions with H₂O, resulting in undesired phase transformations with lower thermal conductivity. To solve this problem, fluorine was used to impart hydrophobicity to the MgO surface. The hydrophobic coating was developed through a sol-gel process using Fluorine Alkyl Silane. This coating provides Si-C and C-F groups, which enhances hydrophobicity as confirmed by contact angle measurements. The developed hydrophobic MgO as a filler for TMIs is expected to enhance the safety of battery systems by preventing undesired phase transformations and improving stability.

Fabrication of MoS₂ Patterns Using a Laser Direct Writer and Emulation of Neuromorphic Device Characteristics

Park Hyehyeon, Kim Minwook, Muhammad Suleman Min Doyoung and Hong Naryeong, Seo Yongho^{*}

> SejongUniversity, 209, Heap-ro, Gwangjin-gu, Seoul, Korea *yseo@sejong.ac.kr

Neuromorphic systems, which mimic the neural structure of the brain, are gaining significant attention due to their potential to reduce hardware size and power consumption. MoS₂ is emerging as a promising material for neuromorphic devices, owing to its high charge mobility and excellent electronic properties. By using ammonium tetrathiomolybdate ((NH₄)₂MoS₄) and exposing it to laser irradiation, single-crystal molybdenum disulfide (MoS₂) can be synthesized.[1] The use of a laser direct writer allows for easy manipulation of the laser to create various patterns, enabling the fabrication of multiple MoS₂ channels arranged to accommodate multi-input neuromorphic devices. This arrangement can effectively mimic the complex synaptic connections between neurons.

To evaluate the basic functions of the neuromorphic device, excitatory postsynaptic current (EPSC) is measured by applying pulse voltages. Short-term pulses can be applied to observe the immediate response, while continuous pulses can be used to assess the short-term plasticity of the synapses.[2] Therefore, in this study, the feasibility of creating precise patterns on MoS₂ surfaces using a laser was investigated, and the fabricated devices were analyzed to understand the impact of these patterns on their electrical and neuromorphic properties. This approach suggests that MoS₂-based neuromorphic devices have significant potential for future applications in artificial intelligence hardware systems.

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Unraveling the sodium storage mechanism of NASICON-type cathode for sodium-ion battery

Junpyo Hur, Jacob Choe, and Jong Min Yuk*

Korea Advanced Institute of Science and Technology (KAIST), Republic of Korea *jongmin.yuk@kaist.ac.kr

Sodium-ion batteries (SIBs) have been proposed as a potential alternative to lithium-ion batteries (LIBs) due to their low cost and plentiful sodium resources. Among the cathode materials explored for SIBs, the Na+ superionic conductor (NASICON)-type polyanionic compounds, including $Na_3V_2(PO_4)_2F_3$ (NVPF) and $Na_3V_2(PO_4)_3$ (NVP), have emerged as a promising candidate due to their high structural stability and high average discharge voltage. However, further research is required to reveal the working mechanism of NASICON-type cathode materials. Herein, the charging and discharging mechanism of NVPF and NVP composite was analyzed. The distinctive two-step crystal structure evolution occurring in each (de)sodiation process was revealed. The oxidation state change of vanadium during the corresponding (de)sodiation process was also conducted. Furthermore, the overall electrochemical performance of the composite cathode was evaluated to assess the impact of the two-step phase transition. This research is anticipated to offer valuable insights into vanadium-based polyanionic cathode materials for developing high-performance cathode materials in SIBs.

Engineering Alloyed Transition Metal Dichalcogenides Nanosheets towards Efficient Electrocatalytic Hydrogen Evolution Reaction

In Hye Kwak^{1*} and Ik Seon Kwon^{2*}

¹Research Center for Materials Analysis, Korea Basic Science Institute (KBSI), Republic of Korea ²Pohang Accelerator Laboratory (PAL), Republic of Korea *ihkwak318@kbsi.re.kr

The rapid increase in fossil fuel consumption has caused global energy and environmental crises, driving the focus toward clean and renewable energy sources like hydrogen, solar, and wind power. Hydrogen stands out due to its high energy density and the fact that it produces only water when used in fuel cells. Key methods for producing hydrogen include gas reforming, electrolysis, solar-driven processes, and biomass conversion. Among these, water-splitting electrolysis is the cleanest, but its costs need to be reduced to compete with fossil fuels [1-2].

One potential solution is using transition metal dichalcogenides (TMDs) as cheaper alternatives to Pt-based catalysts. However, controlling the electronic structure of TMDs for renewable energy applications is challenging [3-4]. A study on ReSe₂-VSe₂ alloy nanosheets synthesized through a colloidal reaction shows that increasing the composition ratio enhances metallic properties and induces a phase transition. These nanosheets also exhibit improved electrocatalytic activity for the hydrogen evolution reaction (HER) when alloyed. The findings provide a strategy for designing TMD alloy nanosheets with better catalytic performance for renewable energy use.

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Fabrication of electrodeposited three-dimensional nickel nanocup array electrode

Jungyu Sung and Yang-Rae Kim*

Department of Chemistry, Kwangwoon University, 20 Kwangwoon-ro, Nowon-gu, Seoul 01897, Republic of Korea *yrkim@kw.ac.kr

Recently, nanolithography has been used to fabricate nanostructures in various fields. It is well-known that there are two nanolithography methods: top-down and bottom-up. The top-down technique requires expensive equipment, such as an electron beam, to create patterned electrodes, adding a complicated process involving etching and masking. However, the bottom-up technique is more cost-effective and straightforward because it fabricates nanostructures through an atomic and molecular assembly process. [1-2]

Nanostructures, with their large specific surface area, exhibit excellent electronic or ionic charge transfer and specific interface effects. In addition, they can revolutionize the catalytic performance and functionalities of many materials. [3]

In this study, various three-dimensional nano-cup array electrodes were fabricated using a bottom-up method.[4] A monolayer of polystyrene was formed on a nickel foil using the Langmuir-Blodgett method. Several nano-cup array electrodes were fabricated through the electrodeposition of nickel. Finally, the structure of fabricated electrodes has been analyzed using a scanning electron microscope and a focused ion beam.

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Surface Properties of Organic Halide Perovskite Thin Films Degraded by Electron Beam Irradiation

HyeonHo Park, HyeonWoo Ju, SeongHeon Kim*

Department of Physics, Jeonbuk National University (Jeonju 54896, Republic of Korea) *shkim97@jbnu.ac.kr

Organic metal halide perovskite has highly efficient photoconductivity, but it has the limitation that it can be degraded severely by external factors. So, there are a lot of studies on the topic of durability and degradation.

In this study, we directly image and characterize the degradation phenomena of Perovskite surface caused by E-beam irradiation under different conditions using Kelvin probe force microscopy (KPFM).

The Perovskite sample area exposed to the E-beam has a distinctly different work function compared to the pristine surrounding area. The work function of the E-beam exposed area was found to be significantly higher than that of the pristine surrounding surface. In addition, we found the newly grown particles around the E-beam exposed area, and the evolution of the newly grown particles was studied by the long-term measurements.

Fine-tuning strategy of supported Au single atom catalyst : atomic-precision hybrid oxide interface modulation

Minkyeong Kim^{*}, Eunji Kang, Jieun Yun, Hongjin Park and Hyun You Kim

Deprartment of Materials Science and Engineering, Chungnam National University, Daejeon 34134, Korea *kimhy@cnu.ac.kr

Single-atoms(SAs) catalysts have attracted much attention, because of their efficient utilization and unique properties. Supported SAs are widely used in various catalytic reactions. CO oxidation is a simple probe reaction which is pivotal in emission control and hydrogen production. Here, Au SAs can successfully be stabilized on the surface of CeO_x -TiO₂ hybrid oxide to achieve superior low-temperature activity and mass activity(MA) toward CO oxidation. By combining density functional theory calculation(DFT) and catalytic characterization with CO oxidation, we found that interface of CeO_x -TiO₂ thermodynamically stabilizes Au as SAs and interaction between Au-SAs and CeO_x -TiO₂ causes low activation energy barrier. The isolated Au-SAs at the CeO_x -TiO₂ interfaces activate the Mars-van Krevelen type CO oxidation. We confirmed that Au/CeO_x -TiO₂(ACT) catalyst exhibit improved low-temperature CO oxidation activity than the conventional Au/TiO₂ catalyst. However, the light-off curve of ACT showed the early activated Au-SAs are not actively involved in CO oxidation. We anticipate that the active sites of overall catalytic activity were attributed to the to the low activation energy barrier of ACT, was delayed the negative impact at high temperatures. Our findings indicate that precise modulation at the atomic level can effectively enhance the catalytic performance and stability of Au-based catalysts.

Electrochemical characteristics of dense PVDF-PEGDME polymer electrolytes for solid state lithium batteries

Yunju Choi¹, Jaeyeong Lee¹, Hyun Gyu Kim¹, Euh Duck Jeong¹, Jong-Seong Bae¹, Yongku Kang^{2*}, Jong-Pil Kim^{1*}

¹Korea Basic Science Institute Busan Center, Busan 46742, Republic of Korea ²Center for Advanced Battery Materials, Advanced Materials Division, KRICT, 141 Gajeong-ro, Yuseong-gu, Daejeon 34114, Republic of Korea *jpkim@kbsi.re.kr

Solid electrolyte lithium-ion battery research is a very interesting research topic as it alleviates the disadvantage (explosiveness) of liquid lithium-ion batteries (LIB) and improves the electrochemical properties of solid electrolyte lithium-ion batteries. In this study, a composite polymer electrolyte was prepared by adding 5 wt.% and 7 wt.% of PVDF, which is used as a binder in electrode manufacturing, to PEGDME-based solid polymer electrolyte. The PVDF-added PEGDME-based solid polymer electrolyte exhibited excellent incombustibility, thermal stability (250 °C), and improved ionic conductivity (7 wt.% PVDF-added P-SPE; 1.14×10^{-4} s/cm at room temperature and 4.27×10^{-4} s/cm at 333 K). From an application point of view, cell design, manufacturing techniques, and material properties significantly impact the cell's electrochemical and safety performance. The charge/discharge characteristics according to the N/P ratio of a solid lithium ion battery full cell (3×4 cm² pouch type, cathode electrode; LFP, anode electrode; graphite) using a PVDF-added PEGDME-based polymer solid electrolyte were presented. The full-cell battery uses 5 wt.% and 7 wt.% PVDF-added PEGDME-based composite polymer electrolyte showed an excellent retention rate of 81.4 % after 100 cycles and a high capacity of 104.9 mAh/g at 0.1 C. The N/P ratio in the full cell of the PVDF-added PEGDME solid polymer electrolyte battery showed a stable capacity value over a wide range.

Interpretation of ToF-SIMS depth profiles of mycelium coils in an orchid mycorrhiza of *Cephalanthera falcata* using sparse autoencoder

Hikaru Yamagushi¹, Shohei Hananoki², Masahide Yamato³, Hiroyuki Hashimoto⁴, and Satoka Aoyagi^{1*}

¹Faculty of Science and Technology, Seikei University, 3-3-1 Kichijoji-kitamachi, Musashino, Tokyo ²Sekisui Chemical Co., LTD., Osaka ³Faculty of Education, Chiba University, Chiba ⁴Comprehensive Research Organization for Science and Society (CROSS), Ibaraki *aoyagi@st.seikei.ac.jp

Cephalanthera falcata is an endangered orchid listed in the red data book of the Ministry of environment. This plant is also known as partial mycoheterotrophy obtaining a part of carbon compound from mycorrhizal fungi. Colonization of ectomycorrhizal fungi in the orchid suggested a symbiotic relationship between the orchid, fungi, and trees [1,2]; however, the process of obtaining nutrients, such as carbon and nitrogen, has not been clarified. In this study, mycelium coils isolated from the mycorrhiza of C. falcata were measured using time-of flight secondary ion mass spectrometry (ToF-SIMS), which provides distribution images of biological molecules. As the interpretation of ToF-SIMS data from biological samples is difficult, the ToF-SIMS data were analyzed using unsupervised learning methods, such as principal component analysis (PCA), multivariate curve resolution (MCR), and sparce autoencoder (SAE), to extract important features [3,4]. The spectral and image information related to the fungi and the orchid was separated from other factors by examining the spectral information and images indicated by each learning method. Depth profiles of the mycelium coils extracted from orchid mycorrhiza were obtained using TOFSIMS 5 (ION-TOF GmbH, Münster) with Bi₃⁺⁺ as a primary ion beam and C_{60}^{++} as a sputtering ion beam. The 3D image data with spectra were converted into numerical matrix data by accumulating 25 layers each out of the 1000 depth profile layers and then analyzed using PLS Toolbox (Eigenvector Research Inc., WA) for PCA and MCR and Neural network toolbox of MATLAB (The Mathworks Inc., MA) for SAE. All of the learning methods extracted the spectra and image data of the biological factors.

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Evaluation of diclofenac permeation into human skin using ToF-SIMS

Atsumi Shinozaki¹, Kazuhiro Matsuda², and Daisuke Hayash¹, Satoka Aoyagi^{1*}

¹Seikei University, 3-3-1 Kichijoji-kitamachi, Musashino, Tokyo ²Toray Research Center, Inc., 3-3-7, Sonoyama, Otsu, Shiga, 520-8567, Japan aoyagi@st.seikei.ac.jp

Molecular imaging in skin tissues is essential for evaluating the penetration of drugs into the skin tissues. Time-of-flight secondary ion mass spectrometry (ToF-SIMS), which enables distribution imaging of organic matters with high spatial resolution (approximately 100 nm two-dimensional resolution and several nm depth resolution), is a suitable analysis method for the evaluation of drugs into the skin tissues. However, ToF-SIMS data of biological samples is generally too complex to interpret manually, and therefore numerical analysis methods such as multivariate analysis [1] have been applied to obtain useful information from complex ToF-SIMS data. In this study unsupervised machine learning methods including principal component analysis (PCA), multivariate curve resolution (MCR), and sparse autoencoder [2,3] were applied to the interpretation of the skin tissues ToF-SIMS data. A model drug was Voltaren lotion (Dojin Pharmaceutical Chemical Co.), which contains diclofenac as an active ingredient. Stratum corneum samples for TOF-SIMS measurements were obtained from Voltaren-treated and untreated skin by tape stripping. The positive and negative ion TOF-SIMS data acquired by TOF-SIMS.5 (ION-TOF GmbH, Munster, Germany) with a Bi₃⁺⁺ primary ion source were converted into numerical matrix data, and then the data were analyzed by the unsupervised learning methods. As a result, positive secondary ion images of cholesterol and diclofenac showed different distributions, inside and outside of the cells, respectively. Diclofenac-derived components were also detected in negative secondary ion spectra. This indicates that diclofenac penetrated into the inside of cells and the deep layers of the skin.

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3D Distribution Imaging Analysis of Components Using Orbitrap/TOF Hybrid SIMS

Ji Yeong Sung and Jong Sung Jin*

Korea1Busan Center, Korea Basic Science Institute (KBSI), Busan, Korea *jsjin@kbsi.re.kr

The chemical structure and distribution analysis of the components of lithium-ion batteries are very important in terms of correlation with energy storage efficiency. TOF-SIMS has the advantages of a wide analysis range from elements to organic/inorganic molecules, excellent detection limits (~ppm), and high image resolution. However, TOF-SIMS has several analytical limitations because it is difficult to interpret numerous mass peaks due to its relatively low mass resolution. Orbitrap/TOF Hybrid SIMS has much higher image resolution and mass resolution than TOF-SIMS.

In this study, we used this instrument to conduct ion imaging studies on the distribution and depth behavior of various components including lithium ions in each layer of a half-cell of a lithium-ion battery. Specifically, we designed a systematic approach to accurately analyze the 3D images of the extracted ions by finding characteristic peaks of molecules of interest according to depth behavior using multivariate curve resolution (MCR) technology. This study will provide a new analytical method to obtain clear information on battery materials, such as confirming the 3D images of the lithium penetration depth of a secondary battery cell.

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Red fluorescent copper nanocluster for fluorescence, smartphone, and electrochemical sensor array to detect the monkeypox A29 protein

Barkavi Dhanasekaran, Kyusik Yun*

Department of Bionanotechnology, Gachon University, Gyeonggi-do 13120, Korea *ykyusik@gachon.ac.kr

MPXV is an orthopox zoonotic infected viral disease it is leading infected disease worldwide from human to human through direct or indirect sexual contact so it is must essentially detect (MPXV) earlier stage to prevent the mortality. In recent years fluorescence-based materials have received significant attention for biomedical application. In this study, we synthesized red-fluorescent copper cluster (CuNCs) with a size of less than 10nm, which was confirmed by high-resolution transmission electron microscopy (HR-TEM) and atomic force microscopy (Bio-AFM) analysis. The synthesized CuNCs had a high fluorescence nature and were utilized for the detection of the MPXV (A29P) by an antigen-antibody conjugation using fluorescence, smartphone colorimetric, and electrochemical sensing techniques. Mechanism of the antigen (A29P) and antibody (Ab A29) were studied by X-ray photoelectron spectroscopic (XPS) analysis. Additionally, fluorescence and electrochemical sensing were performed in PBS with detection limit of 0.096 and 0.114 nM, respectively. For real world applications, the prepared immunosensor array can detect A29P in spike serum samples and point-of-care (POC) analysis a smartphone- integrated sensor array was used to measure the RGB color changes. The final value showed that synthesized CuNCs are potential material for detecting A29P via fluorescence and smartphone colorimetric and electrochemical sensing techniques.

Quartz tuning fork-based viscometry for separating bovine sperm in a biomimetic cervix environment

Dongwon Kim^{*} and Manhee Lee^{**}

Department of Physics, Chungbuk National University 28644, South Korea **mlee@cbnu.ac.kr

In the livestock industry, the acquisition of sperm with superior genetic traits for artificial insemination is in high demand. Separating high-quality bovine sperm from semen is crucial to meet this demand. Here, we obtained high-quality sperm in large quantities using an IVF sperm sorting chip (SSC), which could mimic the viscous environment of the bovine cervix during ovulation and facilitates isolation of progressively motile sperm from semen.

The viscous environment-on-a-chip was created by formulating and implementing polyvinylpyrrolidone (PVP)-based solutions for the SSC medium. To control the viscosity of the SSC, we modulated the concentration of polyvinylpyrrolidone (PVP) in the SSC medium. We used a hand-made micro-viscometer based on a Quartz Tuning Fork (QTF) Atomic Force Microscope to measure the viscosity of the medium with a volume of approximately 100 μ L or less. we were able to create a medium in PVP 1.5% with proper viscosity for sperm separation using the QTF-based micro-viscometer. We used this medium to make a microfluidic chip that mimics a biomimetic cervix environment. The sperm separated through the microfluidic chip has good properties in motility, morphology, and DNA integrity.

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High-Throughput Quantitative Analysis of Amino Acids in Freeze-Dried Drops Using Time-of-Flight Secondary Ion Mass Spectrometry

Heejin Lim^{1*}, Siheun Lee², Jong Sung Jin³, and Min-Sik Kim^{4,5,6*}

¹Center for Scientific Instrumentation, Korea Basic Science Institute (KBSI), Daejeon 34133, Korea

²School of Undergraduate Studies, Daegu Gyeongbuk Institute of Science and Technology (DGIST), Daegu 42988, Korea

⁴Department of New Biology, ⁵New Biology Research Center, ⁶Center for Cell Fate Reprogramming and Control, Daegu

Gyeongbuk Institute of Science and Technology (DGIST), Daegu 42988, Korea

*hjlim0111@kbsi.re.kr

Time-of-flight secondary ion mass spectrometry (ToF-SIMS) has become a promising analytical tool for molecular profiling in biological applications. However, its ultrahigh vacuum environment and matrix effects hamper the absolute quantitation of solution samples. Herein, we present a rapid high-throughput platform for a quantitative ToF-SIMS analysis of amino acids in matrix deposits formed from freeze-dried solution drops through ice sublimation on a parylene film microarray substrate [1]. Droplets of the amino acid solutions, which were mixed with stable isotope-labeled phenylalanine (F*) of high concentration (10 mM), were loaded on wells of the microarray and then frozen and evaporated slowly below the freezing point, forming into continuous solid-phase F* matrix deposits. The amino acids ($\leq 500 \ \mu$ M), adequately well dispersed throughout the F* matrix deposits on each well, were quantitatively analyzed by ToF-SIMS in a rapid and high-throughput fashion. The lower limit of quantitation reached below 10 μ M.

³Busan Center, Korea Basic Science Institute (KBSI), Busan 46742, Korea

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Investigation of Antenna Effect: Enhanced Luminescence of Terbium(III) with Glucoconjugated Ligands

Parmeshthi Parikh, Anuvasita Parikh, Ajay K. Sah*

Department of Chemistry, Birla Institute of Technology and Science, Pilani; Pilani Campus Rajasthan 333031, India. * asah@pilani.bits-pilani.ac.in

The lanthanides exhibit emission across the wavelength range of visible to near-infrared (NIR). This emanating nature of lanthanide ions makes them important in optoelectronic devices, contrast agents, photodynamic therapy, etc. [1]. The lanthanide ions have low molar absorptivity due to the forbidden $f \rightarrow f$ transition making them insignificant for efficient photon. However, the magnitude of emission intensity of Ln(III) ions can be enhanced by coordinating them with chromophoric ligands. [1, 2]

In this work, we have explored the sensitizing effect in terms of the luminescence of various glucoconjugate molecules toward Tb^{3+} . Our results indicate that the presence of glucoconjugate moieties enhances the characteristic emission peaks of terbium ions in solution. Additionally, the terbium complexes formed with these glucoconjugates exhibit the expected emission peaks in the solid phase as well.

The selective antenna effect in terbium ion was explored on the basis of the fluorescence spectroscopic technique. Further, the characterization of terbium complexes involves FTIR, Raman, TGA, PXRD, XPS, FESEM etc.

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Analysis of natural pigments using various instrument and their statistical processing

Youngseo Lee^{1,2}, Won-Yong Lee^{2*}, and Yeonhee Lee^{1*}

¹Advanced Analysis and Data Center, Korea Institute of Science and Technology ²Department of Chemistry, Yonsei University, Seoul 03722, Korea Seoul 02792, Korea *gksten@kist.re.kr

Artifacts and artworks of significant cultural and artistic value often face challenges related to counterfeiting and forgery. Determining authenticity requires both artistic expertise and scientific analysis, including techniques such as dating and material composition analysis. As these objects are getting old, damage may occur, necessitating restoration. In such cases, the scientific analysis of materials and pigments is crucial. Pigments, which are colorants dispersed rather than dissolved in a medium, have evolved over time, making their composition essential for authenticity verification and restoration processes [1-2].

This study aimed to enhance the reliability of art authentication and contribute to the development of a comprehensive pigment database. Thirty-three types of natural pigments were analyzed using spectrophotometry, X-ray fluorescence (XRF), FT-IR, and time-of-flight secondary ion mass spectrometry (ToF-SIMS), with data systematically collected for database construction. Additionally, principal component analysis (PCA) was performed using R to better understand the discriminate among the pigments.

The results revealed that blue, green, and yellow pigments each consisted of a single mineral, with brightness modulated by particle size, whereas red pigments comprised various minerals. A PCA plot was generated to accurately identify pigment compositions, even among those derived from the same mineral. Notably, the application of ToF-SIMS data to PCA demonstrated distinct color-based classifications according to principal components. These findings underscore the utility of PCA in analyzing pigment characteristics and offer valuable insights for art authentication, aiding in authenticity verification and guiding restoration efforts through the precise classification of pigments used in artworks.

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Accelerator Mass Spectrometry-based Quantitative Tracing of Phenol and its Derivatives in Soil and Plants

Gwan-Ho Lee¹, Seong Eun Song², Min-Seok Oh¹, Seo Ra Seo¹, Byung-Yong Yu^{1*}

1 Korea Research Institute of Standards and Science, 2YeonSei University KIST (Hwarang-ro 14-gil, Seongbuk-gu, Seoul 02792, Korea) *ghlee@kist.re.kr

Accelerator mass spectrometry (AMS) is an ultra-sensitive analysis method, differed from conventional mass spectrometry. It accelerates atomic ions generated from carbon isotopes and counts each isotope ion to obtain the isotope ratios ($^{14}C/^{12}C$) in samples. Moreover, AMS analysis requires using much lower radio activity of ^{14}C than other commonly used radioactive experiment, so it has a great advantage of reducing limitations for tracking the isotope and radioactive wastes. Thus, a minute amount of ^{14}C labeled molecules can be traced by AMS, so-called ^{14}C nanotracing.

The soil pollution by chemicals can cause concern over health risks from direct contact, vapors, and secondary pollution. When the place is exposed to pollutant, especially phenol in this study, plants grown on the soil are likely to face second-hand contamination by phenol itself and its metabolites. Thus, precise quantification of a chemical contamination is important to predict and prevent the secondary or tertiary contamination.

Here in, we quantitate phenol, on the behalf of other chemical pollutes, and its metabolites and products of decomposition in soil and plant, using AMS.[1] We planted Arabidopsis thaliana as a model plant in soil polluted with phenol and little of ¹⁴C-phenol (~5 nCi, 7.13 ng), and the plants were grown in controlled circumstances for 3 weeks. Total radio activity (TRA) of ¹⁴C included in 3-week grown plant and soil were analyzed by using liquid scintillation counter(LSC), which was connected with oxidizer. Since, the LSC method has 10^3 to 10^4 times lower sensitivity than AMS, it was hard to accurately quantitate the TRA in the sample. Thus, we introduced the AMS method for quantitation.

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Device-level XPS Analysis for Physical and Electrical Characterization of Oxide-Channel Thin-Film Transistors

Gyungtae Kim^{1*}, Myung Keun Lee¹, Yun-Ju Cho², and Sung-Min Yoon^{2*}

1National Nanofab Center, Daejeon, 34141, Korea

2Department of Advanced Materials Engineering for Information and Electronics, Kyung Hee University, Yongin, Gyeonggi-do 17104, South Korea *gtkim@nnfc.re.kr

This work presents the first device-level XPS analysis of IGZO TFTs using optimized measurement setups for fine patterns. The material is split into four sections. The initial section suggests a methodology for identifying the optimal analysis location at the device level. The second verifies device-level XPS analysis by analyzing atomic ratios and O 1s spectra in IGZO TFTs with different cation compositions. The third investigates the changes in BE at active/GI interfaces experiencing charge-trap events before and after undergoing a positive-bias stress (PBS) test of IGZO TFTs. Finally, this paper presents prospects for improvement and utilization of analysis methods. We successfully demonstrate the technical feasibility of device-level XPS analysis and propose new applications of XPS measurement for more sophisticated analysis of AOS TFTs [1].



Figure 1. Device-level XPS Analysis of Oxide-Channel Thin-Film Transistors

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Design of the High Heat Load Front-End for the 4th Generation Synchrotron in Korea

Hyung-seok Choi, Jong-ha Park, Young Duck Yun, Ki-jeong Kim*

Pohang Accelerator Laboratory 80, Jigok-ro 127beon-gil, Nam-gu, Pohang-si, Gyeongsangbuk-do, 37673, Rep. of Korea *kjkim@postech.ac.kr

Currently, a 4th generation synchrotron(Korea-4GSR) is under construction in Ochang-eup, Cheongju-si, Chungcheongbuk-do, Korea. Korea-4GSR has an electron beam energy of 4 GeV, and its brightness is about 100 times that of Pohang Accelerator Laboratory's PLS-II, making it a linear accelerator(LINAC), booster-ring, and storage-ring were designed. The white beam emitted from the storage-ring to the beamline has a much higher output than the PLS-II, which inevitably imposes a high heat load on each equipment of the beamline. In this design, we analyzed the High Heat Load Front-End structure that minimizes the heat load commonly applied to each beamline of Korea-4GSR in advance and protects the vacuum of storage-ring and the radiation shielding.

Synthesis and application of tungsten disulfide for energy storage devices

Hae Kyung Jeong*

Department of Energy System Engineering, Daegu University, Gyeongsan 38453, Korea *outron@gmail.com

Tungsten disulfide nanostructures with various morphologies were synthesized and investigated, by using a simple and easy hydrothermal method, for flexible supercapacitor applications. The tungsten disulfide synthesized for 24 h (WS₂-24) exhibited flower-like nanostructures composed of numerous aggregated nanosheets, demonstrating high electrochemical performance, in terms of electrochemical surface area, charge transfer resistance, specific capacitance, and rate capability. Electrochemical studies were conducted using a three-electrode system in a 1.0 M potassium hydroxide (KOH) electrolyte. Additionally, the electroactive WS₂-24 electrode was employed on a flexible activated carbon cloth substrate (ACC) to assemble a flexible symmetric supercapacitor with polyvinyl alcohol/ sodium hydroxide (PVA/ NaOH) gel electrolyte in a two-electrode system. The WS₂-24h-ACC device exhibited a specific capacitance of 262.5 F g⁻¹ at 1 A g⁻¹, an energy density of 23.6 Wh kg⁻¹, a power density of 402 W kg⁻¹, excellent cyclic stability of 94.5%, and a rate capability of 86.4% after 5,000 cycles. [1]



Figure 1. Tungsten disulfide with various nanostructure depending the synthesis condition. [1]

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Study on Reversible Multicolor Chromism through Humidity for Short Organic Spacer-based Perovskites: Focusing In-situ Observation

Aelim Ha^{1,2}, Kitae Kim^{1,2}, Seunghwan Kim^{1,2}, Eunki Yoon^{1,2}, Sooyeon Pak^{1,2}, Yeonjin Lee², KyuHyoung Lee^{2*}, Soohyung Park^{1,4*}

¹Korea Institute of Science and Technology, ^{2,3}Yonsei University, ⁴University of Science and Technology

¹Advanced Analysis and Data Center, Korea Institute of Science and Technology, 5 Hwarang-ro 14-gil, Seongbuk-gu, Seoul 02792, Republic of Korea

²Department of material science & engineering, Yonsei University, 50 Yonsei-ro, Seodaemun-gu, Seoul 03722, Republic of Korea *Email: soohyung.park@kist.re.kr, khlee2018@yonsei.ac.kr

Recently, organic-inorganic hybrid perovskites (PVSK) has garnered a surge of attention as nextgeneration optoelectronic materials. This is attributed to their outstanding optical properties and impressive performance of the devices based on them. In the field of perovskites, determining the structural phase of a specific PVSK is crucial. Because the perovskites can exhibit completely different properties depending on their structure even with the same elemental composition. For example, CH₃NH₃PbI₃ and [C₄H₉NH₃]₂PbI₄ are both composed of C, N, Pb, I and H atoms, the former has a three-dimensional (3D) phase, while the latter has a two-dimensional (2D) phase. In this regard, the Goldschmidt tolerance factor is widely used in PVSK structure analysis. It predicts the crystal structure of PVSK based on the radii of constituent organic, metal, and halide ions in the system. If the tolerance factor is above 1, it predicts a 2D structure, while below 1, it predicts a 3D structure. However, it has been pointed out that the tolerance factor has limitations in anticipating perovskite with values very close to 1. EA-based perovskite (EA_xPbI_v), which employs the ethylammonium (EA) as organic molecule, has a tolerance factor of 1.04. It implies that EA_xPbI_y theoretically exists at the boundary on somewhere between 3D and 2D structures. In fact, there is still limited understanding of the structure of reported EAxPbIv and a consensus has not established yet. Hence, a research is needed that (i) accurately elucidates the structure of EA_xPbI_y, and (ii) refines the current Goldschmidt tolerance factor.

In this study, we investigated the structural phase of EA_xPbI_y through in-situ Grazing-Incidence Wide-Angle X-ray Scattering (GIWAXS). We have observed that EA_xPbI_y exhibits interesting phenomena under specific humidity conditions. The film's color reversibly changed from yellow to orange, brown, and colorless as humidity increased beyond a critical point. Changes were also observed in the GIWAXS patterns corresponding to each color. We hypothesized that this multicolor chromism correspond to structural changes in EA_xPbI_y based on humidity. The monitored structural changes imply that the influence of humidity should be considered in relation to the Goldschmidt tolerance factor, beyond just the atomic size. Through this, we aim to broaden the understanding of the physical and material properties of how humidity impacts to the structure of perovskites. Additionally, we anticipate contributing to the ultimate performance optimization of devices utilizing EA_xPbI_y.

Electronic Structure of Silver Phenyl Selenolates [AgSePh]_∞, and Their Dependency on Thickness: A Investigation via Photoemission Spectroscopy

Seunghwan Kim^{1,2}, Kitae Kim^{1,2}, Eunki Yoon^{1,3}, Aelim Ha^{1,3}, Sooyeon Pak^{1,2}, Kyu Hyung Lee³, Yeonjin Yi², Soohyung Park^{1*}

¹Korea Institute of Science and Technology, ²Department of Physics Yonsei University, ³Department of Material Science & Engineering Yonsei University

¹Advanced Analysis and Data Center, Korea Institute of Science and Technology, 5 Hwarang-ro 14-gil, Seongbuk-gu, Seoul 02792, Republic of Korea; Division of Nanoscience & Technology, KIST

School, University of Science and Technology (UST), Seoul 02792, Republic of Korea

²Department of Physics and van der Waals Materials Research Center, Yonsei University, 50 Yonseiro, Seodaemun-gu, Seoul

03722, Republic of Korea

*Email: soohyung.park@kist.re.kr

The study of silver phenylselenolate $[AgSePh]_{\infty}$, a prominent metal-organic chalcogenolate (MOC), has gained a significant attention due to its remarkable electronic properties. This growing interest is driven by its distinctive two-dimensional (2D) layered structure, in which the inorganic planar silver selenolate system is sandwiched by organic phenyl groups. This structure confines carriers within inorganic layers and enables unique anisotropic light emission and absorption characteristics. Notably, $[AgSePh]_{\infty}$ exhibits a direct bandgap in the blue spectral region, highlighting its potential for use in optoelectronic applications. However, experimental investigations of its electronic structure on this material has been limited relative to the high interest. Particularly, the electronic structure of $[AgSePh]_{\infty}$ is expected to be influenced by the substrate, considering it is a layered material. In this study, we conduct an extensive investigation of its intrinsic electronic properties and their thickness dependency. To this end, we refined the synthesis method, allowing for easy control of thickness and the production of high-quality samples. Using photoemission and inverse photoemission spectroscopy (PES and IPES), we accurately measure the material's transport bandgap, ionization potential, and electron affinity. Furthermore, we also investigated the exciton binding energy by comparing its obtained transport bandgap to optical bandgap. To understand the thickness dependence of the electronic structure, the entire experiments were performed with samples with varying thicknesses from few-layers to bulk. This detailed analysis greatly enhances our understanding of [AgSePh]_∞ and provides a solid empirical basis for its use in optoelectronic devices with thickness-based modulation.

Spacer-Assisted Growth of Thin Single-Crystalline Two-dimensional Perovskite Membranes

Sooyeon Pak^{1,2}, Kitae Kim^{1,2}, Seunghwan Kim^{1,2}, Eunki Yoon^{1,2}, Aelim Ha^{1,2}, Kyu Hyoung Lee², Yeonjin Yi², Soohyung Park^{1*}

¹Korea Institute of Science and Technology, ²Yonsei University, ¹Advanced Analysis and Data Center, KIST (5, Hwarang-ro 14-gil, Seongbuk-gu, Seoul 02792 Korea) ²Department of Physic, Yonsei University (50 Yonsei-ro, Seodaemun-gu, Seoul 03722 Korea) *soohyung.park@kist.re.kr

Single-crystalline perovskites have gained significant attention due to their superior optical and electrical properties, which allow precise control over material properties and enhance carrier dynamics compared to polycrystalline forms. These characteristics make them highly suitable for optoelectronic devices because of their susceptibility to external stimuli originating from their thin nature. It allows easy modification of their semiconductor properties, fully exploiting the features of perovskites. Effective fabrication of electronic devices using single-crystalline perovskites requires careful control over thickness and lateral dimensions, especially the thickness needs to be below 10 nm to fully leverage its advantages at the surface or interface.

Various methods have been explored for growing thin single-crystalline 3D perovskites, including the Space-Limited Inverse Temperature Crystal (SLITC) method by Chen et al. [1] However, 3D perovskites are susceptible to moisture, which poses a significant drawback. To address this, 2D Ruddlesden-Popper (RP) phase perovskites offer improved stability due to their layered structure, alternating organic cation and metal halide layers. Liu et al. successfully synthesized thin, large-area single-crystalline (PEA)₂PbI₄ membranes using the Induced Peripheral Crystallization (IPC) method. [2] However, fabricating thin and large single-crystalline 2D RP perovskites is still an ongoing research challenge.

In this study, we propose an improved method inspired by Liu et al.'s crystallization technique. We found limitations of this method as the difficulty in controlling the crystal growth direction due to random seed formation, which leads to overlapping crystals. To overcome these issues, we introduced a spacer into the IPC technique. This spacer-assisted method localizes the seeds on the interface between spacer and precursor, thereby controls the direction of crystal growth, enabling the formation of larger, well-aligned single crystals. Through optimization of synthesis parameters, we successfully grew (PEA)₂PbI₄ single crystals with excellent morphological and structural properties, as confirmed by X-ray dirffaction and photoelectron spectroscopy. We believe this study will enhance our understanding in growth technique of 2D perovskite single crystal and facilitate their integration into various technological applications.

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Cryo-TEM Observation of Ice I

Ji Su Park¹, Namgyu Noh¹, Jungjae Park¹, Yoonsu Shim¹, Sanghyeon Park¹, Yusra Qureshi¹, Sung Kang², Yoon Huh², Chan-Woo Lee³, and Jong Min Yuk^{1*}

¹Department of Materials Science and Engineering, Korea Advanced Institute of Science and Technology, 291 Daehak-Ro, Yuseong-Gu, Daejeon, 34141, Republic of Korea

²Analysis & Assessment Research Group, Research Institute of Industrial Science and Technology, Pohang, 37673, Republic of Korea ³Energy AI & Computational Science Laboratory, Korea Institute of Energy Research, Daejeon 34129, Republic of Korea *Corresponding author: jongmin.yuk@kaist.ac.kr

Ice, as a solid state of water, plays a crucial role in the Earth's cryosphere, influencing fields such as cryopreservation [1-4], climate modeling [5-7], and aviation [8,9]. It exhibits over 20 polymorphic phases [10,11], including the recently identified ice XIX [12], with cubic ice (Ic) and hexagonal ice (Ih) being particularly significant due to their unique properties [13,14]. These phases have tetrahedral hydrogenbonding configurations but differ in stacking sequence and free energy [15]. Researchers have used methods like thermal annealing of vitreous ice [16-18] and hyperquenching [19] to prepare Ic, often resulting in stacking-disordered ice (Isd) [20,21]. While traditional diffraction-based methods struggle to distinguish these phases due to their lattice similarity [22-24], advances in cryogenic transmission electron microscopy (cryo-TEM) and low-dose imaging have enabled detailed, real-space imaging of ice at the molecular level [25]. This study uses cryo-TEM to investigate phase changes in ice on graphene under various conditions. Dark-field micrographs and electron energy-loss spectroscopy (EELS) reveal transitions from Ic to Isd at specific thicknesses. High-resolution TEM shows defect-assisted phase transitions from cubic to hexagonal structures. These findings enhance our understanding of ice polymorphism and the mechanisms driving phase transitions at the nanoscale.

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Defect Analysis of Semiconductor Devices Using SEM, FIB, PFIB : Practical Cases and Results

Junyoung Won, Hee-Soo Kim, Soyeon Kwon, Sunghoon Cho, and Changwoo Byun**

Advanced Institute of Convergence Technology (AICT), 145 Gwanggyo-ro, Yeongtong-gu, Suwon-si, Gyeonggi-do 16229, Suwon, Republic of Korea *corresponding byuncw@snu.ac.kr

This study presents practical cases and results from the defect analysis of semiconductor devices using Scanning Electron Microscopy (SEM), Energy dispersive spectroscopy (EDS), Focused Ion Beam (FIB), and Plasma Focused Ion Beam (PFIB) techniques. The analysis focuses on interposer substrates, semiconductor metal interconnect, and interface defects employing the unique advantages of each technique to precisely determine the causes of these defects.

SEM was utilized for high-resolution imaging of surface and structural features, while FIB and PFIB were used for selective milling and cross-sectional analysis to locate and identify internal defects. PFIB, in particular, demonstrated significant time efficiency for large-area analysis, enabling faster milling of extensive regions compared to FIB, making it especially effective for analyzing defects in complex structures. EDS was used to identify the elemental composition of the defective areas in each device.

The results of this study successfully identified structural defects in the interposer substrates and the root causes of semiconductor wiring failures. These findings are expected to contribute to improving the reliability of semiconductor manufacturing processes and reducing defect rates.

In-Situ Observation of Ag2S-Catalyzed ZnS Nanowire Growth via VLS-SLV Mechanisms

Han-Kyun Shin, Jung Han Kim*

Department of Materials Science and Engineering, Dong-A University, Republic of Korea *junghankim@dau.ac.kr

In this study, we investigated the growth of semiconductor-catalyzed semiconductor nanowires (NWs), specifically Ag₂S-catalyzed ZnS NWs, through a vapor-liquid-solid (VLS) mechanism using metal-organic chemical vapor deposition (MOCVD) with an Ag thin film. Extensive electron microscopy techniques, including in situ heating transmission electron microscopy (TEM), were employed to confirm the formation of ZnS NWs with a wurtzite structure via high-resolution, multi-dimensional surface and interface analyses. To further support the VLS growth of Ag₂S-catalyzed ZnS NWs, in situ heating TEM experiments were conducted, observing temperature changes from room temperature to 840°C. A reverse reaction, consistent with a solid-liquid-vapor (SLV) mechanism, was observed. The melting of the Ag₂S catalyst at approximately 480°C, surrounded by a carbon (C) shell, marked the onset of the process. Complete melting of the Ag₂S catalyst into the ZnS NW occurred around 825°C. As the temperature increased further, both the Ag₂S and ZnS NWs continued to melt and vaporize up to 840°C, leaving only the C-shell. Based on these structural and chemical investigations, a possible growth mechanism is proposed.

Keyword: zinc sulfide nanowire, silver sulfide, growth mechanism, in situ TEM

Isotropic electrical field-driven MEMS chip for electrochemical in situ TEM application

Min Wook Pin^{*}, Joon Ha Chang, Jungjae Park, Yoon Huh and Sung Kang

Analysis & Assessment Research Group, Research Institute of Industrial Science & Technology (RIST), 67, Cheongam-ro, Pohang, 37673, Republic of Korea *minwook.pin@rist.re.kr

Liquid phase electron microscopy (LPEM) is a revolutionary technique that enables the characterization of structural, morphological, and chemical changes in nanoparticles immersed in liquid environments, a feat previously deemed unattainable. LPEM necessitates the utilization of a specially designed holder and a consumable MEMS chip equipped with an ultra-thin silicon nitride window for in situ observation. To delve beyond mere observation and comprehend the electrochemical behavior within liquid cells, a system capable of fabricating electrodes on one side of the MEMS chip via semiconductor processes and facilitating signal application through an external potentiostat is imperative. This advanced setup has facilitated diverse electrochemical experiments encompassing OER/ORR, corrosion analysis, and charging/discharging investigations of secondary batteries. Nevertheless, the implementation of realistic in situ TEM experiments poses numerous challenges in addition to size-related effects. One prevalent issue stems from the inherent inhomogeneity of the electric field resulting from electrode placement on one side of the MEMS chip. Unlike conventional electrochemical devices, in situ TEM MEMS chips exhibit a horizontal electric field characterized by current density distribution, contingent upon the spatial separation between the working and counter electrodes. Commercial MEMS chips often suffer from non-uniform electrode dimensions and spacing, thereby generating anisotropic electric fields leading to undesired hot spots and associated side effects.

In this study, we present an optimized design of isotropic electric field-driven MEMS chips, accomplished through Finite Elemental Method simulations, and investigate the relationship between modifications in electrode design and resulting electrical properties. Furthermore, we demonstrate the exemplary performance of our isotropic electric field-driven MEMS chip via electrochemical experiments showcasing the uniform deposition of copper metal onto the working electrode from a copper sulfate solution. This research will yield crucial insights and serve as a cornerstone for establishing essential guidelines governing the electrode design of MEMS chips, ensuring the reliability of future electrochemical experiments.

Advanced Electron Microscopy Analysis of High-Ni single crystal NCM cathode

Joon Ha Chang^{*}, Min Wook Pin, Jungjae Park, Sung Kang, Jiho Lee, Yoon Huh

Analysis and Assessment Research Group, Research Institute of Industrial Science and Technology (RIST), Pohang 37673, Republic of Korea *e-mail: joondury@rist.re.kr

The High-Ni single crystal LiNi_xCo_yMn_{1-y}O₂ (NCM) cathode is critically important due to its superior energy density and stability, which are essential for next-generation lithium-ion batteries. With the increasing demand for high-performance batteries in electric vehicles and portable electronics, the ability of High-Ni NCM cathodes to deliver enhanced capacity and long-term cycling stability makes them a key material in advanced battery technology. This research aims to deepen our understanding of these cathodes by providing detailed insights into the structural and chemical properties of High-Ni NCM cathodes synthesized from commercial materials.

In this study, we conducted a comprehensive evaluation of High-Ni single crystal NCM particles synthesized from commercial raw materials. To achieve this, we applied various advanced analytical techniques, including scanning electron microscopy (SEM), transmission electron microscopy (TEM), X-ray diffraction (XRD), electron energy loss spectroscopy (EELS), and X-ray photoelectron spectroscopy (XPS), to thoroughly examine the structural stability and surface characteristics of the particles. By precisely measuring the distribution of Ni²⁺ and Ni³⁺, as well as the thickness of the rock-salt structure, we secured fundamental data for assessing the viability of utilizing recycled raw materials in future studies.

The results of this study provide crucial foundational data for understanding the practicality and mechanisms of High-Ni single crystal NCM particles synthesized from commercial materials. In future research, we will extend this analysis to High-Ni single crystal NCM particles synthesized from recycled materials to evaluate their feasibility and potential for use in sustainable battery technologies.

Calculation of light element (Li,C,O) ionization ratio measured by 2D-ERDA method using TOF-MEIS and electrostatic deflector

C.S. Park, J.H. Song, K.S. Park, C.S. Sim, W.S. Kim S.B. Kim, D.W. Moon, W. J. Min*

HB Solution, Techno 8ro 33, Yuseong-gu Daejeon, Republic of Korea, 34028 *wj.min@hb-solution.co.kr

Time of Flight-Medium Energy Ion Scattering (TOF-MEIS) is a technology that can analyze the composition and thickness of thin films at the atomic layer by measuring the time when particles are scattered after colliding energetic ions (He⁺) with a sample. However, light elements with small scattering probabilities have a small scattering cross section and overlap the substrate element spectrum, making it difficult to analyze by backscattering measurement. To analyze light elements is by Elastic Recoil Detection Analysis (ERDA), which is a measurement method of Direct Recoil (DR) nucleus from the sample by incident ions. In TOF-type MEIS, it is possible to analyze hydrogen at a depth of 20 nm from the surface without additional ion optics by using the recoiled hydrogen ion that arrive at the detector faster than scattered He ion during ERDA analysis. [1] However, the hydrogen element has a limit to the analytical depth at thicknesses exceeding 20 nm. Additionally, light elements other than hydrogen cannot be analyzed due to the overlap of DR peaks and scattering spectra. To overcome this, we tried 2D-ERDA analysis to simultaneously obtain energy and TOF of DR elements by introducing an electrostatic deflector between the sample and the position sensitive TOF-detector. This made it possible to analyze by separating the light element ERDA spectrum such as Li, C, and O, which were previously difficult to analyze. In this study, the 2D-ERDA spectra of LiF, SiO₂, MgO, SiC, and DLC were obtained with TOF-MEIS using 100 keV He⁺, and the ionization ratio for Li, C, O, and H included in the sample was compared with the backscattering spectrum to confirm the possibility of light elements quantitative analysis using 2D-ERDA.

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Semiconductor Analysis by Atom Probe Tomography

Bong Ho Lee^{*}, Youngmoo Eun, and Taehoon Cheon

Advanced Analysis Team, INST, DGIST, 333 Techno jungang-daero, Hyeonpung-eup, Dalseong-gun, Daegu 42988, Korea *bhlee@dgist.ac.kr

As semiconductor device sizes have been drastically reduced to just a few nanometers, there is a growing demand for the development of nanoscale analysis techniques to address these challenges. In the case of nanomaterials, the properties can vary significantly depending on compositional changes in nanoregions, clusters, interfaces, and quantum regions. Therefore, analytical techniques for interpreting these variations are crucial.

Atom Probe Tomography (APT) is an analytical method that uses a high electric field and laser pulses on the apex of a needle-shaped specimen to evaporate individual atoms. The flight time and impact position of the evaporated atoms are measured by a position-sensitive detector, and the data is reconstructed over time to create a three-dimensional compositional map. Due to its sub-nanometer probe size and exceptional sensitivity, capable of detecting concentrations beyond parts per million (ppm), APT is highly effective for analyzing the composition of interfaces and quantum regions.

In this presentation, we will examine various case studies of APT analysis applied to Si semiconductors, III-V semiconductors, and power semiconductors. We will also explore analysis examples in the fields of energy and nanomaterials. Through this, we aim to discuss the potential of APT for ultrafine-scale analysis.

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Optimization of SIMS Energy Slit for Dopant Distribution Analysis in SiC Power Semiconductors

Minji Kang¹, Taehun Jang¹, Tae Eun Hong^{1*}

¹Korea Basic Science Institute ¹Busan Center, KBSI (30, Gwahaksandan 1-ro 60beon-gil, Gangseo-gu, Busan, 46742 Korea) *tehong@kbsi.re.kr

Silicon carbide (SiC) is widely used in the production of high-voltage power semiconductors, and the implementation of high-voltage transistors requires ion implantation of various n-type and p-type dopants. Accurately identifying the distribution of implanted dopants is crucial for improving the performance of power semiconductors and preventing defects. However, it has been reported that during sputtering of ion-implanted SiC samples, slight variations in the energy distribution of secondary ions occur. These variations can hinder the accuracy of analysis using secondary ion mass spectrometry (SIMS). Therefore, precise control of the energy slit position in SIMS is essential for accurate dopant distribution analysis [1-2].

In our study, we conducted experiments using nitrogen-implanted SiC samples to observe changes in matrix ion intensity depending on the energy slit position. Based on this experiment, we identified the optimal energy slit configuration for analyzing SiC power semiconductors. The energy slit optimization derived from this experiment is expected to serve as a critical reference for future dopant analysis and evaluation in various SiC power semiconductor applications.



Fig. 1 Depth profile results as a function of energy slit position

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Determining the Radius and Cone Angle of a Probe Tip Using an AFM Tip Characterizer

Young Bum Kim, Jin Chun Woo and Kyung Joong Kim*

Kims Reference Corp., Daejeon, 34129, Republic of Korea *kjkim@kimsreference.com

In the measurement of nano materials by atomic force microscopy (AFM), the measured size is different from the real value by the large offset value due to the radius and cone angle of the used tips. For the reliability of the AFM images by correction of the offset value, the radius and cone angle of the AFM tips should be well determined. A certified reference material (CRM) with a series of trenches having different trench widths from 10 nm to 200 nm was developed to determine the radius and cone angle of the AFM tips. The trench widths of the CRM could be traceably certified by high resolution transmission electron microscopy from the lattice constant of Si(110) plane in the Si(100) substrate. The radius of the tip can be determined in the trenches with the shallower trench depths than the half trench width. On the otherhand, The cone angle of the tip can be determined in the trnches with deeper trench depth than the half trench width. As a result, the radius and cone angle of the AFM tips can be determined from the certified trench widths of the CRM.

Sub-picoliter drug delivery into living cells

Jinwan Cho[†], Hyoju Choi[†], and Manhee Lee^{*}

Department of Physics, Chungbuk National University, Cheongju, Chungbuk 28644, Korea [†]Equally contributed to this work *mlee@cbnu.ac.kr

A novel micro-pipette designed for Scanning Ion Conductance Microscopy has been developed, with the capability of controlled pico-liter scale drug delivery. This micro-pipette utilizes the inversed current rectification, which allows for the selective and regulated release of substances [1]. We directly observe the release of liquid delivery using fluorescence microscopy, as illustrated in Fig. 1. Based on the fluorescence intensity, the amount of the released substance is carefully quantified, as presented in Fig. 2. This technology is suitable for on-demand delivery of sub-picoliter scale drug onto living cells, with significant contribution to microenvironment manipulation in the biological science and industry.



Fig. 1. Direct observation of liquid delivery via fluorescence Fig. 2. Delivered volume as a function of microscopy time

^[1] M. A. Oh, C. I. Shin, T. D. Chung, ACS Appl. Mater, Interfaces (2021), 13, 26748-26758

Study on Crystallinity and Phase Changes of NCA Cathode Material Using Advanced XRD Analysis

Sangyong Lee, Hee-Soo Kim, Juhyun Lee, Changwoo Byun*

Semiconductor Analysis and Development Team, Semiconductor Innovation Center, Advanced Institute of Convergence Technology (145 Gwanggyo-ro, Yeongtong-gu, Suwon-si, Gyeonggi-do, Republic of Korea) *byuncw@snu.ac.kr

Commonly known X-ray diffraction (XRD) analysis methods include Normal XRD, Grazing Incidence XRD (GID), and X-ray reflectivity (XRR). More advanced application methods encompass High Resolution XRD (HR, RSM, etc.), micro-XRD, In-situ Temp. XRD, and In-operando XRD.

The XRD equipment (Bruker, D8 DISCOVER) at the Advanced Institute of Convergence Technology can perform all the aforementioned analyses. Particularly, advanced analyses are feasible using In-situ Temp. XRD and In-operando XRD, which are applicable according to the characteristics of the sample.

In-situ Temp. XRD can analyze thin film samples in reflection geometry and is suitable for powder and sample holder sizes. The sample holder temperature ranges from -190°C to 600°C, and the internal atmosphere of the chamber can be air, inert gas, or vacuum (10^{-4} mbar).

In-operando XRD can analyze batteries such as pouch cells and coin cells in transmission geometry. It supports voltage ranges from -10V to 10V and current ranges from -1000mA to 1000mA.

To examine the crystallinity and phase changes of the NCA (LiNiCoAlO2) cathode material in response to temperature increase and charge-discharge cycles, the diffraction angles were measured and analyzed using the XRD at the Advanced Institute of Convergence Technology.



Figure 1. (a) In-situ Temp.(2D view) (b) In-operando(1D view waterfall display) data

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POSTER II



Optimal Mass Spectra Preprocessing to Extract Mass-Specific Features and Application to Classification

Jin Gyeong Son^{1*}, Hyun Kyong Shon¹, In-Ho Lee², Tae Geol Lee¹

¹Nanobio Measurement Group, Division of Biomedical Metrology, Korea Research Institute of Standards and Science, Daejeon 34113, Korea

²Material Property Metrology Group, Division of Chemical and Material Metrology, Korea Research Institute of Standards and Science, Daejeon 34113, Korea *corresponding author :yeskyoung@kriss.re.kr

Time-of-flight secondary ion mass spectrometry (ToF-SIMS), a type of mass spectrometry specialized for surface analysis, generates large amounts of fragment ions through sputtering, making data interpretation challenging. Conventional methods extract sample-specific peaks through dimensionality reduction such as principal component analysis (PCA) and non-negative matrix factorization (NMF). Recently, various methods have been proposed to improve the efficiency of data interpretation by applying machine learning algorithms and deep learning. All these approaches require data preprocessing, but most widely used software-based peak extraction methods are prone to bias and have difficulty to process large amounts of data at once. The mass segmentation method usually applied in machine leaning makes arbitrary intervals that create problem of non-peak regions being used for training. We propose a method for mass spectra preprocessing that is based on peak extraction but is not user dependent, non-dispersive to the data, and suitable for processing large amounts of data. Based on this approach, we applied tree-based algorithms such as decision tree and ensemble learning. Through which, we effectively categorized ToF-SIMS spectra according to plastic type and extracted relevant features for discrimination. The proposed method utilizes the hierarchical structure of decision trees to systematically analyze spectral data and identify characteristic patterns associated with different plastic types. Furthermore, by utilizing peak extraction techniques during data pre-processing, the extracted features retain interpretable information relevant to the chemical composition of the samples.

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Fabrication and Analysis of Electrode from Rapid Alkaline Depolymerization of PET into Na2TP with High Performance MXene (Ti3C2TX) on Nickel Foam Substrate for Hydrogen Evolution Reaction.

Rahul Ramkumar, Jung Woo Lee*

Department of Materials Science and Engineering, Pusan National University * Corresponding: jungwoolee@pusan.ac.kr

A civilization's technological advancement relies heavily on its ability to effectively utilize its energy resources. Consequently, there is an increasing urgency in the contemporary era to enhance the search for high-performance non-noble metal hydrogen production methods, alongside a critical need to address the mounting issue of polyethylene terephthalate (PET) waste.

In recent times, MXenes, denoted by the naming convention Mn+1XnTx, have garnered significant attention as efficient electrocatalysts for electrochemical reactions. They exhibit promising potential in the hydrogen evolution reaction (HER) due to their structural robustness, expansive surface area, and impressive electrical conductivity. Concurrently, the utilization of small organic molecules has opened significant avenues in the energy sector owing to their environmentally friendly nature, sustainability, and cost-effectiveness, sourced from a variety of outlets. The functionalization of these compounds with MXene material has shown improved performance in HER evolution.

In this study, we propose a novel approach by employing a MXene material, specifically $Ti_3C_2T_X$, deposited on a nickel foam substrate, in conjunction with disodium terephthalate (Na₂TP) derived from the swift microwave alkaline hydrolysis of PET waste. PET depolymerization methodologies have undergone extensive scrutiny, and among them, alkaline hydrolysis stands out for yielding a product amenable to electrochemical applications. As anticipated, the $Ti_3C_2T_X/Na_2TP$ composite on nickel foam (NF) demonstrates superior electrocatalytic performance for HER compared to bare nickel foam and $Ti_3C_2T_x$ on nickel foam configurations.

The resultant electrode architecture, characterized by a sandwich-like structure, proves advantageous for fostering an augmented contact interface and enhanced pathways for electron migration during electrolysis. Additionally, it exhibits low overpotential, high stability, and minimal resistance, thus laying a foundation for the advancement of MXene-derived electrocatalysts for HER while expanding their potential applications. In essence, this study underscores a dual-purpose approach: repurposing waste PET through alkaline hydrolysis into a valuable precursor and integrating it with MXene on nickel foam for hydrogen energy generation.

Key words: Electrocatalyst, Electrode, Hydrogen Evolution Reaction, PET Alkaline hydrolysis, MXene

LDI-TOF Mass Spectrometry for Composition Differentiation of Transition Metal Dichalcogenides

TaeWan Kim, Song Byeong Heon, Seungjae Lim, Jae-Ung Lee and Jooyean Oh

ASTA Inc., 7th FL. AICT Bldg, A, 145, Gwanggyo-ro, Yeongtong-gu, Suwon-si, Gyeonggi-do, Korea *twkim@astams.com

Transition Metal Dichalcogenides (TMDs) are important materials in nanotechnology and electronics, with properties that can vary significantly depending on their composition. This study presents a method for rapidly distinguishing the compositions of various TMDs using Laser Desorption/Ionization Time-of-Flight (LDI-TOF) mass spectrometry.

TMDs exhibit a range of electrical properties, including semiconductor, metal, or insulator characteristics, which can greatly influence their physical and chemical properties based on composition. The study demonstrates that LDI-TOF mass spectrometry can clearly differentiate mass spectra based on the composition of TMDs, allowing for the rapid identification of individual components even in complex mixtures.[1]

The LDI-TOF technique offers high mass resolution and fast analysis speed, making it particularly advantageous for quickly distinguishing between different TMD compositions. This capability represents a significant advancement in analytical methods, providing essential and timely information that accelerates research and development in nanotechnology and electronic devices.

Thus, this research highlights the effectiveness of LDI-TOF mass spectrometry as a reliable and efficient tool for composition analysis of TMD materials, offering a valuable method for rapid and accurate analysis.

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2024년도 TC201 표면화학분석 국가표준 개발 성과 및 향후계획

손정효^{*}, 김영실

KOTITI시험연구원 KOTITI시험연구원 첨단융합산업본부(13840 경기도 과천시 과천대로8나길 48) *kim_ys@kr.kotiti-global.com

표면화학분석 분야는 반도체, 배터리, 디스플레이 등 첨단산업의 근간이 되는 기술로 표준개발이 중요 하다. 본 분야의 표준은 국제표준화기구(ISO/TC201)[1]에서 운영하는 국제표준(ISO)과 국가기술표준원 에서 운영하는 한국산업표준(KS)이 있다.

2024년 9월 기준으로 ISO/TC 201은 국제표준을 83개 제정하였고, 17개를 개발(제·개정) 중이다. 국내에 서는 2003년부터 국제표준을 채택하여 22개(22%)를 KS로 도입하였다. 향후 표면화학분석 분야가 더 활 성화되고 발전하기 위해서는 적극적으로 국제표준 개발에 참여하여 국내 기술을 국제표준에 적용함으로 써 선점 효과를 얻고, KS로 도입하여 산업계에서 쉽게 활용할 수 있도록 기반 강화가 필요하다.

KOTITI시험연구원은 표준개발협력기관(COSD)으로서 TC201분야의 KS 표준을 개발 및 관리하고 있 다. 이에 따라 2024년에는 한국표면분석학회와 협력하여 국가표준 5개(KS D ISO 14237, 14706, 14707, 15472, 17560)를 국제표준 개정에 따라 최신화하고, 용어 표준(ISO 18115-1, ISO 18115-2)을 개발 중이다. 향후 개발 표준은 E나라표준인증 사이트[2]를 통하여 누구나 활용할 수 있다. 특히 용어표준은 표면화학분 석 분야에 통합적으로 적용되는 만큼 파급력 및 활용성이 기대되는 바이다.

2025년에는 용어표준(ISO 18115-3)의 도입을 목표로 하고 있다. 또한, 국가표준 22개 중에 국제표준의 최신화 사항이 반영되지 않은 9개 표준에 대해서도 우선순위를 고려하여 개정할 계획이다. 본 분야의 전문 가 및 산업계의 관심과 참여가 필요하다.



^[1] ISO/TC 201, https://www.iso.org

^[2] https://standard.go.kr/

First Principles Study on CO2 Hydrogenation over Pd Catalysts: Elucidating the Role of C–O Bond Activation

Yejung Choi, Hyuk Choi, Ju Hyeok Lee, Jongseok Kim, Hyun You Kim*

Department of Materials Science and Engineering, Chungnam National University, Daejeon 34134, Republic of Korea *kimhy@cnu.ac.kr

Carbon dioxide (CO_2) is a prevalent greenhouse gas, significantly augmented by industrial emissions and fossil fuel combustion. Hydrogenation of CO_2 presents a viable strategy for mitigating atmospheric CO_2 levels by transforming it into clean fuels and hydrocarbons such as methane, formic acid, and C_2 + products. This study employs density functional theory (DFT) calculations to elucidate the hydrogenation mechanisms of CO_2 over Pd_{22} nanoparticles supported on MgO and CaO. We discovered distinct activation sites for H_2 and CO_2 ; H_2 activation occurs on the metal nanoparticles, while CO_2 activates at the interface between the oxide support and the metal nanoparticle. Moreover, our results indicate divergent reaction pathways on different oxide supports-specifically, carboxyl- and formate-mediated mechanisms on CaO and MgO, respectively. Such variation is attributed to the differential activation of the *C-O bond, which is influenced by the binding energy of CO_2 on the respective oxide supports. Notably, CaO demonstrates higher binding energy, correlating with enhanced *C-O bond strength in the adsorbed CO_2 molecular orbital states. These findings underscore the critical role of *C-O bond activation in the hydrogenation process and offer novel insights into the catalytic behavior under varying support conditions.

Key Words: CO₂ hydrogenation, Density Functional Theory, Activation of *C-O bond
Analysis of electron backscatter diffraction raw data, Kikuchi patterns, using machine learning

Kazuma Takeishi¹, Yoshihisa Matsumoto², Akiko N. Itakura³, Daisuke Hayashi¹, and Satoka Aoyagi^{1*}

¹Faculty of Science and Technology, Seikei University, Musashino, Tokyo 180-8633 Japan

²Depatment of Mechanical Engineering, National Institute of Technology, Oita College, 1666 Maki, Oita City 870-0152, Japan

³National Institute for Materials Science, 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan

*aoyagi@st.seikei.ac.jp

Electron backscatter diffraction (EBSD) provides detailed crystal information such as orientation and strain of a solid sample. EBSD is used to evaluate the crystal structure of various solid samples. Kikuchi diffraction patterns are generated from each measurement point on the surface of a solid sample depending on the crystal structure and the angle. Generally, the dominant Kikuchi bands in Kikuchi patterns are selected and then the crystal structures are identified. A pattern matching method based on the simulation of Kikuchi patterns from the type of crystal lattice of the assumed sample is now available from 2022. This method has increased the possibility of indexing complex regions that had been difficult to index in the past. However, problems remain in predicting unknown structures, because only the known crystal structures are simulated. For example, the minor crystal structures can be omitted. Therefore, the EBSD raw data (Kikuchi pattern at each measurement point) analysis method [1] has been developed to classify crystal structure groups over the measured area using unsupervised machine learning. In this study, the EBSD raw dataset of a pure vanadium sample with an average grain size of 110 μ m, a thickness of 0.5 mm, and a diameter of 18 mm was analyzed using principal component analysis, non-negative matrix factorization (NMF), and autoencoder. A marker for the image fusion process [2] was applied to a square area of approximately 329 μm x 487 μm using a Vickers hardness tester. Each pixel of the Kikuchi pattern map was treated as a variable and each pixel of the measurement area was treated as a sample in the data analysis. Since the data size was too large, the number of pixels in the Kikuchi bands was reduced before the data analysis.

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Effect of pixel binning on principal component extraction in PCA-based denoise of AES spectrum image

Fuyuki Nabeshima^{1*}, Konomi Ikita¹, Tatsuya Uchida¹, Kazushiro Yokouchi¹, Akihiro Tanaka¹, Toshiyuki Ohama¹, Kenichi Tsutsumi¹, and Noboru Taguchi²

¹JEOL Ltd., 3-1-2 Musashino, Akishima, Tokyo 196-8558, Japan ²National Institute of Advanced Industrial Science and Technology (AIST), Ikeda, Osaka 563-8577, Japan *fnabeshi@jeol.co.jp

Development of a spectrum imaging method for a commercially available Auger microprobe enlarges the range of application of Auger electron spectroscopy (AES) [1]. Multivariate analysis for spectrum image data cube is becoming increasingly important to realize faster data acquisition. A denoising technique based on principal component analysis (PCA) is a popular, fast and powerful tool as a preprocessing of spectrum image data cube. However, in the case of data with extremely low signal to noise ratio (S/N), artifacts are likely to occur. This is a significant issue especially in the AES spectrum image because Auger peaks appear in the large background.

In this study, we tried to suppress artifacts in PCA denoise by applying pixel binning in extracting principal component vectors from spectrum image data cube. Figure 1 shows SEI and spectra extracted from a spectrum image data cube of a gold electrode, which has organic and sodium compounds on the surface. Electron counts in each energy channel of the spectrum image data cube are typically 10-50 counts per pixel. The spectrum after denoising with standard PCA (orange line) is quite different from that of the raw data (blue line). As the binning size becomes larger, the spectrum becomes closer to the raw data, demonstrating suppression of artifacts in the denoise process. In the presentation, we will show the detail of the denoise process and also discuss the range of application of this method to AES spectrum image.



Fig. 1. (a) A secondary electron image (SEI) of island-like carbon on a gold substrate. (b) Spectra in the red rectangle area in (a) extracted from the raw and PCA-denoised data.

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Study on the correlation with the characteristic and role of inorganic films for LTPO TFT

Sera Kwon, Jung Min Bae^{*}, Mihyun Yang, So-Hyeon Yang, Hye Kyoung Park, Sang-Moo Park, Young Seok Choi

> LG Display, Production Technology Center, LG Display (245 LG-ro, Paju-si, 10845, Korea) *jungmin.bae@lgdisplay.com

OLED (Organic Light-Emitting Diode) 디스플레이 제품은 TV와 스마트폰 뿐 아니라 노트북, Tablet PC, 스마트 워치, 차량용 디스플레이 등 적용 영역을 점차 확대해나가고 있으며, 그에 맞춰 TFT (Thin-Film Transistor) 기술 또한 계속해서 개선되고 있다. 일반적으로 고해상도 디스플레이의 경우 미세 전류 컨트롤 이 중요하며 LTPS (Low Temperature Poly Silicon) TFT가 주로 활용되어 왔다. 그러나 공정 비용이 비싸 고 균일도가 낮다는 단점이 있어 대면적 적용에 한계가 있다. 반면 Oxide TFT의 경우 공정 비용이 저렴하 고 균일도가 우수하여 대형 OLED 패널에 활용되고 있으나, 여전히 낮은 이동도 및 신뢰성으로 인해 고해 상도 디스플레이 적용에 어려움을 겪고 있다. 최근 LTPS TFT와 Oxide TFT를 하이브리드한 LTPO TFT가 등장하며 스마트 워치 및 스마트폰 등 소형 프리미엄 OLED 제품을 중심으로 적용 영역을 확대하고 있다. LTPO TFT의 경우 구동부는 LTPS TFT로 구성하고 스위치 영역은 Oxide TFT를 적용하여 기존 LTPS TFT대비 누설 전류를 줄여 소비 전력을 크게 절감할 수 있다는 이점을 가지고 있다. 그러나 LTPS TFT와 Oxide TFT 공정을 위한 Mask 증가로 인하여 공정 비용 및 난이도가 높으며, LTPS/Oxide 간 열처리 온도 등 서로 다른 공정 방식으로 인해 소자 특성에 영향을 줄 수 있어 제작이 매우 까다롭고 수율이 낮다는 단점 이 있다. 특히 공정 중 상/하부 막에 영향을 미쳐 소자 특성 저하 및 불량 현상을 유발할 수 있어 막 물성에 대해 제대로 이해하는 것이 중요하다.

TFT 소자 내 무기막의 경우 외부 투습 방지, 상/하부 층 간 수소 침투 방지, 절연 등의 역할을 수행하는데, 이들 역할을 수행하기 위해서는 요구되는 막 물성이 서로 다르다. 이러한 막 물성은 가스 유량비, 증착 파 워, 압력, 온도 등 공정 조건에 의해 결정되는 요소이므로 원하는 막 물성을 얻기 위하여 공정 조건 제어가 필요하다. 본 연구에서는 공정 조건 조절에 따른 막 물성 변동 방향을 확인하였으며, 막 물성과 막 역할 간 상관관계를 도출하였다.

Peculiarities of XPS analysis of ScN based thin films

Stanislav Cichoň^{*}, Joris More-Chevalier, Michal Novotný and Ján Lančok

Institute of Physics, the Czech Academy of Sciences, Na Slovance 1999/2, Prague 18200 Czechia *e-mail: cichon@fzu.cz

ScN is an emerging medium width band gap semiconductor material for applications in the field of advanced electronic devices such as thermoelectrics, acoustic wave resonators, piezoelectrics and others [1-3]. It is a nitride with a cubic rocksalt structure and a very high melting point [4-6]. It is used either pure or in the form of ternary systems such as Al_xSc1-_xN [7]. ScN represents a borderline nitride between ionic nitrides and transition metal nitrides which is indeed reflected in its properties [8, 9]. ScN seems to be the only compound within the Sc-N binary system [10].

Chemical composition of ScN thin films can be easily elucidated by X-ray Photoelectron Spectroscopy (XPS). Many papers dedicated to the XPS of ScN can be found [11]. However, there are several intricacies associated with the XPS analysis and interpretation of ScN. They include: The Sc XPS knowledge base has been limited so far compared to other elements; Sc is very reactive which complicates the ScN fabrication and the subsequent analysis; The Sc 2p core level spectral region typically employed for the analysis comprises strong loss peaks and overlaps with the N 1s core level; Electrical charging may arise during XPS measurements; During depth profiling, the material is prone to sputtering damage which causes spectral distortions or artefacts; Adventitious carbon charge referencing can lead to misinterpretations [11].

We made structurally highly ordered ScN thin films with well-defined properties by high temperature sputter deposition. We show that employment of the binding energy position of the main peak component of N 1s as a means of a reference for binding energy calibration of measured spectra provides a viable approach for XPS interpretation and comparison of various ScN samples. These results are put into a wider context with other composition, structure and microstructure characterizations as well as characterizations of properties. The successful employment of the internal standard approach for binding energy corrections in our study suggests a more general feasibility of this approach.

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Evaluation of quantitative analysis of OrbiSIMS spectra using ANNbased supervised learning method.

Shun Shibayama¹, Anya Eyres², Jean-Luc Vorng², Gustavo F. Trindade, Ian S. Gilmore², and Satoka Aoyagi^{1*}

¹Faculty of Science and Technology, Seikei University, Musashino, Tokyo 180-8633 Japan 2National Physical Laboratory, Hampton road, Teddington, Middlesex, UK, TW11 0LW *aoyagi@st.seikei.ac.jp

Quantitative analysis using secondary ion mass spectrometry (SIMS) and mass spectrometry (MS) can be difficult due to matrix effects that change the intensity of ions from a particular material regardless of the concentration in a sample. Matrix effects greatly affect not only on the accuracy of quantitative analysis, but also on appropriate mass imaging, because mass imaging is based on the intensity of a target ion. Quantitative analysis by correcting matrix effects in mass spectra obtained with SIMS and some of the mass spectrometry methods has been investigated by applying an artificial neural network (ANN)-based supervised learning method to all mass peaks in each mass spectrum in Versailles Project on Advanced Materials and Standards (VAMAS) project TWA2 A31[1]. The previous study [1] mainly investigated time-of-flight secondary ion mass spectrometry (ToF-SIMS) spectra. In this study, the spectra obtained using OrbiSIMS [2] with an Orbitrap mass analyzer which has much higher mass resolution (approximately 240,000) than a ToF mass analyzer. Due to its high mass resolving power, OrbiSIMS detected a large number of mass peaks, which makes the mass spectra processing complex and difficult. We have developed a mass peak integration system that can include all of the automatically searched peaks for each OrbiSIMS spectrum. The data processing was written in Matlab (The Mathworks Inc., MA). The OrbiSIMS spectra of mixtures of organic electroluminescent (OEL) materials, such as Ir(ppy)3 and Alq3, were analysed using the ANNbased quantitative analysis system [1].

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Development of a hybrid quartz tuning fork-atomic force microscope combined with a scanning electron microscope

Jaehoon Sah¹, Seungtae Leem^{1,2}, Seungwon Choi^{1,2}, and Sangmin An^{1,2*}

¹Department of Physics, Research Institute of Physics and Chemistry, Jeonbuk Natioinal University, Jeonju 54896, Republic of Korea 2K-tip Corporation, Jeonju 54896, Republic of Korea *san@jbnu.ac.kr

The atomic force microscope (AFM) is a widely used instrument due to its remarkable versatility in analyzing the surface properties of materials. The quartz tuning fork-AFM (QTF-AFM), which employs a OTF as the probe for AFM, is known for its high sensitivity as a force sensor and simple electrical sensing system, making it suitable for use in various environments. This is made possible by the unique physical properties of the quartz Tuning Fork [1-3]. One of the valuable advantages of using a Quartz Tuning Fork in the AFM system is its ability to prevent jump-to-contact issues that can arise from high stiffness. This feature enhances the accuracy and safety of the AFM measurements. In contrast, the scanning electron microscope (SEM) excels at quickly obtaining high-resolution images of larger areas compared to AFM. However, SEM falls short in providing critical vertical (z-axis) three-dimensional information about the sample. To address this limitation, we introduce the development strategy for a hybrid SEM system that combines SEM with QTF-AFM. The approach involves designing an AFM combined SEM equipment by mounting a QTF on a piezo motor stepper capable of three-dimensional motion. The first thing that needs to be done within this hybrid systems is to see how the QTF unit behaves in a vacuum. We also need to investigate the interaction between the QTF unit and the electron beam. In this study, we focused on the behavior of QTF units with gold-coated Borosilicate tips and bare QTF without tips in the interaction between vacuum and electron beams. It was confirmed that the QTF's quality-factor increased as it went from normal pressure to vacuum, and the amplitude at the resonance frequency decreased when the electron beam touched the QTF unit. This suggests the importance of the QTF unit's mechanism in a hybrid SEM system that combines QTF-AFM.

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Formation of electrochemical solid/liquid interface with hygroscopic electrolyte for ambient pressure hard X-ray photoelectron spectroscopy

Beomgyun Jeong^{1*}, Cheolho Jeon¹, Sooan Bae², Benedikt P. Klein¹, Yasumasa Takagi³, Okkyun Seo³, and Jaeyoung Lee^{2*}

¹Research Center for Materials Analysis, Korea Basic Science Institute, 169-148 Gwahak-ro, Yuseong-gu, Daejeon 34133, Republic of Korea

²School of Environment and Energy Engineering, Gwangju Institute of Science and Technology (GIST), 123 Cheomdangwagi-Ro, Buk-gu, Gwangju 61005, Republic of Korea

³Center for Synchrotron Radiation Research, Japan Synchrotron Radiation Research Institute (JASRI), 1-1-1 Kouto, Sayo, Hyogo 679-5198, Japan.

*bjeong@kbsi.re.krandjaeyoung@gist.ac.kr

The ability to examine the electrode/electrolyte interface is essential for uncovering the underlying chemistry directly linked to electrochemical device performance. Ambient pressure hard X-ray photoelectron spectroscopy (AP-HAXPES) for electrochemical solid/liquid interfaces, using an ultra-thin liquid layer prepared by the dip-and-pull method, is one such technique. However, the bulk liquid reservoir required for this method can cause technical issues, such as splashing due to gas evolution or boiling from excessive pressure reduction, and the current response may not precisely represent the solid/liquid interface where XPS signals are obtained.

To overcome these challenges, we introduce an innovative method for preparing an electrochemical solid/liquid interface for AP-HAXPES through *in situ* hydration of a hygroscopic electrolyte, thereby eliminating the need for a bulk liquid reservoir. We validated this approach using the Pt/KOH(aq) interface under an anodic potential, observing the corresponding binding energy shift for the electrolyte species and Pt oxidation. This technique is expected to be particularly advantageous for studying gas- or water-sensitive electrochemical reactions in moisture-absorbing electrolyzers, gas sensors, and electrochemical gas (CO₂ and N_2) reduction cells.

Highly Sensitive Low Energy Inverse Photoemission Spectroscopy for the Unoccupied State Measurement of Organic Semiconductors

J.-A. Hong¹, K.-M. Lee¹, and Y Park^{1,2*}

¹Dept. of Physics, Kyung Hee University, 26 KyungHeeDae-ro, Seoul 02447, Republic of Korea ²Dept. of Information Display, Kyung Hee University, 26 Kyungheedae-ro, Seoul 02447, Republic of Korea *parky@khu.ac.kr

We have developed highly sensitive low energy inverse photoemission spectroscopy (LEIPS) apparatus employing parabolic mirror for better light collection for the purpose of measuring the LUMO positions of organic semiconductor materials. In combination with ultraviolet photoemission spectroscopy (UPS) for the HOMO measurement, we could determine the transport energy gap values of several organic electronic materials including pentacene and C60. In addition, with the improved LEIPS sensitivity, we were able to follow the evolution of the transport gap values as a function of organic film thickness on substrates with different surface work functions, and therefore the evolution of exciton binding energies. The implication of these results as well as the future prospect of transport gap measurements in various semiconductor materials will be discussed. Additionally, we will also discuss the strategy to further improve the sensitivity of LEIPS will be presented.

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Evaluation of the image fusion data of hydrogen distribution by operando hydrogen microscope and crystal structure distributions

Yuki Sano¹, Yoshihisa Matsumoto², Akiko N. Itakura³, Daisuke Hayashi¹, and Satoka Aoyagi^{1*}

¹Faculty of Science and Technology, Seikei University, Musashino, Tokyo 180-8633 Japan

²Depatment of Mechanical Engineering, National Institute of Technology, Oita College, 1666 Maki, Oita City 870-0152, Japan

³National Institute for Materials Science, 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan

*aoyagi@st.seikei.ac.jp

To understand the mechanism of hydrogen embrittlement in metals, it is necessary to investigate the relationship between the hydrogen permeation process and the crystal structures in metals. Image fusion of different analysis data, such as scanning electron microscope (SEM) and electron backscattered diffraction (EBSD), and time-course hydrogen distributions in metals using an operando hydrogen microscope (OHM) [2], is useful to evaluate important factors related to hydrogen embrittlement at once. Crystal information directly related to hydrogen permeation can be indicated by analyzing the fused images as a multimodal dataset using machine learning. In this study, vanadium, which is expected to be used as a hydrogen permeable membrane, has been studied as a model sample. Hydrogen distribution images obtained by electron stimulated desorption (ESD) and SEM and EBSD images were fused and then analyzed using unsupervised machine learning methods, such as principal component analysis (PCA) and multivariate curve resolution (MCR), to clarify the relationship between hydrogen permeation and crystal structures. The ESD image were measured with OHM every 150 seconds for 40 hours, and then every 30, 60, 90, or 120 min images were accumulated to obtain higher contrast hydrogen images. These ESD images were fused with EBSD images including inverse pole figure (IPF), Kernel Average Misorientation (KAM), band contrast, and Euler angle map images by rotation, cropping and transformation using image registration in Matlab (Mathworks Inc. MA). As a result the relationship between crystal structures and hydrogen permeation was indicated by analyzing the fused image dataset using PLS toolbox (Eigenvector Research Inc., WA) for PCA and MCR.

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Surface-Analysis Approaches to Elucidate Chromium Ion Adsorption on Glycoconjugate-derived Metallopolymer

Anuvasita Parikh¹, Parmeshthi Parikh¹, Rajashri R. Urkude², Ajay K. Sah^{1*}

¹Department of Chemistry, Birla Institute of Technology and Science, Pilani; Pilani Campus, Rajasthan 333031, India. Tel: +91-1596-515662, Fax: +91-1596-244183

²Beamline Development & Application Section, Bhabha Atomic Research Center, Trombay, Mumbai 400085, India *asah@pilani.bits-pilani.ac.in

The interaction of cupric ions with imine derivatives of 4,6-*O*-ethylidene- β -_D-glucopyranosylamine (Fig. 1) results in the formation of a range of complexes, from mono- to tetranuclear assemblies. Various analytical techniques, including single-crystal X-ray diffraction studies, have characterized these complexes. The crystal structures of the complexes reveal mainly square planar and square pyramidal geometry about the metal center, which are influenced by the solvent system and crystallizing conditions.^{1,2} Notably, the ditopic ligand [bis-(4,6-Oethylidene-*β*-D-glucopyranosylamine)-1,4-dihydroxy-2,5dibenzylidene (H₆L)] reacts with Cu(OAc)₂ under various conditions to produce an amorphous one-dimensional (1D) polymeric complex, denoted as (Cu₂H₂L)_n. Field emission scanning electron microscopy (FESEM) of this material reveals rough, pitted surfaces, suggesting its



potential for heavy metal ion absorption. Considering the harmful effect of heavy metal pollutants, we evaluated the effectiveness of $(Cu_2H_2L)_n$ in adsorbing various heavy metal ions from aqueous solutions. The material demonstrated superior adsorption performance for Cr(III) ions. To further elucidate the adsorption mechanism of Cr(III) onto $(Cu_2H_2L)_n$, we employed a range of analytical techniques including powder X-ray diffraction, Raman spectroscopy, X-ray photoelectron spectroscopy, scanning transmission electron microscopy, time-of-flight secondary ion mass spectrometry, and Cr K-edge X-ray absorption spectroscopy (XANES/EXAFS) (Fig. 2).³ These analyses provide comprehensive insights into the molecular interactions involved in Cr(III) adsorption on $(Cu_2H_2L)_n$, underscoring its potential as an effective material for targeted environmental remediation.

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CO cryo-sorption as a surface-sensitive spectroscopic probe of the active site density of single-atom catalysts

Benedikt P. Klein^{1,2}, Beomgyun Jeong^{1*}, Hafiz Ghulam Abbas³, Geunsu Bae⁴, Adith Ramakrishnan Velmurugan³, Chang Hyuck Choi⁴, Geonhwa Kim⁵, Dongwoo Kim⁵, Ki-jeong Kim⁵, Byeong Jun Cha⁶, Young Dok Kim⁶, Frédéric Jaouen⁷, Reinhard J. Maurer², and Stefan Ringe³

¹Korea Basic Science Institute, 169-148 Gwahak-ro Yuseong-gu, Daejeon 34133, Korea

²Department of Chemistry, University of Warwick, Gibbet Hill Road, Coventry CV4 7AL, United Kingdom

³Department of Chemistry, Korea University, 145 Anam-ro, Seoul 02841, Korea

⁴Department of Chemistry, POSTECH, 50 Jigok-ro 127beon-gil, Pohang 37673, Korea

⁵Pohang Accelerator Laboratory, POSTECH, 80 Jigok-ro 127beon-gil, Pohang 37673, Korea

⁶Department of Chemistry, Sungkyunkwan University, 2066 Seobu-ro, Suwon 16419, Korea

⁷ICGM, University of Montpellier, 1919 route de Mende, 34293 Montpellier, France *bjeong@kbsi.re.kr

A reliable way to quantify the number of active sites in a catalyst is crucial to evaluate its performance. One option to achieve the quantification is to utilize selectively adsorbing gas molecules as a probe to identify the catalytically active sites. Once the molecules are adsorbed on the active sites, their surface density can be determined by using spectroscopic techniques. For this approach it is necessary to identify the probe molecules according to their spectroscopic features, a task much helped by the computational simulation of spectra.

In our work, we apply this method to determine the active site concentration of iron-nitrogen-carbon FeNC electrocatalysts for the oxygen reduction reaction (ORR). We present an *in situ* X-ray spectroscopy study for the cryo-adsorption of CO on an FeNC catalyst under near-ambient gas pressure. Using Near edge X-ray absorption fine structure (NEXAFS) spectroscopy, we could detect the adsorbed CO gas molecules on the catalyst surface, and correlate the NEXAFS to the X-ray photoelectron spectroscopic quantification for calculating the ORR active site density. Our state-of-the-art density functional theory (DFT) calculations reaffirm the spectroscopic fingerprint of the CO molecules specifically adsorbed at Fe-N₄ sites, provide the correlation between the NEXAFS and XPS quantifications, and enable additional structural insights to explain the low CO adsorption temperature.

Ultra-high Breakdown Field of Ga₂O₃ Film via Nozzle Tilting of Aerosol Deposition Method

Jun-Woo Lee, Jwa-Bin Jeon, Ki-Seop Lee, Sang-Mo Koo, Won Ho Shin, Jong-Min Oh*

Department of Electronic Materials Engineering, Kwangwoon University, Seoul 139-701, Republic of Korea *jmOH@kw.ac.kr

Recently, power semiconductor devices play a crucial role in modern electronic systems, efficient power management, and conversion. They are applied in various fields such as renewable energy systems and electric vehicles. The most important property of power semiconductor materials for the reliability and energy sustainability of these applied devices is high breakdown electric field strength. Gallium oxide (Ga₂O₃) is being researched as a promising material for power semiconductor applications due to its high breakdown electric field strength (~8 MV/cm), following GaN and SiC. Various processes such as physical vapor deposition and chemical vapor deposition are applied to fabricate Ga₂O₃ films, but these processes require long deposition times, high-temperature treatments, and significant costs. Despite this, achieving a high breakdown electric field strength above 3 MV/cm is extremely challenging. Therefore, in this study, we used the aerosol deposition (AD) process to rapidly produce thick Ga_2O_3 films at room temperature (~460 nm/min) and analyzed the effect of oxygen vacancies on microstructure, dielectric properties, and electrical characteristics through post-annealing at different temperatures to determine the optimal post-annealing temperature. Additionally, we fabricated dense and uniform Ga₂O₃ films using the AD nozzle tilting method and achieved a very high breakdown electric field strength through optimal post-annealing. This indicates that the thick Ga₂O₃ films produced by AD can ensure reliability in high-voltage environments for power semiconductor devices and capacitors.

CsPbBr₃/Al₂O₃ composite; Large-scale synthesis; Thermostability; Green-emitting phosphor

Seok-Hun^{1*}, Sunghoon Kim¹, and, Jong-Min Oh²

^{*1}Department of Applied Chemistry, Dong-Eui University, Busan 47340, Republic of Korea ²Department of Electronic Materials Engineering, Kwangwoon University, Seoul 01897, Republic of Korea hoon@deu.ac.kr (S. K.), jmOH@kw.ac.kr (J.-M. O.)

Metal halide perovskite materials [1] have garnered significant attention for their optoelectronic properties, particularly in displays, due to their high quantum efficiency [2] and narrow emission spectrum [3]. Among them, colloidal perovskite quantum dots [3,4] exhibit superior emission characteristics but suffer from poor thermal stability. This study explores the development of a CsPbBr₃-based green-emitting phosphor, leveraging submicron-sized Al₂O₃ particles as a support, focusing on a scalable synthesis method that achieves high photoluminescence (PL) efficiency and enhanced thermal stability for use in white LED packages. Two synthesis methods were employed: the solvent-free mechanochemical reaction method (MRM) [5,6] and the dissolution-evaporation method (DEM) [7] representing dry and wet approaches, respectively. Notably, the DEM method produced monoclinic CsPbBr₃/Al₂O₃ powder with a superior PL quantum yield compared to MRM method, maintaining over 90% of its initial PL intensity after 15 days at 200 °C. This composite powder was successfully utilized as a green phosphor in a white LED package, combined with red phosphor (K₂SiF₆:Mn⁴⁺), achieving a luminous efficiency of 25 lm W⁻¹ and a wide color gamut of 112.4% NTSC standard. These findings indicate the potential for cost-effective commercial applications CsPbBr₃/Al₂O₃ composites in advanced, thermally stable optoelectronic devices.

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Enhancing the Initial Nucleation Behavior of ALD-Iridium Thin Films via a Surface Pretreatment Process

Myung-Jin Jung and Se-Hun Kwon*

School of Materials Science and Engineering, Pusan National University, Busan 46241, South Korea *Correspondence : sehun@pusan.ac.kr (S.-H. Kwon)

Iridium (Ir) has low figure of merit ($\rho 0 \times \lambda$) and high melting temperature properties, so it has been recently spotlighted as a very important copper (Cu) alternative interconnect material in next-generation semiconductor devices. In particular, in the case of depositing a thin film using atomic layer deposition (ALD) technology, it can be expected to deposit extremely thin film with conformal, uniform and excellent step coverage characteristics even in a very complex structure or a trench structure of several nm dimension due to the inherent self-limiting characteristic of ALD. In this regard, ALD-Ir is considered as one of the most suitable metallization processes for the application of advanced semiconductor interconnects. Therefore, considerable efforts have been conducted to develop a reliable ALD-Ir process having improved film qualities. And, ALD-Ir process with excellent thin film properties such as low electrical resistivity and negligible oxygen impurities was recently reported using Tricarbonyl (1,2,3- η)-1,2,3-tri(tert-butyl)-cyclopropenyl iridium (C₁₈H₂₇IrO₃ or TICP) precursor and oxygen [1]. However, in the case of this TICP precursor, it was difficult to deposit extremely thin and continuous Ir films on the hydroxyl-terminated oxide layer due to its long incubation delay.

Therefore, in this study, a method for depositing a very thin, uniform and continuous ALD-Ir thin film with low resistivity even on oxide materials was explored by reducing the incubation period and promoting nucleation using various surface pretreatment conditions. In addition, the nucleation behavior as well as film properties of ALD-Ir on the oxide material were systemically compared and analyzed according to the surface pretreatment conditions, and finally, ALD-Ir thin film with excellent properties on the oxide surface was obtained.

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Evaluation of PEALD AI2O3 according to deposition temperature for thin-film transistor applications

Hojeong Jo, Ji-Min Park, Jihyeon Min, Hyun-Suk Kim*

Dept.of Energy and Materials Engineering, Dongguk University, 30 Pildong-ro 1(St), Jung-gu, Seoul 04620, Korea *E-mail: khs3297@dongguk.edu

Thin-film transistors (TFTs) are one of the essential devices in modern industry, that serves as switching or driving devices. Gate dielectric, one of the components of TFTs, electrically and physically separates the gate electrode and the active, and plays a role in forming a channel by attracting carriers induced by according to the gate voltage. The higher the dielectric constant of the gate dielectric, the more charges it can attract, thus ensuring a higher drain current in TFTs. Conventional gate dielectrics such as SiO₂ have excellent leakage current characteristics, but their relatively low dielectric constant makes them unsuitable for modern electronic devices. Aluminum oxide (Al₂O₃) is well-known high dielectric constant materials that can be fabricated by various process, such as chemical vapor deposition, sputtering, and atomic layer deposition (ALD).

ALD based on a self-limiting mechanism enables precise thickness control at the atomic layer level and provides high-quality thin films with excellent step coverage. ALD process can largely divided into thermal ALD and plasma enhanced ALD (PEALD). Compared to thermal ALD, PEALD offers several notable advantages: (1) PEALD enables film deposition at lower temperatures because the plasma can break down precursor molecules to create reactive compounds, which promote surface reactions even at lower temperatures. (2) PEALD tends to produce higher quality films as the plasma helps in removing impurities and does not use reactants containing hydrogen. These benefits make PEALD a promising method for applications in cutting-edge highly integrated circuits or 3D structural devices.

In this study, Al₂O₃ was deposited by PEALD process at three different temperatures: 150°C, 200°C, and 250°C. Electrical and dielectric properties of PEALD Al₂O₃ were evaluated in metal-insulator-metal (MIM) devices. Following to this, IGZO TFTs were demonstrated with PEALD Al₂O₃ as gate dielectrics. These results highlight the need for precise control of gate dielectric deposition temperature in PEALD process and TFT applications, providing valuable insights for improving the performance of various electronic devices.

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Impurity Reduction Leading to Enhanced Properties in Atomic Layer Deposited Ru Films by Introducing Additional Reactant for Cu Alternative Interconnects

Jeongha Kim^{1*}, Yeseul Son¹, Sang Bok Kim¹, Tae Eun Hong³, Jong Seong Bae³, Soo-Hyun Kim^{1,2*}

¹Graduate School of Semiconductor Materials and Devices Engineering, Ulsan National Institute of Science and Technology (UNIST), Ulsan 44919, Republic of Korea

²Department of Materials Science and Engineering, Ulsan National Institute of Science and Technology (UNIST), Ulsan 44919, Republic of Korea

> 3Korea Basic Science Institute (KBSI) 618-230, Gangseo-gu, Busan 46742, Republic of Korea *Corresponding. soohyunsq@unist.ac.kr

This study investigates a 6-step Ru ALD process as shown in Figure 1, to achieve high-quality Ru thin films even at high temperatures where precursor decomposition occurs. Compared to the basic 4-step process using Ru(TMM)(CO)₃ precursor and O₂ reactant, the 6-step process with NH₃ as an additional reactant gas results in improved properties such as reduced resistivity, enhanced crystallinity, and decreased impurities. Both processes were evaluated at a Ru thickness of 25 nm and this thickness was measured using Scanning Electron Microscope (SEM). To examine the impact of NH₃ injection on impurity concentration within the thin films, Secondary Ion Mass Spectrometry (SIMS) analysis was performed. SIMS results showed that the concentrations of C and O impurities in the Ru films decreased from 1.5 at.% to 0.3 at.% (Figure 2). This can be explained by the effective reduction of impurities when NH₃ is injected at high temperatures, where precursor decomposition occurs. Additionally, X-ray Diffraction (XRD) analysis confirmed improved crystallinity, and the resistivity of the thin film decreased from 20.1 $\mu \Omega \cdot cm$ to 13.4 $\mu \Omega \cdot cm$. In conclusion, SIMS depth profiling confirmed the reduction of impurity concentrations in the Ru thin film, which contributed to the improvement in film properties, including the decrease in resistivity.



Figure 1. Schematics of the 6-step Ru ALD process

Figure 2. SIMS elemental concentration depth profiles for Ru, C, O, and N signals for the 4–step Ru ALD film and the 6–step Ru ALD film.

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3D integration of CMOS inverters composed of IGZO and Te through a via-hole-less structure

Dong Bin Lee, Seong Cheol Jang, and Hyun-Suk Kim*

Dept.of Energy and Materials Engineering, Dongguk University, 30 Pildong-ro 1(St), Jung-gu, Seoul 04620 *E-mail: khs3297@dongguk.edu

A complementary metal oxide semiconductor (CMOS) inverter is a fundamental component in complex integrated logic circuits, which rely on both p-type and n-type thin-film transistors (TFTs). Although some studies have explored inverters made solely with n-type TFTs, these designs tend to suffer from drawbacks such as low output swing, small input capacitance, high power dissipation, and poor noise margin. Organic materials and metal chalcogenides have been proposed for high-performance p-type TFTs, but their fabrication processes or inherent physical properties are not well-suited for advanced CMOS inverters. Therefore, to achieve high-performance CMOS inverter logic circuits, a high-quality p-type semiconductor with a straightforward fabrication process is essential.

Three-dimensional (3D) integration is a cutting-edge technology that offers reduced system size, shorter interconnects, lower packaging costs, and the ability to integrate various devices. As Moore's Law approaches its limits, the importance of 3D integration technology is growing. Various methods exist for 3D integration, such as wire bonding and 3D through-silicon via (TSV). While wire bonding is an affordable and well-established process, it is limited to the edges of the die, requires an interlayer, offers low freedom in chip connections, and is prone to RC delay. In contrast, 3D-TSV technology provides a smaller footprint, improved silicon efficiency, reduced RC delay, and lower power consumption. However, 3D-TSV is largely confined to silicon semiconductors and faces challenges when applied to other semiconductor materials. A novel approach, 3D via-hole-less integration, is a multilevel system that avoids the use of etchants, enables simultaneous metal interconnections, minimizes damage to underlying devices, and is highly compatible with various substrates.

In this study, 3D integration of CMOS inverter with n-type IGZO and p-type Te were demonstrated. All processes were based on vacuum processes, and all actives were fabricated using sputtering. Optimization and evaluation were performed for various component such as active, gate dielectric, electrodes, and interlayer dielectrics. Finally, the characteristics of CMOS with planar structure and 3D via-hole-less structure were compared.

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Development of highly conductive NbC_x thin films using PEALD for diffusion barrier applications in Cu and Ru interconnects

Chaehyun Park¹, Minjeong Kweon¹, Sang Bok Kim¹, Jong-Seong Bae², Tae Eun Hong², Soo-Hyun Kim^{1*}

¹Graduate School of Semiconductor Materials and Devices Engineering, Ulsan National Institute of Science and Technology (UNIST), Ulsan, Republic of Korea

²Busan Center, Korea Basic Science Institute, 30, Gwahaksandan 1-ro 60beon-gil, Gangseo-gu, Busan, 46742, Republic of Korea *corresponding author: soohyunsq@unist.ac.kr

In this study, niobium carbide (NbC_x) thin films were successfully grown using plasma-enhanced atomic layer deposition (PEALD) with a new liquid niobium precursor and H₂ plasma reactant. X-ray diffraction (XRD) analysis confirmed the formation of crystalline NbC. The resistivity of the as-grown film was around 260 $\mu \Omega$ -cm, attributed to the 20 at.% oxygen impurities detected by RBS analysis [Fig 1a]. To optimize the deposition conditions, we systematically varied the process temperature and plasma power. The composition and bonding status of the films were analyzed using secondary ion mass spectrometry (SIMS) and x-ray photoelectron spectroscopy (XPS). Figure 1b shows SIMS analysis of NbC_x film at optimized conditions, revealing elemental distribution. Figure 1c presents XPS spectra of NbC_x films, highlighting Nb-C and Nb-O bonding as functions of temperature and plasma power. By establishing the optimal processing conditions, we achieved low oxygen impurity and highly conductive NbC_x films with a resistivity of approximately 100 $\mu \Omega$ -cm. We applied the ALD-NbC_x films to a diffusion barrier for Cu and Ru interconnects and the results will be presented at the conference.



Figure 1. (a) RBS spectra of NbC_x film deposited on Si substrate at basic conditions with 2 MeV He²⁺ incident energy. (b) SIMS depth profiles of NbC_x film deposited at optimized conditions. (c) XPS spectra of the ALD–NbC_x films as a function of the temperature and plasma power

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Highly Breathable and Stretchable Temperature Sensor Using Mesh-Shaped Textile and Partially Reduced Graphene Oxide

Hyun Jin Kand and Jung Woo Lee*

Pusan National University, Busandaehang-ro 63 beon-gil 2, Geumjeong-gu, Busan, 46241, Korea *jungwoolee@pusan.ac.kr

The global digital healthcare market is growing rapidly due to factors such as population increase, aging demographics, and the rise of infectious diseases like COVID-19 [1]. Consequently, there is a growing interest in wearable devices for health monitoring [2]. Body temperature, being one of the most fundamental indicators of our body's condition, is critical as both hypothermia and high fever can lead to severe health issues. Therefore, real-time body temperature monitoring has become increasingly important. However, traditional thermometers are often rigid and bulky, making continuous real-time monitoring on the skin challenging. Although polymer-based flexible sensors are commonly used to address this issue [3-4], they often have low breathability, causing sweating and discomfort during extended wear. This underscores the need for a temperature monitoring device that is soft, lightweight, and breathable.

In this study, we developed a partially reduced graphene oxide on a mesh-shaped textile temperature sensor (PMTT) that allows long-term monitoring of body temperature in real-time by taking advantage of the breathability and stretchability of textiles. The PMTT showed excellent breathability, good washability, outstanding stretchability, decent sensitivity, high linearity, and fast response time. Additionally, it could be attached to the human skin, making it possible to use it for wearable applications. Moreover, by integrating a Wi-Fi module, the PMTT enables wireless monitoring, further enhancing its potential for remote healthcare applications.

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Effect of density and crystal structure of InOx samples on D-SIMS depth profiles

Ki-Cheol Song^{1,2}, Jung-Hyeon Yoon¹, Seong-Hwan Ryu², Jin-Seong Park², and Yeonhee Lee^{1*}

¹Advanced Analysis and data Center, Korea Institute of Science and Technology (KIST) ²Division of Materials Science and Engineering, Hanyang University *T23871@kist.re.kr

In this study, the effect of the density and crystal structure of InOx thin film on the SIMS analysis result was investigated. The InOx (Indium oxide) samples on a silicon wafer were prepared by ALD (Atomic Layer Deposition) method. During the thin film deposition process, H₂O, O₃, and O₂ plasma were used as a reactant, respectively, and the deposition temperature of thin film was changed by 50°C from 100 to 250°C.

In order to analyze the light element in the sample in the depth direction, depth analysis was performed using the Magnetic sector-SIMS (IMS 7F-Auto, CAMECA) equipment. During the analysis it was investigated that the sputter rate varies depending on the crystallinity and density of the thin film. In order to check whether the change in the sputter rate affects the RSF (Relative Sensitivity Factor), a light element quantitative analysis was performed using RBS and ERD technique. The results of the quantitative analysis and the RSF calculated from the result were compared, and finally, RSF values were obtained using different sputter rate, the density of the thin film, and the crystal structure and they were compared.

It was investigated that the interface profile between the substrate and the thin film changed as the reactant changed. To investigate the change in the ionization rate, the total intensities were compared using TOF-SIMS analysis, and the analysis results of AES were also compared to investigate the effect of reactant on the interface between the substrate and the thin film.

Research on Silicon Oxynitride Thin Films Deposited by PECVD Processes with Low-GWP Gas

Woo Cheol Jang, Tae Joo Shin*

Ulsan National Institute of Science and Technology, UNIST (50, UNIST-gil, Ulsan 44919, Republic of Korea) *tjshin@unist.ac.kr

Silica-based Dielectrics are the basis of the current semiconductor industry. Plasma-enhanced Chemical Vapor Deposition(PECVD) is a prominent method for producing thin films. The precursor utilized in this process, Nitrous $Oxide(N_2O)$ gas, is a significant contributor to global warming that impedes international efforts toward sustainable development. To replace this N_2O precursor, an alternative method is developing with Nitric Oxide(NO) gas.

Silicon Oxynitride(SiON) is a particularly attractive material because its properties can be customized tailored by varying the composition ratio of the components that comprise the thin film. In this study, SiON thin films were deposited with N_2O and NO gas precursors and then compared for physical properties such as FT-IR, XRR, XPS, Ellipsometry and TOF-SIMS, insulation performance by dielectric property measurements.



Figure 1. (a) Chemical bond analysis by FT-IR and (b) peak deconvolution data from XPS of Silicon Oxynitride thin films.

Controlled Reduction of the Graphene Oxide for Temperature Sensing

Yeong Jun Yun and Jung Woo Lee*

Pusan National University, 2, Busandaehang-ro 63 beon-gil, Geumjeong-gu, Busan, 46241, Korea *jungwoolee@pusan.ac.kr

In a pandemic like the COVID-19 outbreak that has swept the world, temperature measurement is the quickest way to determine the presence of an outbreak. The importance of body temperature monitoring system is becoming increasingly important as society ages and the number of cancer patients increases.

However, conventional thermometers are rigid and heavy, making it difficult to monitor body temperature for a long period of time and in real time, and the metal used in commercial temperature sensors has low sensitivity. Therefore, there is a need for a body temperature monitoring device that is soft, lightweight, and can read body temperature precisely and accurately.

Therefore, we have developed a temperature sensor based on PrGO(Partially reduced Graphene Oxide). GO (Graphene Oxide) is made by partially breaking the sp^2 bonds of graphene into sp^3 bonds. Structurally, there are oxygen functional groups on the top and ends of graphene, which act as electron trap sites and are removed as they are reduced. Therefore, controlling the degree of reduction from GO to reduced rGO(reduced Graphene Oxide) changes the properties of the material.

In this study, we used the flash reduction method to understand how the properties of the material change depending on the flash energy applied to GO, and finally produced a flexible and lightweight temperature sensor with superior sensitivity compared to commercial metal temperature sensors. The fabricated temperature sensor shows good flexibility, reversibility, high sensitivity, good linearity, long-term stability, and fast response time.

Key words: Graphene Oxide, Flash reduction, Temperature sensor, flexible, Reduction control

Crystal Structure Determination of Coordination Polymers Using Combined Computational Simulation and Powder XRD Analysis

Sung-Chul Kim, Byeong-Hyeon Lee, Junho Ha, Min-Sung Bae, and Sung Ok Won*

Advanced Analysis and Data Center, Korea Institute of Science and Technology, 5, Hwarang-ro 14-gil Seongbuk-gu Seoul, 02792, Republic of Korea *sowon@kist.re.kr

In this study, we introduced an enhanced approach combining computational simulations and powder X-ray diffraction (XRD) analysis to accurately determine the crystal structures of coordination polymers, which are challenging to crystallize as single crystals. Since X-rays primarily interact with electrons, the inherent weak diffraction signal from the organic components complicates XRD analysis. Furthermore, the presence of thermal vibrations in ligands and low crystallographic symmetry results in complex diffraction patterns, making initial structure modeling particularly difficult. To address these challenges, computational simulations were employed to predict the thermodynamically stable positions of atom clusters, which served as the initial models for XRD analysis. The rigid body method and simulated annealing techniques were then applied to refine the atomic positions. Finally, Rietveld refinement was performed to obtain the final crystal structure, which was subsequently validated for structural stability using molecular dynamics calculations. This integrated analytical approach holds significant potential for advancing the structural analysis of various coordination polymers.

Analysis of ZnO/HfO₂ thin film grown Discrete Feeding Method using ToF-SIMS and GIXRD

Haegyeong Kim¹, Eun Jeong Ok¹, Ji Yeong Sung², Tae Joo Shin^{1*}

¹Graduate School of Semiconductor Materials and Devices Engineering, UNIST ²Busan center, Korea Basic Science Institute (KBSI) Ulsan National Institute of Science and Technology, 50, UNIST-gil, Ulsan 44919, Republic of Korea tjshin@unist.ac.kr*

Atomic layer deposition (ALD) is a technology that forms a thin film layer by depositing the desired material on the surface of the substrate in atomic layers. The deposition process can be performed at relatively low temperatures and is characterized by excellent step coverage.[1]

ALD is a process comprising four stages: precursor injection, precursor purging, reactant injection, and reactant purging. The precursor and reactant are introduced sequentially, allowing for the deposition of a mono layer of atoms (or molecules) with each cycle. The limitation of subsequent molecular adsorption is a consequence of the inability of a precursor to react where it has already done so. This process allows for precise control of the film thickness at the atomic level, a phenomenon known as 'Self-limiting surface reaction'.[1]

However, in actual ALD reactions, steric hindrance and screening effects are present, impeding the chemical adsorption of precursor molecules. This can result in the precursor molecules being unable to cover the substrate surface effectively, leading to the formation of thin films of inferior quality.

Discrete feeding ALD (DF-ALD) can be employed to enhance the quality of thin films by effectively eliminating physisorbed precursor molecules and by-products. DF-ALD permits a specific number of individual precursor injections/precursor purges without modifying the overall process time.[2]

In this study, the impurities present in ZnO/HfO₂ thin films deposited by the DF-ALD process were analyzed using a combination of techniques, including time-of-flight secondary ion mass spectrometry (ToF-SIMS) depth profiling, Orbitrap-SIMS. Grazing incidence X-ray diffraction (GIXRD) analysis was conducted to assess the uniformity of the thin films produced using the DF-ALD process.

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Fabrication of Titanium Carbonitride (Ti₃CN) MXene Quantum Dots for Optical Detection of Fe³⁺ ions

Annas S. Ariffin, Anir S. Sharbirin, Afrizal L Fadli, Jeongyong Kim*

Department of Energy Science, Sungkyunkwan University, Suwon 16419, Korea *Email: j.kim@skku.edu

MXene Quantum Dots (MQDs), a zero-dimensional nanomaterial derived by fragmenting the twodimensional MXene to a quantum size (typically <10 nm) have earned a lot of attention lately [1]. This burgeoning quantum material, possess an exceptional quantum effect such as remarkable photoluminescence (PL) [2] excellent photostability, biocompatibility and dispersion stability [3]. MQDs have been applied in vast fields of applications, including fluorescence sensing. The presence of Fe^{3+} is crucial in natural environmental and biological system, but the overabundance and deficiency of these ions could lead adverse effect on health [4]. Thus, a quick, reliable and accurate detection systems for Fe^{3+} ions are in demand. While various reported work on applying MODs for sensing Fe (III) have been reported before by using Ti3C2 MXene [5], reported on another group of MXene such as carbonitride (CN) MXene has been lacking. CN MXene which has been reported to possessed enhanced physical and electronic properties due to stronger Ti-N bond and stability owing to presence of carbon and nitrogen atoms [5] could potentially demonstrate enhanced performance in fluorescence. Herein, a detection system for iron (III) ions (Fe^{3+}) has been designed by utilizing titanium carbonitride (Ti₃CN) MQDs, a hetero-MXene containing both nitrogen and carbon, belong to a class of MXene that received less spotlight compared to the counterpart MXene groups [7]. We showed that Ti_3CN provides high selectivity of Fe^{3+} ions and showed high degree of PL guenching effect in the presence of Fe³⁺ ions in as low as 5 μ M. The PL guenching mechanism of the probe can be examined through time-resolved fluorescence and Stern-Volmer analysis. The as-designed fluorescence probe for Fe sensing Ti₃CN MQDs can be further improved into a practical and effective sensing system in various sample for water quality assessment and soil contamination.

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Machine Learning-Assisted Discrimination Strategy of Acetone and Hydrogen Based on Hybrid SnO2/WO3 Breath Sensors

Heesu Hwang, Jeong Won Cho, Huisu Shin , Wooseop Lee, and Jin-Ha Hwang*

Department of Materials Science and Engineering, Hongik University, Seoul 04066, KOREA *jhwang@hongik.ac.kr

Hybridization of SnO2- and WO3-based semiconducting metal oxide sensors are exploited to predict the status of an exercise-driven diet and irritable bowel syndrome. The dissimilar SnO2- and WO3- sensors were exposed to acetone and hydrogen environments under the interference of ethanol. The SnO2- and WO3-based sensors suffer from poor classification, even under the assistance of machine learning if sensors are separately applied. However, hybrid SnO2/WO3 sensor integration is proven to be highly effective in discriminating acetone from hydrogen even in a two-sensor mode through the synergistic contribution of neural network algorithms. The current machine learning methodology incorporated principal component analysis and neural network-based classification approach involving numeric-based deep neural networks and image-based convolutional neural networks with the aim to discerning biomarkers from the interfering environment. The proposed hybrid sensor concept is proven to be highly effective in functioning as the high-performance breath sensors under harsh environments.

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Nonequilibrium electrical conductivity-induced particle aggregation in slurry

Jeong mok Cho[†], Byung wook Park[†], and Manhee Lee^{*}

Department of Physics, Chungbuk National University, Cheongju, Chungbuk 28644, Korea [†]These authors contributed equally to this work. *mlee@cbnu.ac.kr

The slurry used in the CMP process exhibits excellent dispersibility due to the precise control of properties such as electrical conductivity. However, when the electrical conductivity of the slurry solution increases, the electrostatic repulsion between particles weakens, leading to particle aggregation and the formation of large particles. These large particles causes defects during the polishing process. Large particles can also form when the electrical conductivity is stable in an equilibrium state. This occurs when impurities are introduced in the solution, causing a localized ion burst that rapidly increases the electrical conductivity. During this process, particles can aggregate before the conductivity reaches equilibrium, a phenomenon referred to as 'Conductivity-shock.' We conducted an experiment using micro-scale salt crystals as impurities to compare particle aggregation under both equilibrium and nonequilibrium conditions at the same ion concentration. The results showed that large particles, which were not observed in the equilibrium state, formed in the nonequilibrium state. Therefore, it is crucial to rigorously control the introduction of impurities when using slurry solutions in the CMP process



Figure 1. Nonequilibrium electrical conductivity induces particle aggregation in slurry

Enhancing Sodium-Ion Battery Performance: Advanced Synthesis Methodology for Prussian White Cathodes

JaeEun Joo and Jong Min Yuk*

Korea Advanced Institute of Science and Technology, Republic of Korea *E-mail address: jongmin.yuk@kaist.ac.kr

Currently, sodium-ion batteries are considered more suitable than lithium-ion batteries for large-scale energy storage systems (ESSs) due to the abundance and lower cost of sodium. Prussian blue analogues (PBAs) have emerged as promising materials for sodium-ion battery cathodes because of their straightforward synthesis and cost-effectiveness. PBAs have the chemical formula $AxM1[M2(CN)_6]y\Box_{1-y} \cdot zH_2O$, where M1 and M2 are transition metals bonded by CN^- ions, forming a three-dimensional open structure. The symbol \Box represents vacancies in the M2(CN)₆ group. This structure features a rigid open framework with large interstitial sites that facilitate Na⁺ ion mobility and accommodate volume changes during Na⁺ insertion and extraction. Moreover, PBAs are synthesized via co-precipitation in aqueous solutions at room temperature, making the process economical and environmentally friendly.[1] However, PBAs typically contain vacancies and water within their crystal structure, which can affect their intrinsic electrochemical performance.

Prussian White (PW), with a higher sodium content than Prussian Blue, is being researched to enhance its electrochemical performance. However, PW is more sensitive to air and moisture exposure compared to PBAs.[2,3] This study aims to reduce PW's sensitivity by optimizing the co-precipitation process to limit air and moisture exposure. Our research underscores the importance of managing PW's susceptibility to air and moisture in sodium-ion battery cathodes. By developing innovative synthesis methods that minimize exposure during co-precipitation, we aim to enhance PW stability and performance. This advancement is crucial for advancing sodium-ion battery technology in large-scale energy storage applications.

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Phase evolution induced by irreversible reactions in metal sulfide anodes

Jacob Choe, Junpyo Hur, and Jong Min Yuk*

Department of Materials Science & Engineering, Korea Advanced Institute of Science and Technology (KAIST), 291 Daehak-ro, Yuseong-gu, Daejeon, 34141, Republic of Korea. *jongmin.yuk@kaist.ac.kr

Transition metal sulfides (TMS) are promising materials for anodes in sodium-ion batteries (SIBs) due to their high theoretical capacity and natural abundance. However, their primary sodium storage mechanism, which involves conversion reactions, leads to significant volume changes during the charge and discharge cycles. This expansion and contraction can result in the loss of contact with the conductive agent and cause pulverization of the active materials. Additionally, the slow diffusion of sodium ions in the TMS matrix and these associated issues can lead to irreversible conversion reactions, thereby limiting the practical use of TMS as anodes in SIBs.

In typical battery systems, copper is the most common material used for current collectors in anode electrodes. Sodium polysulfides (NaPSs), formed by the incomplete and irreversible conversion of Na₂S, are key contributors to the corrosion of copper foil. This corrosion leads to the transformation of TMS into copper sulfides. Although the corrosion process is recognized, the detailed mechanisms of this phase transition, as well as the eventual states of the transition metals and their impact on battery performance, are not fully understood.

In this research, we explore the general phase transition phenomena of TMS into copper-incorporated phases during electrochemical cycling. We performed a comprehensive analysis using transmission electron microscopy (TEM), scanning electron microscopy (SEM), X-ray diffraction (XRD), and X-ray photoelectron spectroscopy (XPS).

Our study reveals several factors that influence irreversible conversion reactions and phase evolution in TMS. These findings enhance our understanding of the fundamental processes involved in TMS phase evolution and provide valuable insights for designing TMS-based sodium-ion batteries.

Unveiling the Surface Reaction Mechanisms of Nickel Nitride@ N-doped Carbon for Hydrogen and Oxygen Evolution Through In-situ Raman Spectroscopy

Gnanaprakasam Janani^{1†}, Subramani Surendran^{1†}, Dae Jun Moon^{1,2†}, Joon Young Kim^{1,2}, Yoongu Lim¹, and Uk Sim^{1,2*}

¹Hydrogen Energy Technology Laboratory, Korea Institute of Energy Technology (KENTECH), Naju, 58330 Jeollanamdo, Republic of Korea ²Research Institute, NEEL Sciences, INC., Naju, Republic of Korea e-mail: usim@kentech.ac.kr (U. Sim)

Knowledge of the mechanisms at catalytic surfaces and interfaces is essential for identifying reaction intermediates and understanding the surface structure of catalysts during reactions. In this research, we have prepared the nitride-based heterostructure, Ni/Ni₃N, decorated on nitrogen-doped carbon (Ni/Ni₃N@NC) via a one-step nitridation process and utilized them as the dual functional catalyst in water splitting. Water splitting hinges on electrochemical oxygen evolution reaction (EOER) and hydrogen evolution reaction (EHER), which occurs at the anode and cathode of the water electrolyzer. As a dual functional catalyst, Ni/Ni₃N@NC should possess the active surface for both reactions, which were analyzed using the in-situ Raman spectroscopy. The designed catalyst takes full advantage of its ambipolar behavior, leading to Ni/Ni₃N and Ni/NC acting as the active surface during EOER and EHER. The results of the time/potential dependent in-situ Raman spectroscopy depict the vibrations of Ni-OH and Ni-OOH at 476 cm⁻¹ and 554 cm⁻¹, which are the indicators of EOER activity at Ni/Ni₃N and the peaks at 1115 cm⁻¹ and 1502 cm⁻¹ correspond to H₂O dissociation at Ni and H₂ adsorption on NC involving the adsorbed intermediates during EHER. The water electrolyzer consists of Ni/Ni₃N@NC as both the anode and cathode were constructed, achieving 10 mA cm⁻² with a low voltage of 1.52 V. These results reveal the mechanism and the involvement of active surface at the interface between the surface of an ambipolar catalyst and electrolyte.



Figure 1. Graphical illustration of dual-functionality on Ni/Ni₃N@N-C for simultaneous hydrogen and oxygen evolution reactions, unveiling through *In-situ Raman Spectroscopy*.

Enhanced Electrochemical Properties of Li_{1.6}Ni_{0.6}Co_{0.2}Mn_{0.2} Cathode Thin Film by Post-annealing Process in Oxygen Atmosphere

Saac Lee, Subhashree Behera and Hyun-Suk Kim*

Dongguk University, 30 Pildong-ro 1-gil, Jung-gu, Seoul, 04620, Korea *khs3297@dongguk.edu

Recent progress in electronic devices has generated robust demand for compact energy sources boasting outstanding power density. Among the potential solutions, thin-film lithium-ion batteries (TF-LIBs) emerge as promising contenders. These TF-LIBs exhibit significant potential to energize diverse diminutive devices [1]. The performance of TF-LIBs batteries is influenced by the cathode materials, and while extensive research is being conducted on various cathode materials, lithium nickel cobalt manganese oxide has been gaining significant attention (LiNi_xCo_yMn_zO₂, x + y + z = 1) [2].

In this work, Li_{1.6}Ni_{0.6}Co_{0.2}Mn_{0.2} cathode material was successfully manufactured using RF (radio frequency) sputtering and annealing was performed to enhance the crystallinity and performance of the synthesized Li_{1.6}NCM622 cathode material. The optimal annealing temperature was determined by comparing various annealing temperatures and different atmospheres. Li_{1.6}NCM622 annealed in an oxygen atmosphere exhibited a high initial capacity and improved cycle life for the batteries.

The results showed the oxygen-annealed $Li_{1.6}NCM622$ thin-film batteries with a high capacity value of 646 mAh/cm³ with improved cycle performance of 81% at 100 charge-discharge cycles. In the future, it can be a viable material combination for thin-film battery applications.

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Oxidative Stability of PEO based Polymer Electrolyte

P-74

Suhyeon Kim¹, YoonJi Park², and Taeho Yoon^{1*}

¹Department of Chemical Engineering, Kyung Hee University, 1732 Deogyeong-daero, Giheung-gu, Yongin-si, Gyeonggi-do, 17104, Republic of Korea

²Department of Chemical Engineering, Yeungnam University,280 Daehak-ro, Gyeongsan-si, Gyeongsangbuk-do, 38541,Republic of Korea

*tyoon@khu.ac.kr

As the secondary battery market expands, there is a growing interest in applying lithium-ion batteries with enhanced safety and superior performance across various fields. Among the proposed approaches, the use of polymer solid electrolytes based on Poly Ethylene Oxide (PEO) has emerged as a promising area of research due to its ease of synthesis, high compatibility with accompanying salts, and processability. However, the low oxidative stability of PEO imposes constraints on the selection of cathode active materials and the design of battery energy density. In this study, we aim to elucidate the relationship between the oxidative stability of solid electrolytes based on PEO and the coordination with accompanying ions, and propose strategies to enhance the oxidative stability of polymer electrolytes.

In this research, we varied the size of accompanying cations, such as Li^+ , Na^+ , and K^+ , to introduce differences in the coordination number within the solid electrolyte used alongside PEO. Specifically, we synthesized polymer solid electrolytes by incorporating each of these cations with PEO. Spectroscopic and thermal analyses were conducted to verify the coordination state within the synthesized polymer solid electrolytes, and linear sweep voltammetry was employed to assess the oxidative stability of the electrolyte.

The analysis revealed that as the size of the cation increases, the coordination number also increases, resulting in improved oxidative stability of the polymer electrolyte. This study highlights the significance of adjusting the coordination degree between PEO and cations in PEO-based polymer solid electrolytes to enhance oxidative stability, with the potential to create polymer solid electrolytes that operate reliably even at voltages exceeding 4V.

Structure and electrochemical properties of Li-Ti-O anode material for Li-ion battery

Se-Hyun Nam^{1*}, Sang-Woo Ahn¹, Kwan-Mo Yang¹, Sei-Jin Lee², Jong Bae Park², and YangSoo Kim^{2*}

Marchal Cap, D11, 520, misa-daero, Hanam-si, Gyeonggi-do, Korea Korea Basic Science Institute, 540-742, Republic of Korea *corresponding author. caolion@nate.com, kimyangsoo@kbsi.re.kr

We investigated the structural and electrochemical properties of new compositions Li-Ti-O (LTO) for anode material in secondary Li-ion batteries using various techniques.

The material was selected by first principles calculation and its real properties as a negative electrodewere measured after it is synthesized by solid state reactions.

The study focused on elucidating the effects of the microstructural evolution in LTO on battery functionality and assess its suitability for use in anode material in secondary Li-ion batteries.

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New Strategy to Improve the Accuracy of Quantitative Analysis of Energy Dispersive Spectroscopy

Won-Jin Moon¹, Seul Gi Yu¹, Yang Soo Kim², Byung-Kyu Park³, Wan-Gil Jung^{1*}, and Ho-Jun Song^{4*}

¹Korea Basic Science Institute, Gwangju Center, Gwangju 61186, Republic of Korea
²Korea Basic Science Institute, Jeonju Center, Jeonju 54907, Republic of Korea
³ThermoFisher Scientific, Gyeonggi-do 17111, Republic of Korea
⁴School of Dentistry, Chonnam National University, Gwangju, 61186, Republic of Korea
*wgjung7873@kbsi.re.kr, songhj@jnu.ac.kr

Elemental quantification of several single crystalline TEM samples of intermediate thickness range that cannot be quantified by the thin-film approximation method and the ZAF correction were investigated using wedge-shaped samples of known thickness fabricated by the FIB technique. '*Thickness factor* (T_F) ' and 'Thickness correction coefficient (T_c) ' were proposed as error correction items of 'thin-film approximation method' to minimize the quantitative error that occurs when quantifying samples of intermediate thickness with TEM-EDS. As the result of T_F correction, the quantification error in an Al₂O₃ TEM sample by TEM-EDS was reduced from about 52.15% to less than 3.28 (\pm 2.57)% by the correction of only one time. The self-absorption corrected line profiles and self-absorption corrected elemental mapping images in TEM samples of intermediate thickness range were also obtained by T_F correction. As an example of application by T_F correction, we proposed a novel method measuring thin-film thickness in normal TEM without the EELS system. The T_F correction technique is a unique method to overcome the limitation of EDS quantification in the intermediate thickness range. This technique can effectively quantify characteristic x-ray lines less than 1,000 eV in the sample having intermediate thickness ranges using the conventional TEM-EDS system. It is expected to contribute significantly to understanding various characteristics or material nature related to material composition and sample thickness in nanomaterials because it provides more precise quantitative analysis information than current commercial EDS systems.

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Characterization of ocean plastics using ToF-SIMS and machine learning

Miku Kimura¹, Motomi Shiojima², Shohei Hananoki², Daisuke Hayashi¹, Satoka Aoyagi^{1*}

¹Faculty of Science and Technology, Seikei University, Musashino, Tokyo 180-8633 Japan ²Sekisui Chemical Co., LTD., Osaka *aoyagi@st.seikei.ac.jp

Environment issues such as global warming, extreme weather events, and pollution have been attracting more and more attention. Ocean plastics are involved in such issues. Many products are made from plastic because it is light, sturdy, and easy to mass produce. Some of the plastic products are spill out of the garbage collection system and they have spoiled the landscape. Moreover, one of the main problems with ocean plastics is that it has harmed marine life by accidentally eating plastic products such as a plastic bag. In addition, ocean plastics are broken down by waves and sunlight into smaller pieces that become microplastics [1]. It is also a problem that we have not clarified the mechanism of microplastic generation. Ocean plastics are difficult to characterize by appearance. Therefore, their identification at the molecular level is necessary before studying the degradation processes. It is also important to know the chemical composition of these plastic products and their additives, in order to effectively recycle used plastic products. Therefore, in this study, we analyzed ocean plastics by using Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS), a surface analysis method that provides the information of chemical composition high with sensitivity. Since ToF-SIMS spectra of unknown plastic samples are generally too complex to interpretate, we applied machine learning principal component analysis (PCA), multivariate curve resolution (MCR) and autoencoder (AE), to categorize the TOF-SIMS data into several characteristics [2,3]. Among them, we focused on characteristics that associated with plastics, even more, we compare with fragment ions of polystyrene, polyethylene, polycarbonate and so on.

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Surface Analysis of CaCO₃ Nanoparticles Modified by a Silane Coupling Agent Methyltrimethoxysilane

JuYeon Lee, JeongMin Lee, JongChoo Lim*

Dept. of Chemical and Biochemical Eng., Dongguk Univ., Seoul 100-715, Korea *jongchoo@dongguk.edu

Calcium carbonate (CaCO₃) nanoparticles have been widely used as one of the major ingredients in various areas of industrial applications since CaCO₃ is one of the most plentiful substances and perhaps one of the most inexpensive inorganic particles in the world. However, the uses of CaCO₃ particles in many areas are often limited due to their hydrophilic characteristics. For instance, excessive hydrophilic property of CaCO₃ nanoparticles does not allow accumulation of CaCO₃ nanoparticles at most of fluid-fluid interfaces and does not provide compatibility with hydrophobic macromolecule surfaces. Thus, proper surface alteration of CaCO₃ nanoparticles is a prerequisite to a wide expansion of industrial uses in various fields.

The surface activation of CaCO₃ nanoparticles has been performed by using various types of hydrophobic compounds possessing functional ligands [1,2]. Recently, we carried out in situ surface treatment of CaCO₃ nanoparticles by employing 2 kinds of anionic surfactants and confirmed the amount of adsorbed surfactant layer on CaCO₃ substrate by using a quartz crystal microbalance (QCM) [1]. However, the maximum hydrophobicity of CaCO₃ nanoparticles obtained with an optimum dosage of surfactant was not sufficient for industrial applications. For example, the maximum contact angles under optimum conditions were less than 60° in both surfactant systems, indicating that surface modified CaCO₃ nanoparticles was also carried out by interaction with the anionic fluorinated surfactant Zonyl TBS and very stable foam was generated at 0.17 wt% of surfactant concentration where the contact angle was measured to be about 90° [2]. Even though Zonyl TBS was found to be an excellent surface modifier, industrial applicability in various areas is still limited due to extremely high cost of fluorinated surfactant Zonyl TBS.

In this study, the surface modification of CaCO₃ nanoparticles was performed by using a silane coupling agent methyltrimethoxysilane (MTMS) as shown in Scheme 1. In order to confirm surface modification of CaCO₃ nanoparticles by MTMS, Fourier infrared spectroscopy, differential scanning calorimetry, and thermogravimetric analysis have been carried out. Atomic concentration of CaCO₃ particle surface treated by MTMS has been identified by using x-ray diffractometer and x-ray photoelectron spectroscopy analysis.



Scheme 1. Surface modification of CaCO₃ nanoparticles with a silane coupling agent methyltrimethoxysilane (MTMS)

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Bimetal MOF based electrochemical sensor for the detection of serotonin in serum

Veerapandian Mekala, Kyusik Yun*

Department of Bionanotechnology, Gachon University, Gyeonggi-do 13120, Korea *ykyusik@gachon.ac.kr

Serotonin (SER) is the neurotransmitter that plays a major role in the neural activities, imbalance of serotonin leads to the various physiological and psychological disorders. Therefore, accurate detection of serotonin level is essential for the diagnosis of neural disorders. This study presents the electrochemical sensor based on bimetallic Metal-Organic Framework (MOF) for detection of serotonin. The bimetallic MOF (ZnCuMOF) was synthesized using zinc and copper as metal centers and exhibit good physical and chemical properties. The ZnCuMOF modified with carbon cloth electrode (CCE) and electrochemical activity towards sensing of SER was analyzed using cyclic voltammetry (CV) and differential pulse voltammetry (DPV). The ZnCuMOF/CCE exhibit sensitive and selective detection of SER. The sensor demonstrates the wide linear range (0.01-70 μ M), low detection limit (8.5 nM) and better reproducibility. The selectivity towards SER against several interference such as glucose, L-cysteine, dopamine and epinephrine. The fabricated sensor was successfully demonstrated to detect SER in serum with accuracy and reliability. This bimetallic MOF based sensor for the detection of SER, paving the way for advanced diagnostic strategies.

Infrared Nano-Spectroscopy of Single Extracellular Vesicles via Photo-Induced Force Microscopy

Mingu Kang^{1,2}, Hwi Je Woo¹, yeonjeong Koo², Kyoung-Duck Park², Eun Seong Lee^{1*}, and Junghoon Jahng^{1*}

¹Hyperspectral Nano-imaging Team, Korea Research Institute of Standards and Science (KRISS), Daejeon, 34113, Republic of Korea ²Department of Physics, Pohang University of Science and Technology (POSTECH) *eslee@kriss.re.kr, phyjjh@kriss.re.kr

Photo-induced force microscopy (PiFM) enables high-resolution imaging with the suppression of background components by detecting the photo-induced dipole- or thermal forces at the tip using heterodyne mode. Extracellular vesicles (EVs), including small EVs (exosomes) ranging from 20 to 200 nm, play a crucial role in intercellular communication by transporting DNA, RNA, lipids, and proteins. Identifying the molecular fingerprints of EVs is essential for diagnostic and therapeutic applications. Conventional microscopy techniques, such as Raman spectroscopy and Fourier-transform infrared microscopy (FT-IR), have limitations in analyzing EV compositions and differentiating between EV types. In our work, we utilize heterodyne mode PiFM to reveal the protein heterogeneity of EVs derived from HCT116 and HT29 cells at the single-vesicle level. Unlike FT-IR, PiFM distinctively identifies different protein and nucleic acid responses between these EVs, attributed to their microsatellite stability characteristics [1]. Specifically, the reduced IR responses of DNA components (adenine and thymine) in HCT116 indicate a malfunction in the DNA repair mechanism. Moreover, the altered ratio of α -helix to β -sheet in the amide I band suggests higher tumor malignancy in HT29 cells [2]. This work paves the way for revealing molecular features of nano-sized biochemical materials and the rapid and noninvasive diagnosis of cancer cells at the nanoscale.

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Post-functionalization of diazonium-modified surfaces in the presence of redox inhibitor

Sojin Park and Yang-Rae Kim*

Department of Chemistry, Kwangwoon University, 20 Kwangwoon-ro, Nowon-gu, Seoul 01897, Republic of Korea yrkim@kw.ac.kr*

Electrografting of aryldiazonium salts for tunable surface modification has been extensively studied on various electrode materials. The above methods have several advantages. First, the modified electrode exhibits long-term stability even under air exposure due to covalent bond formation with the surface and diazonium compound. Second, relatively short modification time ranges from a few seconds to several minutes. Finally, it is possible to modulate the degree of modification while controlling experimental conditions, such as when a redox inhibitor is added to the precursor solution. [1]

In this study, 4-iodobenzene-1-diazonium tetrafluoroborate (4-IBD) has been used as an aryldiazonium compound to modify highly ordered pyrolytic graphite. For tunable surface coverage, the electrografting of 4-IBD was carried out in the presence of 2,2-diphenyl-1-picrylhydrazyl. Subsequently, the Sonogashira coupling reaction was performed to attach ferrocenyl groups to the modified iodophenyl monolayers. [2,3] These processes were intensively investigated by chronoamperometry and cyclic voltammetry. In addition, atomic force microscopy and X-ray photoelectron spectroscopy estimated the surface coverage.

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Nanoscopic Investigation of Real-Time Conformational Dynamics of Condensins using High-Speed Atomic Force Microscopy

Lim Keesiang¹, Kazuhisa Kinoshita³, Tatsuya Hirano^{3*}, Richard W Wong^{1,2*}

¹WPI-Nano Life Science Institute, Kanazawa University, Kakuma-machi, Kanazawa, Ishikawa 920-1192, Japan.

²Cell-Bionomics Research Unit, Institute for Frontier Science Initiative (INFINITI), Kanazawa University, Kakuma-machi, Kanazawa, Ishikawa 920-1192, Japan.

> ³Chromosome Dynamics Laboratory, RIKEN, Wako, Saitama 351-0198, Japan. *Corresponding. rwong@staff.kanazawa-u.ac.jp, hiranot@riken.jp

Condensins are considered as the universal organizers of chromosomes as they have multiple roles in organizing chromosomal structure such as formation of mitotic chromosome, maintenance of gene stability, and cell differentiation and development [1]. Condensins consist of SMC 2/4 heterodimer and non-SMC complex. The heterodimer has flexible coiled-coil "arms", a proximal "dimerized" hinge domain, and distal ATPase head domain, forming a distinctive V-shape [2]. The non-SMC subunits are HEAT-repeat subunits and a kleisin protein. Conventional structural methodologies such as X-ray crystallography and cryo-EM do not resolve condensins structural dynamics because the images acquired are rather static. In addition, fluorescent-based assays only reflect the structural dynamics of fluorescent labels but not condensins. High-speed atomic force microscopy (HS-AFM) has been developed for direct visualization of biomolecules and organelles in a real-time manner without labeling [3-4]. In this study, we intend to elucidate native structure and conformational dynamics of human condensins with high spatiotemporal resolution at nanoscopic level using HS-AFM. We first obtained the structural details of yeast condensin in PDB format downloaded from the RCSB webserver. After that, we performed HS-AFM simulation to obtain simulated HS-AFM images of condensins as our references. Furthermore, we used AlphaFold3 to predict the structure of human condensins. After in silico analysis, we then scanned condensins in a near physiological buffer with different types of substrates such as bare mica, APTES-coated mica, and PLL-coated mica. We found different degree of mobility of condensins on different substrates. Condensins were more dynamic on substrates with weaker adsorption force. Flexible coiled-coil arm and transient conformations were clearly seen. In summary, HS-AFM is a powerful nanoimaging tool to resolve innate conformational dynamics of condensins under a near physiological environment.

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Application of AFM Measurements in Various Environments

Jihye Lee^{*} and Yeonhee Lee

Korea Institute of Science and Technology Advanced Analysis & Data Center, KIST (5, Hwarang-ro 14-gil, Seongbuk-gu, Seoul 02792 Korea) *023461@kist.re.kr

Atomic force microscopy (AFM) technology is based on the interaction between a sharp tip and the atoms of the sample surface providing three-dimensional information on the surface roughness of samples. The initial purpose of AFM was to measure the surface morphology of a sample, but with the development of AFM analysis technology, it is also widely used to measure the electrical and mechanical properties of various samples. One of the biggest features of AFM is the ability to measure non-conductive or non-solid materials. It also has the advantage of being able to measure samples under any kinds of atmosphere such as air, liquid, or vacuum. Therefore, AFM is a very attractive equipment that can be applied to various research fields.

In this study, we provide some examples of AFM analysis measured in glove box system or in the liquid environment. The use of AFM in glove box shows higher accuracy and better repeatability than measurements under ambient conditions, as it can exclude moisture adsorption or oxidation process in the air. In particular, it is very useful equipment for analysis of air-sensitive materials such as semiconductors and batteries. Liquid AFM is widely used in organic and bio fields because it is almost the only measurement method that can measure the surface morphology, Young's modulus, and adhesion of soft materials in the liquid environment.

Verification of therapeutic effect through Accelerator Mass Spectrometry based single cell level quantification of hESC-endothelial cells distributed into an ischemic model

Min-Seok Oh¹, Gwan-Ho Lee¹, Seongeun Song^{1,3}, Seul-Gi Lee², Hyung Min Chung^{2*}, Byung-Yong Yu^{1*}

¹Advanced Analysis and Data Center, Korea Institute of Science and Technology, Hwarang-ro 14-gil 5, Seongbuk-gu, Seoul, Republic of Korea, 02792

²Department of Stem Cell Biology, School of Medicine, Konkuk University, 120 Neungdong-Ro, Gwangjin-Gu, Seoul Republic of Korea, 05029

³Department of Pharmacy and Yonsei Institute of Pharmaceutical Sciences, Yonsei University Yeonsu-gu, Incheon, 21983 South Korea *yu2997@kist.re.kr

As the potential of pluripotent stem cell-derived differentiated cells has been demonstrated in regenerative medicine, differentiated vascular endothelial cells (ECs) are emerging as a therapeutic agent for the cardiovascular system [1-2]. To verify the therapeutic efficacy of differentiated ECs in an ischemic model, we induced human embryonic stem cells (hESCs) as EC lineage and produced high-purity ECs through fluorescence-activated cell sorting (FACS). When hESC-ECs were transplanted into a hindlimb ischemic model, it was confirmed that blood flow and muscle regeneration were further improved by creating new blood vessels together with autologous ECs than the primary cell as cord blood endothelial progenitor cells (CB-EPCs). In addition, previously reported studies showed detection of transplanted cells engrafted in blood vessels through various tracking methods, but failed to provide accurate quantitative values over time. In this study, we demonstrated that hESC-ECs were engrafted approximately 7-fold more than CB-EPCs by using an accelerator mass spectrometry (AMS)-based cell tracking technology that could perform quantification at the single cell level. An accurate quantification index is suggested. It has never been reported in in vivo kinetics of hESC-ECs that can act as therapeutic agents.

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Cutting-edge analysis technology for various materials of the semiconductor industrial research field by X-ray Photoelectron Spectroscopy in AICT

Gyung Hyun Kim, Ju Hyun Lee, and Chang Woo Byun*

Advanced Institute of Convergence Technology (AICT), 145 Gwanggyo-ro, Yeongtong-gu, Suwon-si, Gyeonggi-do 16229, Suwon, Republic of Korea *corresponding. byuncw@snu.ac.kr

We introduced XPS (X-ray Photoelectron Spectroscopy) analysis technologies, including the temperature dependence curve of the elastic scattering peak of REELS (Relative Electron Energy Loss Spectrum) and the depth profile curve using an equipped electron and ion gun. To investigate the work function with VBM (Valence Band Maximum), UPS (UV Photoelectron Spectroscopy) data acquisition was also conducted. Furthermore, the Ar ion sputtering yield for the carbon film was calculated to be 0.124 nm/s by observing the etched spot via FIB-SEM (Focused Ion Beam-Scanning Electron Microscope). Based on these observations, the time axis (time unit) can be converted to a real depth axis (length unit) in an atomic percent versus time curve plot.



Figure. (a) Atomic concentration versus depth plot with (b) observed etched spot image via FIB-SEM.

Alloying of ReS₂ and VS₂ Nanosheets for Enhanced Electrocatalytic Hydrogen Evolution Reaction

Ik Seon Kwon^{1*}, In Hye Kwak², Jeunghee Park³, Jae-Hong Lim¹, and Ki-jeong Kim¹

¹Beamline Science Team, 4GSR Accelerator Research Division, Pohang Accelerator Laboratory, POSTECH, Pohang, Republic of Korea

²Research Center for Materials Analysis, Korea Basic Science Institute (KBSI), Daejeon, Republic of Korea

³Department of Advanced Materials Chemisty, Korea University, Sejong, Republic of Korea

*iskwon@postech.ac.kr

Modulating the electronic structure of transition metal dichalcogenides (TMDs) via alloying is challenging despite the additional potential applications. In this study, a solvothermal reaction is used to synthesize composition-tuned ReS₂-VS₂ (Re_{1-x}V_xS₂) alloy nanosheets featuring an expanded interlayer distance. Increasing x induces a phase transition from the semiconducting 1T'' phase ReS₂ to the metallic 3R-stacking 1T phase VS₂. Alloying via homogeneous atomic mixing renders the nanosheets more metallic

and with less oxidation than VS₂. Firstprinciples calculations consistently predict the 1T"-1T phase transition of the atomically mixed alloy structures. The calculation also suggests that intercalation drives the 3R stacking of 1T phase VS₂. The $Re_{1-x}V_xS_2$ nanosheets at x = 0.3-0.8 exhibit enhanced electrocatalytic activity toward watersplitting hydrogen evolution reaction (HER) in an acid electrolyte. In situ X-ray absorption fine structure measurements reveal that the metallicity of the alloys is fully retained during HER. The density of states and Gibbs free energy calculations show that alloying increases the metallicity and thus effectively activates the basal S atoms toward the HER, supporting the observed increased HER performance of the alloy nanosheets.



Scheme 1. Schematic illustration for developing highperformance $\text{Re}_{1-x}V_xS_2$ alloy nanosheets toward electrocatalytic water-splitting hydrogen evolution reaction (HER), which includes preparation method of 11 samples (with a step of $\Delta x = 0.1$), DFT calculations, and ex situ/in situ characterization using synchrotron X-ray beam.

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Study on Oxygen Vacancies in Oxide Semiconductors under Thermal Treatment using XPS

Ae Jin Choi^{1,2}, Seunghwan Kim¹, Hee Kyoung Kang¹, Soohyung Park^{1,2*}

¹Advanced Analysis and Data Center, Korea Institute of Science and Technology (KIST) 5, Hwarang-ro 14-gil Seongbuk-gu Seoul 02792, Republic of Korea

2Division of Nanoscience & Technology, KIST School, University of Science and Technology (UST), Seoul 02792, Republic of Korea *soohyung.park@kist.re.kr

Oxygen vacancies directly affect the electronic structure and physical properties of oxide semiconductors. These vacancies occur when oxygen atoms are removed from the crystal structure, leaving behind sites that trap electrons and induce an n-doping effect, thereby increasing the concentration of conductive electrons. The above process requires a significant amount of energy, which can be provided by atomic vibrations (i.e., thermal energy), physical impacts (such as ionic sputtering), or other means. In commercial semiconductor fabrication, thermal treatment is widely used and sometimes it is essential for optimizing semiconductor performance. However, there are no general and systematic approaches to understand their relation behinds. In this reason, universal understanding the relationship between temperature and oxygen vacancies is essential for successful semiconductor manufacturing.

In this study, we investigated the formation and diffusion characteristics of oxygen vacancies in ZnO (Zinc Oxide) and ITO (Indium Tin Oxide), which are representatively widely used n-type semiconductors with broad bandgaps and are commonly utilized in various electronic and optoelectronic devices due to their excellent electrical conductivity and optical transparency. The ZnO and ITO samples were subjected to stepwise thermal treatment in a vacuum chamber using a halogen lamp, with temperatures ranging from 0°C to 700°C at intervals of 100°C, while varying the applied voltage and current. Following the thermal treatments, the samples were analyzed using X-ray Photoelectron Spectroscopy (XPS) under vacuum. The O1s peaks were specifically analyzed to examine the formation, diffusion, and annihilation of oxygen vacancies. With quantitative evaluation of oxygen vacancies, the structure changes under different thermal treatment conditions provides essential insights that can be used to optimize the performance of electronic and optoelectronic devices.

Influence of Neutralizer on the ITO Surface in XPS Analysis

Hee kyoung Kang, Ae jin Choi, So hee Kim, Soo hyung Park*

Advanced Analysis Center, Korea Institute of Science and Technology, Hwarang-ro 14-gil, Seongbuk-gu, Seoul 02792, Republic of Korea *soohyung.park@kist.re.kr

X-ray Photoelectron Spectroscopy (XPS) is a powerful analytical technique that enables the precise characterization of surface chemical states by analyzing photoelectrons emitted from a material when exposed to X-ray irradiation. However, in the case of insulating materials or those with low electrical conductivity, the emission of photoelectrons often leads to positive charge accumulation on the sample surface, which can cause significant distortions or shifts in the binding energy of the detected electrons. To counteract these charging effects, the use of a neutralizer is commonly employed in XPS analysis. Despite its widespread use, neutralizers are frequently applied without adequate consideration of the sample's specific properties, potentially leading to detrimental impacts on surface integrity, including damage and spectral alterations.

In this study, we investigated the effects of neutralizer application on the surface of Indium Tin Oxide (ITO), a metal oxide with high electrical conductivity. Surface damage was visually assessed using Scanning Electron Microscopy (SEM), and the chemical state and quantitative variations of oxygen were evaluated via XPS. The objective of this study is to establish optimal analytical conditions tailored to the unique characteristics of oxide materials.

In recent years, there has been a sharp increase in the number of research papers utilizing XPS, with the use of electron beams in analysis becoming widespread for most samples. However, this can cause physical and chemical alterations to the sample, posing challenges in accurately determining its intrinsic properties. Therefore, this study seeks to propose a method that selectively uses electron beams based on the material properties, enabling analysis with minimal damage.

Mechanism of Light-induced Surface Degradation in Two-Dimensional Halide Perovskites: Impact of Light during Fabrication and a Passivation Strategy

Kitae Kim^{1,2}, Chanhui Park², Eunseo Cha², Donghee Kang¹, Jeehong Park¹, Sylke Blumstengel³, Nicholas Zorn-Morales³, Emil J.W. List-Kratochvil³, Sang Wan Cho¹, Hyunbok Lee⁴, Soohyung Park^{2,5}, Yeoniin Yi^{1*}

¹Yonsei University, ²Korea Institute of Science and Technology, ³Humboldt University, ⁴Kangwon National University, 5University of Science and Technology ¹Department of Physics, Yonsei University, 50 Yonsei-ro, Seodaemun-gu, Seoul 03722, Republic of Korea *yeonjin@yonsei.ac.kr

In last several years, organic-inorganic two-dimensional halide perovskites (2DHPs) have achieved significant advancements in perovskite-based photovoltaics, including applications in solar cells, light-emitting diodes, and photodetectors. By incorporating organic spacer molecules above and below each metal halide layer, the 2DHPs are endowed with layered structure where each layer interacts via van der Waals interaction. The 2DHPs have much enhanced stability against exposure to heat, oxygen, and moisture than 3D perovskites.

However, despite these benefits, the photostability of 2DHP perovskites has not been sufficiently explored, even though they are used as light-absorbing materials. A few studies have reported that the 2DHPs are rapidly degraded under light illumination. This light-induced degradation accompanies loss of volatile organic spacers and iodine ions. And eventually it leads to a critical deterioration on optical properties. Despite the significance of the issue, there has been a lack of research to figure out the causes and mechanisms of light-induced degradation of 2DHPs or its prevention strategy.

In this study, we thoroughly investigate the surface photodegradation of the 2DHP using $[C_8H_{12}N]_2PbI_4$ ([PEA]₂PbI₄) films. We illuminated the samples with light sources with varying wavelengths in stepwise manner. The evolution of the surface was monitored through photoelectron spectroscopy, photoluminescence spectroscopy, SEM, and AFM. The results indicate that photodegradation of the 2DHP occurs when exposed light has photon energy exceeding the band gap, leading to the formation of electron-rich metallic defects. Also, we highlight the effectiveness of blocking the short-wavelength light during the film fabrication, because degradation accelerates at this stage. Additionally, we propose useful passivation strategy using molecular acceptors to prevent photodegradation of 2DHP surfaces. We believe our findings offer valuable understandings on 2DHPs and their potential applications.

Round Robin Test for the Calibration of Magnification and Offset in SEM and AFM Measurements using a Nanostructured Certified Reference Material

Park, Young Su¹, Kang, So Hee¹, Kim, Hyun Joung¹, Woo, Jin Chun¹, Kim, Kyung Joong^{1,2*}

¹Kims Reference Corp. (KRC), Republic of Korea ²Korea Research Institute of Standards and Science (KRISS), Republic of Korea

A high magnification calibrator (HMC) has been developed for the calibration of magnification and offset value in the horizontal nanoscale surface shape measurement by scanning electron microscopy (SEM) and atomic force microscopy (AFM). The five pitch values ($P_1 \sim P_5$) and five line width values ($W_1 \sim W_5$) shown in Figure 1(a) were traceably certified by high-resolution TEM measurement from the basis of Si lattice constant measured in the Si(100) substrate.

The magnification can be calibrated using the five pitch values shown in Figure 1(a) by a linear regression equation between the certified and measured pitch values. The offset value can be also calibrated by a linear regression equation between the certified and the measured line width values. The locations to measure the pitch values and line width values can be clearly determined from the contrast line profile of SEM and the linear height profile of AFM images as shown in Figure 1 (b). Moreover, using a magnification calibration program, the magnification correction factor and the offset correction factor can be automatically calculated as shown in Figure 1 (c).

The calibration of magnification by the high magnification calibrator and the measurement of critical dimension of a nanostructured material with a silicon line were compared in a domestic round robin test using SEM and AFM. The effects of measurement conditions such as electron energy and magnification in SEM measurement and the radius and cone angle of the used AFM tips were systematically investigated.



Figure 1. (a) Structure of the high magnification calibrator, (b) contrast line profile of SEM and height line profile of AFM, (c) calculation program of magnification and offset correction factor

Comparative study of time-resolved electroluminescence and photoluminescence of light emitting devices

Weon-Sik Chae^{1*}, Keum-Jin Ko², and Jong-Soo Lee²

¹Daegu Center, Korea Basic Science Institute (KBSI), Daegu 41566, Republic of Korea ²Department of Energy Science and Engineering, DGIST, Daegu 42988, Republic of Korea *wschae@kbsi.re.kr

Light emitting devices (LEDs) are operating at active semiconductor layer by recombination of charge carriers (electron and hole) which are supplied from negative/positive electrodes under applied electrical bias. The LED materials typically show highly-emitting characteristics under light irradiation through electron and hole recombination at the active layer. In this study, we comparatively studied time-resolved electroluminescence (EL) and photoluminescence (PL) in the fast time regime from nano- to micro-second time window. Interestingly, we could extract electron-hole recombination information from the time-resolved PL spectroscopy, whereas the transient EL signal provides the information of electron diffusion at the active layer and subsequent recombination characteristics. Furthermore, time-resolved EL and PL imaging enables valuable information about the homogeneity/inhomogeneity of the emitting materials and effectiveness of charge injection over the device area.

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In-situ liquid phase TEM for revealing suppression effect of Mo etching by solid by-products

Sanghyeon Ji, Jacob Choe, Jeongmin Kim, Sanghyeon Park, and Jong Min Yuk*

Korea Advanced Institute of Science and Technology, Republic of Korea jongmin.yuk@kaist.ac.kr

Recent progress in semiconductor technology demands highly integrated devices with interconnects reduced to just a few nanometers. While copper (Cu) has been commonly used, its performance declines at scales smaller than 10 nm, leading to the investigation of alternative materials. Molybdenum (Mo) has emerged as a promising substitute due to its superior electrical properties. However, challenges arise in wet etching processes for Mo, as the traditional etchant, an aqueous hydrogen peroxide solution, reacts aggressively with Mo, often resulting in uneven surfaces after etching.

In this study, we developed two distinct etching conditions—acidic and alkaline—based on the Mo-H2O phase diagram. We observed the etching dynamics in real-time using in-situ liquid phase transmission microscopy (LPTEM). Under acidic conditions, solid by-products form during the wet etching process, leading to delays or cessation of etching. We investigated the formation mechanism of these solid by-products, tracking their development from nucleation to the formation of larger particles, and identified the by-products through post-mortem TEM analysis. Conversely, under alkaline conditions, the Mo film is etched cleanly without the formation of solid by-products. By comparing the two conditions through quantitative analysis, we determined the impact of solid by-products on incomplete etching. This quantitative assessment is anticipated to inform future research aimed at developing more effective etchants.

Automatic analysis program for the TEM diffraction patterns (REDI, RIST Electron Diffraction Interpreter)

Sung KANG^{*}, and Yoon HUH

Analysis and Assessment Research Group, Research Institute of Industrial Science and Technology, Pohang 37673, Korea *sungkang@rist.re.kr

In order to analyze the microstructure of materials using TEM, it is necessary to obtain an electron diffraction image such as SAED or NBD, or analyze the crystal phase through a diffraction image obtained after FFT conversion of high-resolution image of an atomic level. Also, the crystal phase analysis requires a separate S/W such as Digital-Micrograph to measure the distance and angle between diffraction points (spots) in the obtained diffraction images, and has the disadvantage of being highly dependent on the researcher's experience. Therefore, in order to solve the inconveniences that have been felt while analyzing diffraction patterns, 1) integrate the SWs used for diffraction pattern analysis into one platform, 2) combine the necessary material information (DB), and 3) develop a system that can obtain analysis information about the crystal phase only by inputting diffraction pattern images and components.

In this presentation, I would like to introduce REDI, an automatic analysis program for the TEM diffraction patterns that accurately recognizes and measures the distance and angle between spots in the diffraction pattern images, and interprets the crystal phase, automatically.



[Welcome to REDI(Main image)]

ZnS/Diamond-Like Carbon Heterostructure Nanowires: Synthesis and Characterization

Ki-Young Lee, Jung Han Kim*

Department of Materials Science and Engineering, Dong-A University, Republic of Korea *junghankim@dau.ac.kr

The stability of nanomaterials is critical for their practical applications, including in nanodevices and waveguides. To optimize ZnS nanowires for such uses, overcoming oxidation challenges is essential. ZnS nanowires exhibit high reactivity, making surface passivation crucial to prevent deformation, oxidation, corrosion, and contamination. In this study, we fabricated ZnS/diamond-like carbon (DLC) core-shell heterostructure nanowires using the vapor-liquid-solid (VLS) method combined with radio frequency plasma-enhanced chemical vapor deposition. Au-catalyzed ZnS nanowires, with widths of 70-80 nm and an outer DLC layer thickness of 20-30 nm, were synthesized. The nanowires were analyzed through extensive electron microscopy and chemical composition studies. Raman spectroscopy of the DLC layer revealed typical peaks at 1550 cm⁻¹ (G peak) and 1330 cm⁻¹ (D peak), indicating hydrogenated diamond-like amorphous carbon. IR transmittance measurements showed that ZnS/DLC nanowires exhibit a transmittance of 90-98%, with enhanced IR transmittance observed at 2100 cm⁻¹ and 3000 cm⁻¹, showing a 1-1.4% improvement over ZnS nanowires.

Keyword: zinc sulfide nanowire, diamond-like carbon, growth mechanism, heterostructure

Impact of n-Doping on Defect States and Energy Level in Two-Dimensional Hybrid Organic-Inorganic Ruddlesden-Popper Perovskites

Eunki Yoon^{1,2}, Kitae Kim^{1,2}, Seunghwan Kim^{1,2}, Aelim Ha^{1,2}, 2Sooyeon Pak^{1,2}, Yeonjin Yi², Kyu Hyoung Lee^{2*}, Soohyung Park^{1,3*}

¹Korea Institute of Science and Technology, ²Yonsei University, ³University of Science and Technology

¹Advanced Analysis and Data Center, KIST (5, Hwarang-ro 14-gil, Seongbuk-gu, Seoul 02792 Korea)

²Department of Materials Science & Engineering, Yonsei University (50 Yonsei-ro, Seodaemun-gu, Seoul 03722 Korea) ³Division of Nanoscience & Technology, KIST School, University of Science and Technology (UST), Seoul 02792, Republic of Korea

*soohyung.park@kist.re.kr

Two-dimensional organic-inorganic hybrid Ruddlesden-Popper (2D RP) perovskites have emerged as next-generation materials, particularly gaining attention as key layers in various optoelectronic devices. Doping perovskites plays a crucial role in enhancing the efficiency of these devices. However, research on the structural changes induced by doping remains insufficient. Therefore, this study aims to conduct an in-depth analysis of the changes in perovskites caused by different n-type dopants.

In this study, we doped the perovskite surface with two n-type dopants, [RuCp*Mes]2 and Decamethylcobaltocene (DMC), and prepared samples with doping thicknesses ranging from 0.5 nm to 7 nm under UHV conditions. We plan to observe the chemical changes on the perovskite surface using XPS and measure the energy levels as a function of dopant concentration using UPS and IPES. Through this analysis, we aim to investigate the effects of n-doping on perovskites. This research is expected to provide a deeper understanding of the interactions between perovskites and dopants, contributing to the future design and performance enhancement of optoelectronic devices.

Depth Profiling of Thick Samples Excluding Sputtering Damage Using TOF-MEIS and Ar Sputter

Jwasoon Kim, Chang Seon Park, Haejoon Hahm, Kyungsu Park, Soobang Kim, Won Ja Min*

Analysis Technology Team, HB Solution Co., Ltd, 33, Techno 8-ro, Yuseong-gu, Daejeon 34028, Republic of Korea *wj.min@hb-solution.co.kr

TOF-MEIS (Time-Of-Flight Medium Energy Ion Scattering) can analyze the composition depth profile non-destructively and with superior depth resolution for thin film samples of about 2 to 20 nm thickness using medium energy ions. [1, 2] However, TOF-MEIS experiences increased straggling and multiple scattering at depths greater than 20 nm, causing a degradation in thickness resolution and composition accuracy. By using sputtering as a method to overcome these limitations in depth of analysis, the thickness resolution and composition accuracy for films thicker than 20 nm can be maintained at the same level as for samples less than 20 nm thick.

Typically, during depth profiling with sputtering in techniques like XPS and SIMS, the composition ratio at the surface layer of 2 to 10 nm changes due to the varying sputter yields of different elements and the mixing effects induced by the sputter beam. [3, 4] Most surface measurement equipment measures this area, which can distort the composition depth profile. To avoid this sample damage effect, surface measurement equipment that can separate measurement results from deeper areas rather than damaged areas is required.

Since MEIS can analyze the non-destructive depth profile in a 20 nm thick region, even if sputtering is used, the composition depth profile without distortion caused by sample damage can be obtained by connecting the non-destructive composition depth profiles below the damage region.

In this study, TOF-MEIS measurement and analysis using Ar sputter were optimized, and a function to merge the depth profiles obtained by MEIS measurement after sputtering, excluding the sputter damage region, was added to the analysis program. This study presents measurement and analysis results of thick samples obtained using Ar sputter and TOF-MEIS.

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Determination of Screening model for Quantitative analysis in ToF-MEIS for 150 keV He^+

Haejoon Hahm, Kyungsu Park, Wansup Kim, Hoseong Jang, Soobang Kim, Wonja Min*

HB solution, Techno 8ro 33, Yuseong-gu Daejeon, Republic of Korea, 34028 *wj.min@hb-solution.co.kr

Due to the high integration of semiconductor devices, thin films with a thickness of several to tens of nanometers are being used in the semiconductor and display industries. Managing the composition and thickness of nanoscale thin films is critical for the process. Therefore, reliable measurement and analysis methods are necessary.

MEIS technology is particularly suitable for these needs as it can provide nanoscale thin film composition, thickness, and quantification of each element (atoms/cm²) at the atomic layer level. In particular, Time-of-Flight Medium Energy Ion Scattering (TOF-MEIS) is attracting attention as a method that allows quantitative analysis without considering ion neutralization because of measuring the flight time of scattered particles after ions are incident into the sample. A numerical approach is used when analyzing the MEIS ion scattering spectrum, and various theoretical models are included. To obtain accurate elemental quantification (atoms/cm²), it is important to select an appropriate screening model for the incident ions.

MEIS has a scattering process mechanism the same as RBS, but the range of the incident ion energy is different. In the 1-2 MeV region used for RBS, the screening effect can be ignored. Allowing accurate quantification using Rutherford cross sections that consider only inter-nuclear interactions, which can serve as a reference for quantification. [1] To determine the most suitable screening model for MEIS, the quantitative values for various elements were compared by analyzing ion scattering spectra obtained from the same sample with 150 keV He⁺ and 1-2 MeV He ions incident

In this study, MEIS spectra were measured using 15 nm Cr, Ti, In, Mo, Ti; 20 nm Ge; 50 nm IGZO; and 60 nm PtNi alloy samples. Quantitative values for each element were analyzed using Anderson, Molière, and ZBL screening models. Among these, the screening model with the best quantitative consistency compared to RBS was determined to be the most appropriate model.

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Elemental distribution analysis of nanoparticles by atom probe tomography

Ji Yeong Lee^{1*}, Su-Jin Yoon², Yun-Sik Nam¹, Yanghee Kim¹, Gi Hoon Park¹, Young Woo Jeong¹, Min Ju Cha¹, Ye Ji Lee¹, Hae-Ryoung Kim¹, Byung Yong Yu¹, and Jae Pyoung Ahn¹

¹Advanced Analysis Data Center, Korea Institute of Science and Technology, Seoul, Korea ²Center for Water Cycle Research, Korea Institute of Science and Technology, Seoul, Korea *leejy@kist.re.kr

Atom probe tomography (APT) has many kinds of advantages like as three-dimensional atomical resolution, high sensitivity of 10 ppm. Accurate imaging and compositional analysis have also been the key driving technological factor for advances in semiconductor, Li ion battery, display, thermoelectric devices, and oxide semiconductors. APT has been developed to characterize nanoscale feasures of materials, which is a unique instrument for three-dimensional analysis with atomic resolution.

We introduce the specimen preparation method for APT analysis of nanoparticles. We measured several kinds of nanoparticles such as Au nanoparticles, core-shell nanoparticles, ZnSe nanoparticles, silver nanoparticles. Herein, we investigated highly sensitive colorimetric determination of chlorite ion based on selective etching of concave cubic gold naoparticles lie as figure 1.



Figure 1. Schematic illustration of the concave cubic Au nanoparticles etching process upon the adition of $CIO_{2^{-}}$ (0.15 μ M) after 30 min incubation.

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Enhancing nanoscale resolution in AFM images using deep learning algorithm

Jeongwoo Yang,* Jintae Moon, Panithan Sriboriboon, Yunseok Kim*

Sungkyunkwan University, Suwon 16419, Korea *yunseokkim@skku.edu

As the size of devices in the semiconductor industry shrinks to nanoscale, the importance of acquiring improved image resolution and analyzing the accurate surface of devices have increased. Atomic force microscopy (AFM) is one of the most powerful practical techniques for investigating the properties of materials at the nanoscale dimension. However, it requires a fairly long time to obtain clear and accurate images from AFM measurements. So, the needs for research that can achieving high-resolution images from AFM with high throughput has increased. In previous reports, convolutional neural networks have applied to enhance image resolution, improving the study of medical images such as CT scans and MRIs. Referring to previous studies, we utilized deep neural networks to improve the resolution of images of patterned silicon oxide, which were obtain from AFM measurements. We demonstrate that the result of our study would be applied to not only augments the quality of low-resolution images but also reduces the time required for high throughput. We also anticipate that our approach can be extended to various other patterned materials, fascinating more efficient data analysis.

Evaluation of atomic-level interfacial layer using AFM

Minhyung Kim¹, Seungjae Heo¹, Yong Hyeon Cho², Hongseok Kim¹, Min Hyuk Park², and Yunseok Kim^{1*}

¹School of Advanced Materials Science and Engineering, Sungkyunkwan University (SKKU), Korea ²Department of Materials Science and Engineering, Seoul National University (SNU), Korea *vunseokkim@skku.edu

As the scale of semiconductor shrinks to nanoscale, the space occupied by dielectric films is decreasing. In order to obtain large capacitance and high reliability in a narrow space, it is important to understand the characteristics of the interfacial layer in the dielectric films. Typically, the interfacial layer is evaluated using the C-V based EOT method. Because top electrode is deposited for the measurement, the measured value includes both upper and lower interfacial layers. Although electrical properties of these upper and lower interfacial layers can be different with each other due to the different formation mechanisms, it is difficult to evaluate them separately based this method. In this study, we propose an evaluation method of atomic-level interfacial layer based on atomic force microscopy (AFM). We employ a model system consisting of HfO₂ and Al₂O₃ in which Al₂O₃ with low dielectric constant is assumed as the interface layer and HfO₂ is assumed as the dielectric layer. The model systems with varied thicknesses are analyzed using impedance based AFM technique to evaluate the presence of an interfacial layer and changes in physical properties according to thickness. Through this approach, we are able to effectively evaluate the interfacial layer. It shows that the characteristics of the interfacial layer could be detected. AFM imaging can be served as an effective tool to explore the electrical properties of interfacial layer in dielectric films at the atomic level.

Calibration of lateral piezoelectric coefficient in atomic force microscopy

Jina Kim, Panithan Sriboriboon, and Yunseok Kim*

¹School of Advanced Materials Science and Engineering, Sungkyunkwan University (SKKU), Korea *Corresponding author: yunseokkim@skku.edu

Atomic Force Microscopy (AFM) has been widely used for studying lateral properties of materials at the nanoscale. However, quantifying lateral force signals in an AFM system is a challenging task for researchers. Lateral forces often involve complex interactions between the tip and surface, including friction and twisting effects, which can complicate measurements. Therefore, calibrating lateral forces requires a more complex calibration process compared to vertical forces. In this study, we used the Flat-Wedge method, which is based on varying the lateral output on surfaces with flat and sloped inclines to calibrate lateral forces for piezoelectric materials. Finally, we could determine the sensitivity of the lateral signal, which allowed us to calibrate the lateral piezoelectric coefficient in atomic force microscopy.

Enhancement of valley polarization of monolayer transition metal dichalcogenides by plasmonic surface lattice resonance

Changwon Seo, Eunji Lee, and Jeongyong Kim*

Department of Energy Science, Sungkyunkwan University, Suwon 16419, Republic of Korea *j.kim@skku.edu

Plasmonic resonance by collective oscillation of conduction electrons on metallic nano objects occurs at specific frequencies of illuminated light of which resonance condition depends on size, shape and kind of materials forming the metal nano object. Surface lattice resonance (SLR) that can be formed by periodically modulating the local dielectric properties usually in nanoscale dimension can be used as additional resonance mechanism to the plasmon resonance if SLR is used in metallic structures [1,2]. Simultaneous presence of these two resonances mechanism or plasmonic SLR (PSLR) can provide enhanced light-matter interaction for periodic metallic nanostructures [3]. Transition metal dichalcogenides (TMDc) is a two-dimensional semiconductor with a band gap in optical range and strong exciton emission in monolayer [4]. Due to the asymmetric atomic lattice constant between transition metal and dichalcogenide atoms, the electronic state in different valleys (K and K') are degenerate, and they can be selectively populated by using circular polarized excitation, of which phenomenon is known as a valley polarization [5].

Here, we demonstrate the method to enhance the valley polarization in monolayer molybdenum disulfide (1L-MoS₂) using an array of gold nano-rods involving PSLR. By adjusting the lattice constant of the array of gold nano-rods, PSLR frequency was matched to the exciton emission energy of 1L-MoS₂. We used lab-made angle-resolved reflectance imaging system to investigate photonic band structure of our PSLR configuration. The enhancement of the valley polarization in TMDc can offer the opportunity to develop valley polarization based quantum optical devices.

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Operando Electrochemistry: NAP-XPS on electrolyte/electrode interfaces - studies of liquid electrolytes and their interfaces to battery cathodes for Lithium ion battery applications

Paul M. Dietrich¹, Lydia Gehrlein², Julia Maibach², Andreas Thissen¹

¹SPECS Surface Nano Analysis GmbH ²Institute for Applied Materials (IAM-ESS), Karlsruhe Institute of Technology (KIT)

In this article, we present NAP-XPS results from model and commercial liquid electrolytes for lithium-ion battery production using an automated laboratory NAP-XPS system. The electrolyte solutions were i) $LiPF_6$ in EC/DMC (LP30) as a typical commercial battery electrolyte and ii) LiTFSI in PC as a model electrolyte. We analyzed the LP30 electrolyte solution, first in its vapor and liquid phase to compare in-dividual core-level spectra. In a second step, we immersed a V₂O₅ single crystal as a model cathode material in this $LiPF_6$ solution. Additionally, the LiTFSI electrolyte model system was studied to compare and verify our findings with previous NAP-XPS data. Photoelectron spectra recorded at pressures of 2-10 mbar show significant chemical differences for the different lithium-based electrolytes.



at 10 mbar and of LiTFSI in PC (lower curves) at 2 mbar. The chemical structure of LiTFSI is shown in the inset of 4b.

We demonstrate the enormous potential of laboratory NAP-XPS for investigations of solid-liquid inter-faces in electrochemical energy storage systems at elevated pressures, also illustrating the ease of use of the setup used.

Keywords: NAP-XPS, Electrochemistry, Operando Studies, Solid-Liquid Interfaces, Lithium Ion Batteries

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Quantification and reporting of XPS data taken under Near Ambient Pressure conditions – chances and challenges in acquision speed, beam damage, sensitivity, reliability, reproducibility and repeatability

Paul Dietrich and Andreas Thissen

SPECS Surface Nano Analysis GmbH, Voltastraße 5, 13355 Berlin, Germany

Over the last fifty years significant developments have been done in photoelectron spectroscopy instrumentation and thus opened new fields of application. Especially XPS or ESCA developed into a standard analytical method in many labs for surface and material characterization. The number of users and the number of publications using XPS data has tremendously increased. But as a side effect it is a challenge to keep the level of knowledge about the method and correct data interpretation at a high level for all users of these data.

To avoid errors in the interpretation of XPS data instrument manufacturers put efforts inside their instruments and software packages to help and guide the user through data acquisition, data quantification and interpretation and finally also through data reporting. By this data can be made compatible with existing ISO and other community standards. But even more, data quality becomes transparent also in times of open source publications and open data repositories.

For the last ten years XPS under near ambient pressure conditions (NAP-XPS) has gained significant attention in the XPS community. The technique allows for standard analysis of samples under pressures up to about 50 mbar. This opens XPS to liquids, solid-liquid interfaces, gas-solid-interfaces, gas-liquid-interfaces. New fields like operando studies on electrochemical systems, corrosion experiments, analysis of food samples, but also studies of biological samples have been added to the XPS portfolio. The background gas pressure in such experiments is beneficial for the analysis of materials, because it avoids beam damages and degradation due to UHV conditions and also enables true non-destructive analysis of all types of degassing samples and insulators. On the other hand, the absorption of X-rays in the gas atmosphere, the emitted electrons from the gas molecules and inelastic electron scattering in the gas influences the spectral distribution of photoelectrons significantly strongly influencing elemental identification, quantification and detection sensitivity. This presentation summarizes the special challenges in the interpretation of NAP-XPS data and uses several reference samples (mostly published in Surface Science Spectra) from different fields of application. Basic concepts for identification and quantification of spectral features are demonstrated. Finally an outlook is presented how close NAP-XPS is to be a routine metrology technique.

Using lab-based HAXPES for angle resolved XPS reconstructed depth profiles of thin-films

JDP Counsell¹, <u>CJ Blomfield</u>¹, C Tupei2 and Y Li²

¹Kratos Analytical Ltd, Wharfside, Manchester, UK ²School of Electrical and Electronic Engineering, Nanyang Technological University, Singapore Email: adam.roberts@kratos.co.uk

Lab-based, high-energy X-ray photoelectron spectroscopy (XPS) was employed to determine the structure and chemical composition of HfOx thin films deposited on Alumina substrates. The demand for enhanced uniformity and control of layer thickness, driven by the reduction in device dimensions, has led to an increased adoption of atomic layer deposition (ALD). ALD has proven valuable in depositing high dielectric constant (high-k) films, enabling their widespread application in optical, optoelectronic, and electronic devices.

While standard Al K α excited XPS permitted the determination of film thicknesses up to 7nm, accurate quantification of the Si 2p peak from the substrate beyond this range was unfeasible. Employing Ag L α excitation, which results in higher kinetic energy (KE) electrons for the same photoemission peak, increased the effective attenuation length of the overlayer. In practical terms, this led to a roughly twofold increase in the sampling depth.

In this study, high-energy Ag XPS (Ag L α radiation - 2984eV) was used in a conventional angle-resolved XPS (ARXPS) experiment. The ARXPS data was analysed using a maximum entropy algorithm [1] to generate a reconstructed depth profile over an extended sampling depth provided by the higher energy excitation source. This methodology facilitated the non-destructive determination of the structure of ALD thin films composed of hafnia, alumina, and a combination of both. Importantly, the use of the higher photon energy excitation source removed the need for destructive depth profiling involving Ar-ion beams, minimizing the risk of ion beam-induced chemical changes.

The focus of the investigation included the determination of film thickness, the examination of chemistry at the interfaces, and the assessment of the utility of Ag L α excited XPS for such applications.

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Using cryo-XPS for XPS analysis of lithium-sulfur battery materials

C.J. Blomfield, J.D.P. Counsell

Kratos Analytical Ltd, Wharfside, Manchester, UK. M17 1GP

Lithium-sulfur batteries (LSBs) are appealing due to their high theoretical energy density and the low cost of raw materials. However, their commercialization has faced significant challenges, such as the volume expansion of the sulfur electrode during cycling and the polysulfide shuttle effect. To overcome these obstacles, a comprehensive understanding of the Li-S system's underlying mechanisms and chemistry is essential.

X-ray photoelectron spectroscopy (XPS) is a powerful tool for analyzing LSBs, as it can reveal the oxidation states of sulfur and carbon in the electrode materials. Sulfur can exist in multiple oxidation states, ranging from -2 to +6. In LSBs, the most frequently observed states are +2 and 0, which correspond to lithium sulfide (Li₂S) and elemental sulfur (S₈), respectively. The detection of higher oxidation states, such as +4 and +6, often indicates the presence of polysulfide intermediates, which contribute to the shuttle effect.

XPS has also been used to probe the oxidation states of carbon, which can exist in various forms, such as sp^2 hybridized carbon in graphene-like structures or sp^3 hybridized carbon in amorphous carbon. The presence of sp^2 hybridized carbon suggests the formation of conductive carbon networks, enhancing electron transport and improving LSB performance.

XPS analysis can introduce spectral artifacts and alter the sample's surface chemistry due to potential surface damage. This may result in the formation of new chemical species that do not accurately represent the true surface chemistry. To address this limitation, cryo-XPS can be employed, where the sample is cooled to cryogenic temperatures prior to analysis. This approach helps stabilize the surface and minimize the formation of artifacts, providing a more accurate depiction of the surface chemistry.

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transformations. Until now these studies were limited to UHV compatible samples. EnviroMetros overcomes this constraint due to its NAP-XPS functionality and, with its HAXPES capabilities, offers new exciting possibilities for surface and bulk sensitive analysis of surface phases and generic bulk properties. The influence of gases and vapours can be studied up to 50 mbar.



Nanomaterials

Nanomaterials have attracted a lot of attention from research and industry in the past decades. Questions about the influence of the

surrounding atmosphere on the chemical composition and potential core-shell structure are ideally addressed by EnviroMETROS. The non-destructive depth profiling capabilities with different excitation energies combined with Raman and IRRAS give exciting new insights into nanomaterial structures. The variable environment allows for reactivity studies.



(주)아이엔에이코리아 서울특별시 마포구 만리재로 110 DK빌딩 12층 Tel: 02-714-5456 Fax: 02-714-5457

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Ultra low-voltage application for battery materials





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It shows the SEM images of binder residues adhering on the lithium-ion battery anode active material surface using a normal optical system at the accelerating voltage of 20 V without applying the sample bias. If the accelerating voltage were set to a several hundred volts, topographic features of the sample disappeared due to the charge-up effect, and morphology of the binder would be difficult to see. However, by decreasing the accelerating voltage to 20 V as shown in image (left), the binder was shown clearly. Image (right), enlarged from the yellow frame in image.

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Figure 1: EDS maps (same count rate/total time) from IC cross section at 15kV and 6kV using a W SEM and an FE SEM



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