NIMS AWARD SYMPOSIUM 2024

State-of-the-art Characterization to Accelerate Materials Innovation

INNOVATION CHARACTERIZATION

Abstracts

National Institute for Materials Science

Contents

Greetings from President

It is with great pleasure that I welcome you to the NIMS Award Symposium 2024. This annual event stands as a celebration of scientific excellence and innovation, recognizing outstanding contributions that have advanced the frontiers of materials science and brought transformative benefits to society. As we gather for this year's Award Symposium, I am excited to acknowledge the profound work being honored and the impact it will continue to have in shaping our future.

The 2024 NIMS Award is presented to two distinguished scientists who have made remarkable contributions to the field of materials characterization and nanoscience. Prof. Yuichi Ikuhara, from the University of Tokyo, has revolutionized our understanding of materials at the atomic scale through his pioneering work on transmission electron microscopy (TEM). His innovative techniques in high-resolution microscopy have enabled breakthroughs in the study of grain boundaries, interfaces, and dislocations, particularly in ceramics and semiconductors, leading to the development of new functional materials with far-reaching industrial applications.

Similarly, Prof. Franz J. Giessibl, from the University of Regensburg, has profoundly impacted the field of non-contact atomic force microscopy (AFM) through his invention of the qPlus sensor. This sensor has enabled atomic-level imaging with unprecedented precision and sensitivity, facilitating major advances in the study of nanomaterials and surface science. His work has provided crucial insights into atomic and molecular structures, furthering our ability to engineer materials at the nanoscale.

This year's symposium, under the theme "State-of-the-Art Characterization to Accelerate Materials Innovation", brings together experts from around the world to share their latest research and advancements. We are living in a time where the development of innovative materials is critical to addressing global challenges such as energy efficiency, sustainability, and technological transformation. The work of Prof. Ikuhara and Prof. Giessibl exemplifies how cutting-edge characterization tools are at the heart of these innovations, driving the discovery and optimization of materials that will underpin future technologies.

I would like to express my deepest appreciation to our awardees for their contributions, as well as to the distinguished speakers and participants who have traveled from near and far to be a part of this important event. I am confident that the symposium will spark meaningful discussions, inspire future collaborations, and foster new ideas that will propel the field of materials science forward.

On behalf of NIMS, I wish you all a fruitful and stimulating symposium.

Kazuhiro Hono

Kazuhiro Hono

President, National Institute for Materials Science

Program: Day1

Nov. 6, Wednesday

9:30 Registration

10:00 Opening Remarks by NIMS President Dr. Kazuhiro Hono

10:05 Greetings from MEXT

10:10 Introduction of NIMS by NIMS President Dr. Kazuhiro Hono

10:20 NIMS Award Ceremony [Chair: Dr. Takashi TANIGUCHI]

10:35 NIMS Award Winning-lecture I.
Prof. Yuichi Ikuhara (The University of Tokyo, Japan)
"Breakthrough Developments in Atomic Resolution Electron Microscopy and Its Applications for Materials Science"

11:25 NIMS Award Winning-lecture II.
Prof. Franz Josef Giessibl (Unversity of Regensburg, Germany)
"The Atom"

12:15 Photo Session and Lunch Break

Session 1: Advanced Characterization for Materials Innovation

[Chair: Dr. Koji KIMOTO]

13:30 Invited Talk ***S1-1***
Prof. Rafal E. Dunin-Borkowski (Institute for Microstructure Research, Germany)
"Advanced Transmission Electron Microscopy of Microstructure-property Relationships in Magnetic Materials"

14:00 Invited Talk ***S1-2***
Prof. Kazutomo Suenaga (Osaka University, Japan)
"Single-atom Spectroscopy in Low-dimensional Materials"

[Chair: Dr. Oscar CUSTANCE]

14:30 Invited Talk ***S1-3***
Prof. Takayuki Uchihashi (Nagoya University, Japan)
"Beyond the Static: Unveiling Single-Molecule Dynamics with High-Speed Atomic Force Microscopy"

15:00 NIMS Talk S1-4
Dr. Shigeki Kawai (Group Leader/Nanoprobe Group/CBRM)
"On-surface Synthesis Studied with High-resolution Scanning Probe Microscopy"

15:20 Coffee Break

[Chair: Dr. Yuichi YAMASAKI]

15:40 Invited Talk ***S1-5***
Prof. Masaki Takata (Tohoku University, Japan)
"Building a New Range of Synchrotron Radiation Facility"

16:10 Invited Talk ***S1-6***
Prof. Simon J. L. Billinge (Columbia University, USA)
"Real Materials in Action: Studying Structure on Different Length and Time-scales"

16:40 NIMS Talk ***S1-7***
Dr. Shinji Kohara (Group Leader/Quantum Beam Diffraction Group/CBRM)
"Structure and Thermophysical Properties of High-temperature Levitated Liquids"

17:00 Dr. Masanobu Naito (Deputy Editor-in-Chief of STAM / Deputy Director, Research Center for Macromolecules and Biomaterials, NIMS)
"Introduction to Science and Technology of Advanced Materials (STAM), a leading international open access journal in materials science"

17:10 Poster Session/Coffee Break

18:00 NIMS Award Reception

Program: Day2

Nov. 7, Thursday

9:30 Registration

Session 2: Synchrotron Spectroscopy and Imaging

[Chair: Dr. Koichiro YAJI]

10:00 Invited Talk ***S2-1***
Prof. Changyoung Kim (Seoul National University, Korea)
"Manipulation & Detection of Electronic States of Atomically Thin Films of Quantum Materials"

10:30 Invited Talk ***S2-2***
Dr. Hendrik Ohldag (Lawrence Berkeley National Laboratory, USA)
"Complex Materials at Device Relevant Time- and Length-scales - A Soft X-ray Spectromicroscopy Study"

11:00 Invited Talk ***S2-3***
Prof. Yukio Takahashi (Tohoku University, Japan)
"Visualization of Nanoscale Structures and Chemical States by Coherent X-ray Diffraction Imaging"

11:30 NIMS Talk ***S2-4***
Dr. Yuichi Yamasaki (Team Leader/Synchrotron Radiation Imaging Team/ CBRM)
"Synchrotron Radiation Imaging for Magnetic Materials Research"

11:50 Lunch Break

Session 3: Scanning Probe Microscopy

[Chair: Dr. Shigeki KAWAI]

13:00 Invited Talk ***S3-1***
Prof. Lifeng Chi (Soochow University, China)
"From N-alkane to Conjugated Polyene and Their Aromatization via On-surface Chemistry"

13:30 Invited Talk ***S3-2***
Prof. Yasuhiro Sugawara (Osaka University, Japan)
"Optical Imaging of a Single Molecule with Subnanometer Resolution by Photoinduced Force Microscopy"

14:00 Invited Talk ***S3-3***
Prof. Soo-hyon Phark (Institute for Basic Science (IBS), Korea)
"A Qubit Platform Crafted Atom-by-atom"

14:30 NIMS Talk ***S3-4***
Dr. Shunsuke Yoshizawa (Senior Researcher/Nanoprobe Group/CBRM)
"Imaging Quantum Phenomena with Scanning Tunneling Microscopy"

14:50 Coffee Break

Session 4: Advanced Electron Microscopy

[Chair: Dr. Kazutaka MITSUISHI]

15:10 Invited Talk ***S4-1***
Prof. Yasukazu Murakami (Kyushu Univeresity, Japan)
"Electron Holography Studies on the Charging State of Catalyst Nanoparticles"

15:40 Invited Talk ***S4-2***
Prof. Colin Ophus (Stanford University, USA)
"New Dimensions in Phase Contrast Scanning Transmission Electron Microscopy"

16:10 NIMS Talk ***S4-3***
Dr. Naoyuki Kawamoto (Principal Researcher/Electron Microscopy Group/CBRM)
"Thermal Transport Measurements Using Thermocouple Probing in Pulsed STEM"

16:30 Poster Award Presentation/ Closing

16:40 Poster Session (with Light Meal)

Poster Presentation List

1. Advanced Characterization for Materials Innovation

No	Name	Affilication/Company	Presentation Title	Award Nominee
P1-01	Tatsuya Nakamura	Institute of Science Tokyo	Thickness-dependent Electronic Structures and Transport Properties of K-intercalated Graphene	🎀
P1-02	Riku Gotoh	Tokyo Univ. of Science	Operando Study of Graphene Charge Transfer Through Micro-Raman Spectroscopy and Machine Learning	🎀
P1-03	Koji Ohara	Shimane Univ.	Lithium ion Transport Environment in Ion-Conducting Glasses	🎀
P1-04	Hajime Matsumoto	Mitsubishi Chemical Co.	Microstructure of Light-emitting Phosphor of (Sr, Ca)$AlSiN_3$:Eu^{2+}	
P1-05	Shuya Sato	Tokyo Univ. of Science	Structural Analysis of Densified SiO_2 Glass Synthesized under Extreme Conditions using Quantum Beam	🎀
P1-06	Yohei Onodera	NIMS	Investigation of the Formation of a Zirconium Oxide Crystal Nnucleus in the Initial Nucleation Stage in Aluminosilicate Glass	🎀
P1-07	Yen-Ju Wu	NIMS	Structural Insights into Thermal Conductivity of Amorphous Germanium Using Topological Data Analysis	🎀
P1-08	Shino Hayafune	Tohoku Univ.	Structural Properties of Na_2O-SiO_2 Melts under High Pressure, as Revealed by X-ray Diffraction and Molecular Dynamics Simulation	🎀
P1-09	Koji Kimura	Nagoya Institute of Technology	Phonon Dispersions of Element-doped Fe_2VAl Thermoelectric Compounds Studied by Inelastic X-ray Scattering	🎀
P1-10	Yasuaki Miyakawa	Institute of Science Tokyo	Formation of Ultrathin Oxide Films and Controlled Single-Photon Emitters at SiC Interfaces	🎀
P1-11	Sumbal Jamshaid	Univ. of Erlangen-Nürnberg	Synthesis and Characterization of $BaZrS_3$ Thin Films for Photovoltaic Applications using a Stacked Elemental Layer Methodology	🎀
P1-12	Mitsunori Kurahashi	NIMS	Spin-dependent O_2 Chemisorption and Catalytic CO Oxidation on Magnetized PtCo Surface	
P1-13	Masataka Tansho	NIMS	Adjacent Elemental Analysis of Oxide Fuel Cell Materials by High Field Solid-state NMR	
P1-14	Atsushi Goto	NIMS	NMR Techniques for the Detection of Photo-induced Effects in Solids	
P1-15	Kenjiro Hashi	NIMS	Development and Application of High-temperature NMR	
P1-16	Ta-Te Chen	Nagoya Univ.	Characterization of the Tensile Properties of GAN-generated 3D Microstructures in Dual-Phase Steels	🎀
P1-17	Dayuan Liu	NIMS	Characterization of Mechanical Properties of Alloys Using Neighboring Indentation Test	🎀
P1-18	Sherjeel Mahmood Baig	NIMS	Pt_5Ce Single Crystal Ingot: Nanophase Separation from Synthesis to Characterization	🎀
P1-19	Ryo Murakami	NIMS	Automatic Identification of Crystalline Phases Using Bayesian Estimation in XRD	🎀
P1-20	Keyun Gu	NIMS	Revealing the Surface Adsorbates of Diamond Using MEMS Resonators	🎀
P1-21	Rabindra Nath Acharyya	NIMS	Nitrogen-Doped Cobalt/Carbon Composite from Metal Organic Framework on Fullerene Self Assemblies (MOFOF) for Energy Conversion Application	🎀
P1-22	Yasutaka Imanaka	NIMS	Magneto-optical Studies in 2D Carrier Systems of Semiconductor and Semimetal under High Magnetic Field	

2. Synchrotron Spectroscopy and Imaging

No	Name	Affilication/Company	Presentation Title	Award nominee
P2-01	Shingo Takezawa	Tokyo Univ. of Science	Electronic State Analysis of Ultra-thin Cu Film on FeCo/MgO(100)	
P2-02	Thang Dinh Phan	NIMS	Electronic Properties of Chemical Vapor Deposition-grown Graphene on Ni (111) Investigated by Spin- and Angle-resolved Photoemission Spectroscopy	
P2-03	Koichiro Yaji	NIMS	Visualization of Spin-polarized Electronic States by Imaging-type Spin-resolved Photoemission Microscopy	
P2-04	Shunsuke Tsuda	NIMS	Angle-resolved Photoemission Spectroscopy of Polycrystalline Materials Using an Imaging-type Photoemission Microscope	
P2-05	Jiangwei Liu	NIMS	Calibrating Binding Energy for Insulating/Semi-Insulating Carbon-Related Materials in X-Ray Photoelectron Spectroscopy Measurements	
P2-06	Yuta Ishii	NIMS	Time- and Space-resolved Soft X-ray Microscopy for Magnetic Materials	
P2-07	Naoka Nagamura	NIMS	Machine-Learning Based Analysis for Synchrotron X-ray Spectral Imaging	
P2-08	Kentaro Fuku	Tokyo Univ. of Science,	XANES Spectral Analysis of Ni Complexes Using Machine Learning	
P2-09	Yasuhiko Igarashi	Univ. of Tsukuba,	Sparse Coding-Based Multiframe Superresolution for Efficient Synchrotron Radiation Microspectroscopy	
P2-10	Naoki Yamane	Univ. of Tsukuba	High-speed Measurement of MOF Using Sparse-view XAFS-CT Reconstruction with Compressed Sensing	
P2-11	Masashi Ishii	NIMS	Implementation of an Ontology Framework for Integrating Synchrotron Radiation Data	

3. Scanning Probe Microscopy

No	Name	Affilication/Company	Presentation Title	Award Nominee
P3-01	Oscar Custance	NIMS	Defect Identification at Confined CO_2 Islands Using SPM	
P3-02	Tatsuhiro Hirai	Keio Univ.	Water Adsorption on the Magnetite surface studied by scanning tunneling microscopy	
P3-03	Kewei Sun	NIMS	On-Surface Synthesis of Silicon Incorporated Carbon Nanostructures	
P3-04	Donglin Li	NIMS	On-surface Synthesis of Triaza Triangulene and Its Magnetism	
P3-05	Hironobu Hayashi	NIMS	Synthesis and Characterization of Oligoacenes	
P3-06	Yuji Isshiki	NIMS	On-surface Synthesis of Azobenzene-linked porphyrin	
P3-07	Masayuki Abe	Osaka Univ.	Studying Adsorbates on Rutile TiO_2(110) – (1×2) Surface Using Tip-enhanced Raman Spectroscopy	
P3-08	Ridwan Putraz	Hokkaido Univ.	Unveiling the Nanomechanical Phenomena in Silicon Thin Film Electrodes by Real-time Bimodal Atomic Force Microscopy Imaging	
P3-09	Masahiro Nakayama	Osaka Univ.	Mechanism of Triboelectric Charging in Fluorine-containing Monolayers Using Amplitudefeedback Frequency Modulated Scanning Force Microscopy	
P3-10	Nobuyuki Ishida	NIMS	Quantitative Characterization of Built-in Potential Profile Across GaAs p–n Junctions Using Kelvin Probe Force Microscopy	
P3-11	Tomoki Misaka	Osaka Univ.	EFM, KPFM Measurement of Photo-induced Charge Separation on F8T2 Monolayer/ TiO_2 Interface	
P3-12	Naoki Shima	Kanazawa Univ.	Surface Rsistivity Measurements Using Frequency Modulation Atomic Force Microscopy in Ultrahigh Vacuum	
P3-13	Yuya Hattori	NIMS	Measuring Electronic Structure of Thermoelectric Materials by Scanning Tunneling Microscopy	
P3-14	Junya Okazaki	The Univ. of Tokyo	Structures and Surface Conductivity on Dense Pb Monolayers Formed on Si(111) Studied by Low Ttemperature Scanning Tunneling Microscopy/Potentiometry	
P3-15	Kazuki Miyata	Kanazawa Univ.	High-speed Subnanoscale-resolution 2D/3D-AFM Imaging of Calcite Dissolution Process	
P3-16	Masahiro Haze	The Univ. of Tokyo	Role of Steps on Transport Measurements Studied by Scanning Tunneling Potentiometry	
P3-17	Yuta Okabe	Kanazawa Univ.	Preparation and Evaluation of a High-temperature Flame-etched Tungsten Tip for Scanning Probe Microscopy	

4. Advanced Electron Microscopy

No.	Name	Affilication/Company	Presentation Title	Award Nominee
P4-01	Takuro Nagai	NIMS	Visualization of Magnetic Soliton Using Aberration-Corrected Lorentz Microscopy	
P4-02	Ayako Hashimoto	NIMS	In-situ TEM Observation of Ni-based Catalysts for DRM	
P4-03	Toshiki Shimizu	Tokyo Univ. of Agriculture and Technology	In-situ Observation of Post-nucleation Process of NaCl Nanocrystals in an Aqueous Environment Using Liquid-cell Transmission Electron Microscopy	
P4-04	Kei Nakayama	Japan Fine Ceramics Center	In Situ Scanning Transmission Electron Microscopy of the MoS_2 Lithiation Process	
P4-05	Koji Harano	NIMS	Real-Time Electron Microscopic Imaging and Analysis for Single Molecules and Atomically-Precise Nanomaterials	
P4-06	Jun Kikkawa	NIMS	Application of Nanometric Thermometry Based on Electron Spectroscopy of Phonons	
P4-07	Masahiko Shimizu	Mitsubishi Chemical Co.	Direct Observation of Cu Sites in SCR Zeolite Catalysts Using Electron Ptychography	
P4-08	Hieu Duy Nguyen	NIMS	Phase Mapping of Temperature Waves in Submicron-structured Ceramics Using PSTAM	
P4-09	Ryuto Eguchi	NIMS	Interpretable Structural Evaluation of Metal-Oxide Nanostructures in STEM Images via Persistent Homology	
P4-10	Masato Suzuki	Univ. of Tsukuba	Image Processing Techniques for Unveiling the Internal Structure of Crosslinked Rubber	
P4-11	Kodai Niitsu	NIMS	Observation of Skyrmionic Vortex Using Electron Holography	
P4-12	Ovidiu Cretu	NIMS	Direct Imaging of Thermal Vibration Modes Using Frequency-Selective Electron Microscopy	
P4-13	Kazutaka Mitsuishi	NIMS	Deriving Sample Information from 4DSTEM Dataset by Electron Ptychography	
P4-14	Yu Jimbo	JEOL Ltd.	Characterization of Aberration-Corrected Lorentz TEM and STEM	
P4-15	Ankit Singh	NIMS	Observation Conditions for Grayscale HREM Image Interpretation via Persistent Homology	
P4-16	Katsuaki Nakazawa	NIMS	Development of 5-dimensional STEM and Application to Glass Transition Phenomenon	
P4-17	Han Zhang	NIMS	High Resolution and High Probe Current Electron Microscopy Application for LaB6 Nanostructured Emitter	

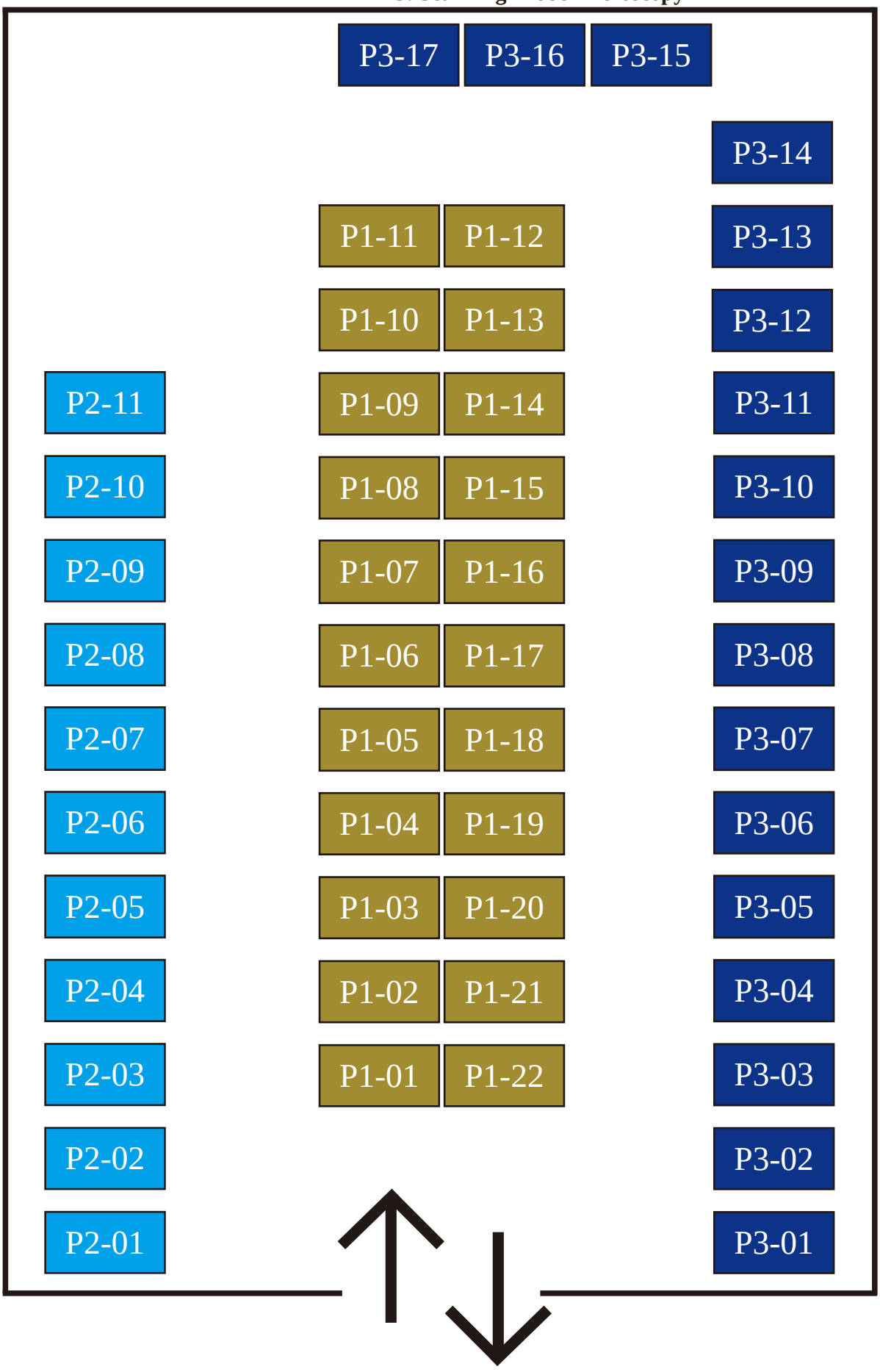
5. Others

No	Name	Affilication/Company	Presentation Title	Award Nominee
P5-01	Bo Da	NIMS	Simulation of Diffractive Electron Lenses Using Monte Carlo Method	
P5-02	Ikumu Watanabe	NIMS	Computational Simulation of Material behavior using Image-based Finite Element Modeling	
P5-03	Yibin Xu	NIMS	Development of Fundamental Technologies for Data-Driven Battery Material Exploration	
P5-04	Yukinori Koyama	NIMS	Exploration of Novel Eu^{2+}-Activated Phosphor Materials Using a Data-driven Approach	
P5-05	Fumihiko Uesugi	NIMS	A Feature Mining Method Composed of Wavelet Filtering and PCA	
P5-06	Daichi Ishikawa	Tokyo Univ. of Science	Information Extraction from Fermi Surfaces Using Unsupervised Machine Learning	
P5-07	Keisuke Sagisaka	NIMS	Predictive Modeling of Two-Dimensional Electron Gas Formation at the β-$FeSi_2$/Si(001) Interface	
P5-08	Yukari Katsura	NIMS	Starrydata: an Open Database of Experimental Measurement Data from Published Plots	
P5-09	Soichi Takase	Tokyo Univ. of Science	Fermi Surface Analysis of Multi-component Co-based Heusler Alloys Using Machine Learning	
P5-10	Toshiro Osawa	Tokyo Univ. of Science	Real-time in-situ Machine Learning Analysis of RHEED Images for MBE Film-growth	
P5-11	Yoshiaki Toda	NIMS	Exploration of New Alloy Compositions Using Prediction Model of Precipitation by Energetics	
P5-12	Masahiko Demura	NIMS	Inverse Design Based on the Concept of Materials Integration	
P5-13	Hitoshi. Izuno	NIMS	A Tandem Bayesian Model for Probabilistic Search to Improve Weld Joint Creep Property	
P5-14	Atsushi Togo	NIMS	First-principles Calculation of Electron-phonon Interaction	
P5-15	Naoki Kikugawa	NIMS	Physical Properties of Quantum Materials under Low Temperature and High Magnetic Field	
P5-16	Yuhang Zu	The Univ. of Tokyo	Observation of Nematicity in the Normal Sstate in Sr-doped Bi_2Se_3	
P5-17	Supicha Trakuldit	Waseda Univ.	Enhancing Corrosion Resistance by Electrodeposition of Mg-Al Layered Double Hydroxide (LDH) for AA6061 Alloy	

No.	Name	Affilication/Company	Presentation Title	Award Nominee
P5-18	Akito Tateyama	Hokkaido Univ.	Supercooled π-Gels Based on A Chiral Alkylated–Carbazole Liquid	
P5-19	Kanji Takehana	NIMS	Development of the Terahertz Magneto-spectroscopic System with Helium-3 Refrigerator	
P5-20	Robert Saraczyn	Warsaw Univ. of Technology	Physical Modelling of Spatial Geometries at the Micro- and Macroscale Based on the Percolation Phenomenon	
P5-21	Maria Thea Rane Clarin	Univ. of Tsukuba	Anti-inflammatory Nanoparticles as Potential Treatment for Aortic Dissection	
P5-22	Cong Zhang	NIMS	Rational Ligand Design for Enhanced Carrier Mobility in Self-powered SWIR Photodiodes Based on Colloidal InSb Quantum Dots	
P5-23	Ai Koizumi	NIMS	Does Uncertainty-based Active Learning Work in Materials Science?	
P5-24	Nur Shamimie Nadzwin Hasnan	Univ. Kebangsaan Malaysia	Kapok Microtubules Incorporated Carbon-Doped Graphitic Carbon Nitride for Photocatalytic H_2O_2 Production	
P5-25	Souta Miyai	Oita College	Differences in Hydrogen Behavior Depending on Vanadium Grain Size	
P5-26	Sabina Shahi	Univ. of Tsukuba	Energy Performance Advancement by Tuning Nanospace of Hollow Carbon Spheres	
P5-27	Shinji Matsumoto	NIMS	Water-cooled Bitter Magnet for Measurement in High Magnetic Fields	
P5-28	Meiqi Zhang	NIMS	Accelerating the valid of Solid Electrolyte Candidates through Machine Learning Force Fields: A Case Study on Li_8SeN_2 and $Li_{10}GeP_2S_{12}$	
P5-29	Jiyi Yang	Tokyo Institute of Technology	AI-Assisted Crystal Plasticity Analysis of Anisotropic Cold Rolling behavior in Ni_3Al	
P5-30	Biplab Manna	NIMS	Decoding Polymer Chain Using Nano Porous Material	
P5-31	Sarita Manandhar	NIMS	Biomass-derived Carbon Nanostructures for Energy Storage Technology	
P5-32	Nasrat Hannah Shudin	NIMS	Oxidation-Triggered Nanophase Separation: Numerical Simulation and Experimental Study.	

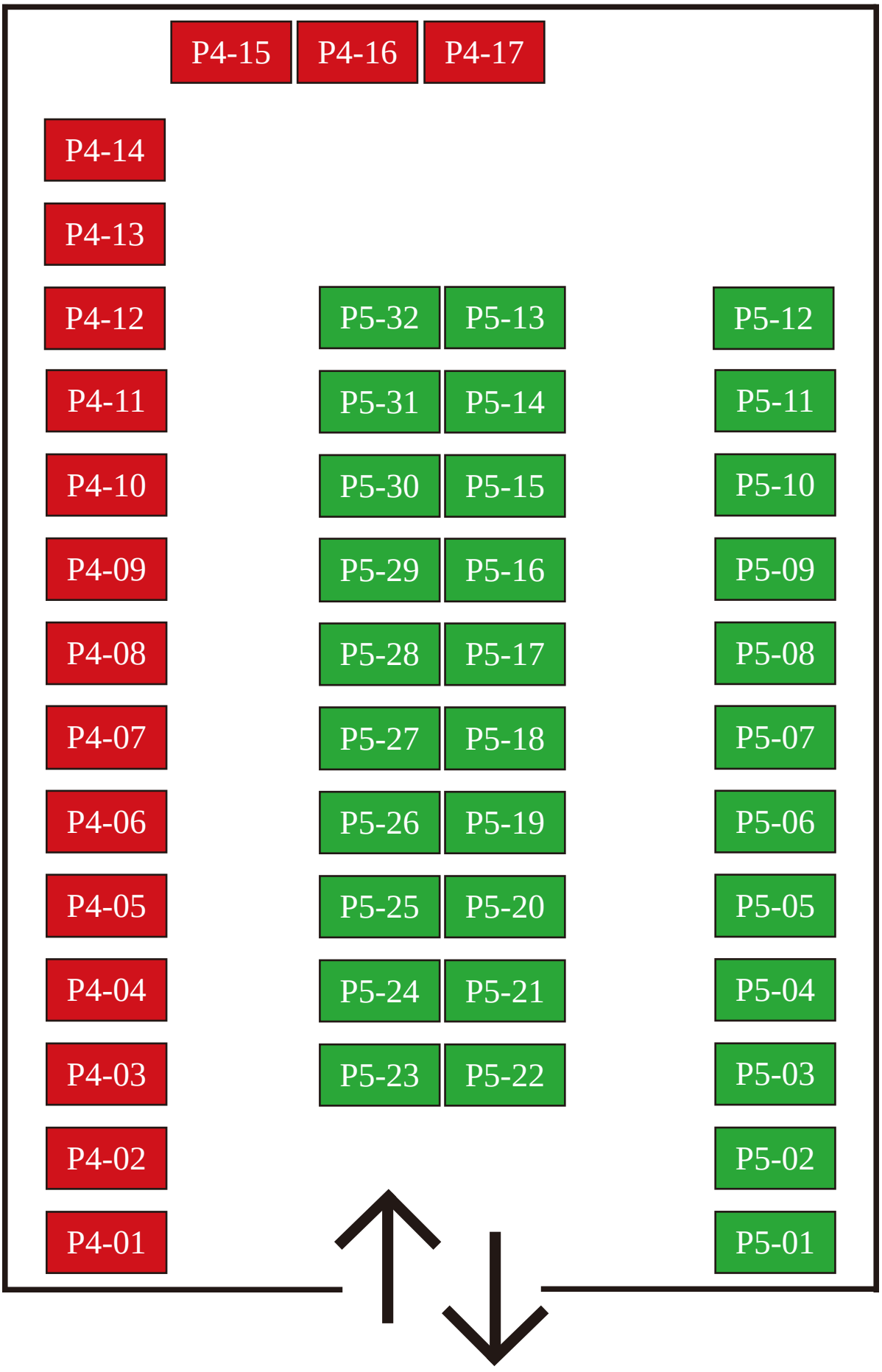
Poster Map (Room #304)

P1: Advanced Characterization for Materials Innovation
P2: Synchrotron Spectroscopy and Imaging
P3: Scanning Probe Microscopy



Poster Map (Room #303)

P4: Advanced Electron Microscopy
P5: Others



Corporate Sponsor List

NIMS AWARD 2024

NIMS Award 2024 Winner

Professor Yuichi Ikuhara from the University of Tokyo was recognized for his contributions to materials interface research through innovations in transmission electron microscopy.

Professor Yuichi Ikuhara

Institute of Engineering Innovation, School of Engineering
The University of Tokyo, Japan

[Field of Research]
Electron microscopy, grain boundaries / interfaces

Research Summary and Impact on the Adacemic and Industrial Sections

Research Acheivement Title

Contribution to material interface research through innovations in transmission electron microscopy

Outline of Awarded Research Achievement

Prof. Yuichi Ikuhara has led the development of high-resolution measurement techniques for atomic structures, electronic states, and dopant elements at grain boundaries and interfaces for many years by developing instruments and methods that expand the potential of material analysis and evaluation methods using transmission electron microscopy (TEM) [1]. Also, by combining chemical composition/chemical bonding state measurements through energy dispersive x-ray spectroscopy and electron energy loss spectroscopy[2], and theoretical analysis by first-principles calculations, he established quantitative evaluation methods for grain boundaries, interfaces, and dislocations in materials. Additionally, collaborating with electron microscope manufacturers, he developed a 300kV electron microscope with a new spherical aberration corrector and achieved the world's highest spatial resolution in scanning transmission electron microscopy (STEM) [3] using annular dark-field imaging[4]. He also developed annular bright-field STEM[5], which allows to observe light elements that are difficult to observe by conventional imaging, enabling the observation of hydrogen and lithium. These innovations in electron microscopy techniques and equipment, as well as their application to the analysis of grain boundaries and interfaces, have led to the elucidation of various mechanisms of functional expression in materials such as ceramics, thereby contributing greatly to materials science.

Ripple Effects of Achievements on Academia and Industry

Prof. Yuichi Ikuhara's achievements have had significant impacts on materials science from two perspectives: the development of innovative material measurement techniques and equipment using transmission electron microscopy, and the elucidation of grain boundary and interface atomic structures.
STEM instruments with the world's highest spatial resolution and annular bright-field STEM detectors have been commercialized and are used worldwide as innovative electron microscopes and related equipment. Additionally, research applying these innovative electron microscopy techniques to a wide range of materials such as ceramics, batteries, catalysts, semiconductors, and magnetic materials have revealed many new findings into grain boundaries and interfaces, leading to the establishment of design guidelines for new materials and the creation of novel materials.

---

1. Transmission Electron Microscopy (TEM) : A microscopy technique where electrons accelerated by high-voltage are irradiated to a thin sample, and then the electrons passing through it form a magnified image. This method provides information on the internal structure and composition of the sample.
2. Electron Energy Loss Spectroscopy: A measurement technique where the energy loss by electrons as they interact with atoms in a sample during passing through the sample is measured. This provides information on the elemental composition, chemical bonding states, and electronic structure of the sample.
3. Scanning Transmission Electron Microscopy (STEM) : A microscopy technique where a finely focused electron beam is scanned across a thin sample, and the electrons passing through it are detected to form a magnified image synchronized with the beam scan. Like TEM, this provides information on the internal structure and composition of the sample.
4. Annular Dark-Field Imaging: A technique in STEM where an annular detector is used to collect electrons scattered at high angles and form a magnified image. The contrast is generally proportional to the square of the atomic number of the sample.
5. Annular Bright-Field STEM: A technique in STEM that collect electrons scattered at low (rather than high) angles with an annular detector, forming a magnified image. Unlike annular dark-field imaging, it enables clear observation of light elements.

History

1983 - 1985	Department of Materials Science, Kyusyu University (MS)
1985 - 1988	Department of Materials Science, Kyusyu University (Dr. Eng.)
1988 - 1991	Researcher, Japan Fine Ceramics Center
1991 - 1993	Visiting Assistant Professor, Case Western Reserve University.
1993 - 1996	Managing Principal Researcher, Japan Fine Ceramics Center
1996 - 2003	Associate Professor, Department of Materials Science, The University of Tokyo
2003 - 2008	Full Professor, Institute of Engineering Innovation, The University of Tokyo
2008 -	Japan Fine Ceramics Center (Concurrent Post)
2008 -	PI, WPI-AIMR Professor, Tohoku University(Concurrent Post)
2024 -	Distinguished Research Professor, School of Engineering, The University of Tokyo

Major Awards

2023	Japan Academy Prize
2023	Henry Clifton Sorby Award, IMS, ASM International
2019	Distinguished Lecture Award, FEMMS 2019 (The Frontiers of Electron Microscopy in Materials Science International Conference)
2018	Hatsujiro Hashimoto Medal, International Federation of Societies for Microscopy
2017	Hattori Hoko Prize, Hattori Hoko Foundation
2016	Medal with Purple Ribbon, Government of Japan
2015	Sosman Award, American Ceramics Society
2015	George Weatherly Distinguished Lecture Award, Microscopy Society of Canada
2013	Academician, World Academy of Ceramics
2013	Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology
2011	Fellow, The American Ceramics Society
2010	Humboldt Research Award , Alexander von Humboldt Foundation
2010	Honda Frontier Prize from Honda Memorial Foundation
2010	Lee Hsun Lecture Award, The Institute of Metal Research, Chinese Academy of Sciences
2008	Ross Coffin Purdy Award, American Ceramics Society
2007	The Seto Prize (Academic Prize), Microscopy Society of Japan
2002	Fulrath Award (Academic), American Ceramics Society
2001	The Academic Prize, Ceramics Society of Japan
1990	Honda Silver Award, Honda Memorial Foundation

Major Publications/Books

1. Physics of Ceramics", Y.Ikuhara, Nikkan-Kogyo-Shinbun Pb. Co. (1999)
2. Transmission Electron Microscopy", S.Horiuchi, Y.Ikuhara and K.Hojo Maruzen Pub. Co.(1999)
3. Grain Boundary Engineering in Ceramics", Ed. T.Sakuma, L.Shepard and Y.Ikuhara, Ceramic.Transaction Vol.118, Am.Ceram.Soc. (2000)
4. Practical Nanomaterial Analysis", T.Yonezawa, K.Asakura and Y.Ikuhara, Kodansya Scientific (2016)

Breakthrough Developments in Atomic Resolution Electron Microscopy and Its Applications for Materials Science

Yuichi Ikuhara

[1] Institute of Engineering Innovation, The University of Tokyo, Tokyo, 113-8656, Japan
[2] Nanostructures Res. Lab., Japan Fine Ceramics Center, Nagoya, 456-8587, Japan
[3] WPI Research Center, AIMR, Tohoku University, Sendai, 980-8577, Japa

Abstract

The advent of aberration-corrected scanning transmission electron microscopy (STEM) has made it possible to analyze the atomic structure of interfaces in materials, as well as individual atomic columns, not only by identifying their positions and elements but also by assessing local composition and electronic states. Additionally, the ability to precisely apply stress and control the electron beam within the electron microscope allows for the direct high-resolution observation of dynamic phenomena such as fracture, deformation, and diffusion in materials. In this presentation, I will introduce the latest observation techniques applied to various ceramic materials and discuss the insights gained for material design guidelines and the elucidation of functional mechanisms.

Ceramic materials are composed of light elements such as oxygen and nitrogen, making the direct observation of light elements essential. However, conventional annular dark field ADF-STEM methods have made it difficult to observe light elements. To address this, our group developed the annular bright field (ABF)-STEM method, which captures electrons scattered at low angles, enabling the direct observation of light elements in materials. Using this method, we successfully observed lithium atoms in lithium-ion battery materials, which are gaining attention as energy and environmental materials, as well as hydrogen atom columns in hydrides. Moreover, we collaborated with the University of Tokyo and JEOL to enhance the resolution of STEM instruments, achieving a spatial resolution of 40.5 pm in 2017, which remains the world record for STEM spatial resolution.

In terms of material applications, in 2005, the University of Tokyo was the first in Japan to equip an existing STEM instrument with an aberration corrector, applying it to structural analysis of various materials' interfaces, grain boundaries, and dislocations. For example, the addition of trace amounts of various dopants to ceramic materials can significantly alter their mechanical and electrical properties. This method has been used to elucidate the causes and mechanisms behind such property changes. By examining ceramic interfaces with different dopants, we identified dopant segregation sites and, through the combined use of atomic-resolution EDS and EELS, were able to determine the specific elements that had segregated and measure their electronic states. We quantitatively clarified the mechanisms of these dopants by comparing the observation results with first-principles calculations. Further applications of aberration-corrected STEM include identifying the atomic positions of light elements in inorganic materials, understanding the core structures of dislocations and lattice defects, and discovering one-dimensional ordered crystals formed at grain boundary triple junctions—clarifying previously elusive material phenomena.

On the other hand, to quantitatively assess the reliability and lifespan characteristics of materials, it is essential to fundamentally understand the elementary processes of material fracture and deformation. In this context, in-situ observation and evaluation techniques within (S)TEM are invaluable for observing these elementary processes. We incorporated nanoindentation within TEM and performed dynamic observations of dislocations and microcracks during the fracture and deformation of ceramics. This allowed us to reveal previously unknown elementary processes, such as dislocation motion, dislocation-grain boundary interactions, dislocation emission from crack tips, grain boundary migration, and twin dislocation motion. Recently, we have also succeeded in atomic-level observation of grain boundary migration phenomena induced by electron beams and have developed TEM holders incorporating MEMS technology, enabling the direct observation of fracture and deformation processes at the atomic level. In this presentation, I will also discuss the impact of these cutting-edge aberration-corrected STEM techniques and high-resolution in-situ observation methods on the field of materials science.

[1] J. Yan et.al., ***Nano Letters,* 24 (10),** 3112-3117 (2024)
[2] R Ishikawa et.al., ***Microscopy,* 72 (2),** 78-96 (2023)
[3] T.Futazuka et.al., ***Nature Communications,* 13(1),** 5299, (2022)
[4] J.K.Wei et,al., ***Nature Communications,* 13(1),** 1455, (2022)
[5] J. K. Wei et al., ***Nature Materials,* 20,** 951-955(2021).
[6] C.Yang et.al., ***Acta Mater.,* 201,** 488-493, (2020)
[7] D. Yin et.al., ***Nature Materials,* 18[1],** 19-23 (2019).
[8] S. Kobayashi et al., ***Nature Communications,* 9,** 2683 (2018).
[9] S. Kondo et al., ***Science Advances,* 2 (11),** e1501926 (2016).
[10] C. Chen et al., ***Nature Communications,* 6,** 6327 (2015).
[11] I. Sugiyama et al., ***Nature Nanotechnology,* 8[4],** 266-270(2013).
[12] N. Shibata et.al., ***Nature Physics*,8[8],** 611-615(2012).
[13] Z. Wang et,al., ***Nature*,479[7373],** 380-383(2011).
[14] J. P. Buban et.al., ***Science,* 311[5758],** 212-215(2006).
[15] Y. Ikuhara, ***J. Electron Micros., Review paper,* 60,** S173 -S188 (2011).

NIMS Award 2024 Winner

Professor Franz J. Giesible from the University of Regensburg was honored for his contributions to nanomaterials research through innovation in non-contact atomic force microscopy.

Professor Franz Josef Giessibl
Institute of Experimental and Applied Physics,
University of Regensburg, Germany

[Field of Research]
Atomic force microscopy

Research Summary and Impact on the Adacemic and Industrial Sections

Research Acheivement Title

Contribution to nanomaterial research through innovations in non-contact atomic force microscopy"

Outline of Awarded Research Achievement

Prof. Dr. Franz J. Giessibl achieved atomic resolution with non-contact atomic force microscopy (AFM) for the first time in the world in 1995. He then developed the qPlus sensor[(1)], a self-sensing force sensor originally based on a quartz tuning fork, significantly enhancing the capabilities of non-contact AFM. In non-contact AFM, the probe oscillates near the sample surface and the minute forces between the sample surface and the probe are detected. Compared to the previously-used cantilever sensors, the qPlus sensor has a very high spring constant, enabling it to detect short-range forces with high sensitivity at amplitudes as small as tens of picometers, which was unattainable with cantilever sensors. This has dramatically improved the contrast at the atomic level. Using the self-sensing qPlus sensor, he also developed a scanning probe microscope capable of operating at extremely low temperatures, which is challenging with cantilever sensors, and proposed the necessary theories for high-resolution measurements. He has demonstrated the significance of these developments through numerous studies on nanomaterials.

Ripple Effects of Achievements on Academia and Industry

Atomic force microscopes utilizing the qPlus sensor developed by Prof. Dr. Franz J. Giessibl have been commercialized and over 500 units have been sold worldwide. The qPlus sensor is incorporated in nearly all atomic force microscopes operating at extremely low temperatures and ultra-high vacuum. The use of these instruments has significantly advanced academic fields of surface science, surface physics, surface chemistry, and the like. Notably, the use of the qPlus sensor has enabled the observation of the internal structure of molecules for the first time, making low-temperature atomic force microscopes equipped with the qPlus sensor essential tools in surface chemistry.

1. qPlus sensor: In conventional AFM, a cantilever is vibrated, and the changes in its resonance characteristics due to interaction with the sample surface are detected using a laser or similar method to obtain information about the sample surface. On the other hand, the qPlus sensor is a force sensor modified from a watch quartz oscillator (in other words, a force sensor based on a tuning fork quartz oscillator), which unlike a cantilever, enables it to detect changes by itself. It is therefore called a self-sensing force sensor.
2. The spring constant of a cantilever ranges from 0.1 to 100 N/m, whereas the qPlus sensor has a spring constant of 1000 N/m, making it much stiffer. This stiffness allows for smaller amplitudes and makes the qPlus sensor suitable for detecting short-range interaction changes. For example, it can improve the measurement accuracy of interactions that are highly distance-dependent, such as the simultaneous measurement of tunneling currents.

History

1981 - 1982	Prediploma in precision engineering at Munich University of Applied Sciences
1982 - 1986	Master studies, Department of Physics, Technische Universität München, Germany
1986 - 1987	Exchange student, Eidgenössische Technische Hochschule Zürich, Switzerland
1987 - 1988	Diploma student with Gerhard Abstreiter, TU Munich Diplom-Physiker Univ.
1988 - 1991	PhD Student at IBM Research Munich, advisor: Nobel Laureate Gerd Binnig
1992	PhD (Dr. rer. nat.) Faculty of Physics, Ludwig-Maximilians-Universität München, Germany
1992	Postdoctoral Fellow at IBM Research Group Munich
1992 - 1995	Senior Scientist, Director of Vacuum Products, Park Scientific Instruments, USA
1995 - 1996	Senior Asscociate, McKinsey & Company, Munich office, Germany
1996 - 2006	Permanent senior researcher and lecturer at Institute for Experimental Physics, University of Augsburg, Germany
2001	Habilitiation (venia legendi), Fakultät Physik, Universität Augsburg, Germany
2005	Offers for Chaired Professorships at Universities of Bristol (UK) and Regensburg (D)
1998 – 2021	Board Member, Nanosurf AG, Liestal, CH

Major Awards

2024	Heinrich-Rohrer Grand Medal by the Surface Science Society of Japan
2023	Fellow of the American Physical Society
2023	Innovation in Materials Characterization Award, Materials Research Society, USA
2016	Feynman Prize in Nanotechnology (Experimental Category) by Foresight Institute, USA
2015	Rudolf-Jaeckel Prize of the German Vacuum Society, Germany
2014	Joseph F. Keithley Award of the American Physical Society, USA
2009	Karl Heinz Beckurts-Prize, Germany
2001	Rudolf-Kaiser-Prize, Germany
2000	German Nanoscience Prize, Germany
1994	R&D 100 Award (jointly with Brian Trafas), USA

Major Publications/Books

1. Physics of Ceramics", Y.Ikuhara, Nikkan-Kogyo-Shinbun Pb. Co. (1999)
2. Transmission Electron Microscopy", S.Horiuchi, Y.Ikuhara and K.Hojo Maruzen Pub. Co.(1999)
3. Grain Boundary Engineering in Ceramics", Ed. T.Sakuma, L.Shepard and Y.Ikuhara, Ceramic.Transaction Vol.118, Am.Ceram.Soc. (2000)
4. Practical Nanomaterial Analysis", T.Yonezawa, K.Asakura and Y.Ikuhara, Kodansya Scientific (2016)

“The atom”

Franz J. Giessibl
Chair for Quantum Nanoscience, Institute for Experimental and Applied Physics,
University of Regensburg, Germany

Abstract

A few weeks after starting a one year abroad study of physics and mathematics in the late summer of 1985 at the Federal Institute of Technology in Zurich, Switzerland, I heard rumors that in the nearby IBM Research Laboratory Rüschlikon, a new type of microscope had been invented that was capable to “see” atoms. Following a proven habit, I spent my semester breaks working in outstanding laboratories, so I applied at the IBM laboratory with a hand-written letter asking for a job in the next break. The reply suggested two projects:

a) Performing X-ray crystallography on oxides with Georg Bednorz, who later won a Nobel Prize together with Karl-Alex Müller for finding oxide based high temperature superconductors. B) Improving a six-pass tandem Fabry-Perot Interferometer with Eric Courtens such that it could resolve the tiny Brillouin scattering signals of fractons - eigenvibrations of silica aerogels [1]. I chose the second project, because I loved lasers and optics at that time and I had already done X-ray scattering on crystals at the Technical University of Munich. Eric was happy with my work and recommended me to Gerd Binnig, who was on a sabbatical at Stanford at the time. Shortly before Binnig won the 1986 Nobel Prize for Physics with Heinrich Rohrer for the invention of the scanning tunneling microscope (STM), shared with Ernst Ruska, he inspired me to finish my master degree quickly and offered to join him for a PhD thesis. He suggested three possible projects: 1. Sequencing DNA by STM; 2. Designing a tunneling detector that could measure gravity waves; 3. Improving the newly introduced atomic force microscope (AFM) such that it could resolve atoms. I chose project 3 and it has kept my life full of challenges, joy, frustrations and breakthroughs up to this day. The AFM can resolve conductors and insulators alike, so it is an incredibly useful tool for materials science and many other branches of science and technology. Imaging “the atom” has turned into a life-long passionate journey with similarities to captain Ahab’s quest for Moby Dick [2]. This journey might look utterly random, turning from an industrial research lab to a Stanford spinoff company, to management consultant McKinsey and back to academia at the Universities of Augsburg and Regensburg and revealing its captivating logic only towards the end [3].

[1] E. Courtens, J. Pelous, J. Phalippou, R. Vacher, T. Woignier, ***Phys. Rev. Lett.*, 58,** 128 (1987).
[2] H. Melville, Moby-Dick, **Harper and Brothers,** New York (1851).
[3] F. J. Giessibl, MRS Bulletin, https://rdcu.be/dGhgQ (2024).

Session1: Advanced Characterization for Materials Innovation

Invited Talk: S1-1

Advanced Transmission Electron Microscopy of Microstructure-property Relationships in Magnetic Materials

Rafal E. Dunin-Borkowski
Director, Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons,
Forschungszentrum Jülich, Germany

Abstract

The transmission electron microscope is a powerful tool for measuring not only local variations in microstructure and composition in materials, but also functional properties and dynamic processes. In particular, electron optical phase measurement techniques such as off-axis electron holography and electron ptychography can be used to record local variations in magnetic field and electrostatic potential within and outside materials with nm to atomic spatial resolution. In this talk, I will illustrate how such measurements, which can be made in the presence of external stimuli such as applied voltage, magnetic field, reduced or elevated temperature, reactive gas and light, can be used to provide unique information about microstructure-property relationships in nanoscale and nanostructured magnetic materials. The examples that I will present include: a) studies of magnetic moments in nanoscale spintronic devices of confined geometry that contain magnetic solitons; b) measurements of local variations in Curie temperature in layered oxides; c) highly complex magnetic behaviour resulting from hierarchical phase separation in multicomponent magnetic high entropy alloys. Quantitative analysis of the results is enabled by the application of a model-based iterative reconstruction algorithm, which can be used to retrieve the projected in-plane magnetization distribution from the magnetic contribution to a recorded electron optical phase image, or alternatively the three-dimensional magnetization distribution from a set of at least two tilt series of magnetic phase images. The technique is based on the optimized implementation of a forward model, which maps a given magnetization distribution onto one or more phase images, as well as on the use of a priori information about the positions and sizes of magnetic objects in the field of view. I will conclude with a brief description of plans for next-generation electron microscopes in the Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons in Forschungszentrum Jülich and plans for a European Distributed Research Infrastructure for Advanced Electron Microscopy.

Rafal Dunin-Borkowski is Director of the Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons in Forschungszentrum Jülich, Germany. He specializes in the characterization of magnetic and electronic materials at the highest spatial resolution using advanced transmission electron microscopy techniques, including aberration-corrected high-resolution transmission electron microscopy and off-axis electron holography. In 2009 he was awarded the Ernst Ruska Prize of the German Society for Electron Microscopy. In 2012, 2017 and 2019 he was awarded Advanced, Proof of Concept and Synergy Grants by the European Research Council. He has published more than 970 journal papers, conference papers and book chapters, has given more than 375 invited lectures and seminars and has received 20 prizes for papers presented at conferences and 6 prizes for science as art.

Invited Talk: S1-2

Single-atom Spectroscopy in Low-dimensional Materials

Kazu Suenaga
Distinguished professor, Osaka University

Abstract

Electron microscopy and spectroscopy are widely used to characterize various low-dimensional materials. Identifying the atomic structures and/or measurements of local optical properties are of great importance in designing nanoscale devices based on hybrid nanostructures.

Electron energy-loss spectroscopy (EELS) has been widely used for elemental identification at the single-atom limit in transmission electron microscopes (TEM) by using core-level excitations. Recent developments of monochromators after the e-beam guns have enabled us to access optical and vibrational information from the valence EELS ranges of nanometric materials with high-spatial/energy resolution. Here we show our latest studies to demonstrate the possibilities of EELS applied for low-dimensional materials. Examples for atomic defects in in-plane hybrid TMDCs, monolayer structures of metal chlorides intercalated in bi-layer graphene, surface adatoms for catalysis, two-dimensional iodine-monofluoride epitaxy, and isotopically heterogeneous graphene will be shown.

[1] Y.-C. Lin et al., Adv. Mater., article number 2007819 (2021).
[2] Y.-C. Lin et al., Adv. Mater., article number 2105898 (2021).
[3] Y.-C. Lin et al., Nano Lett., 21, 10386-10391 (2021).
[4] G. Liu et al., Nature Chem., 810-816 (2017).
[5] S. Wu et al., J. Am. Chem. Soc., 143, 9105-9112 (2021).
[6] R. Senga et al. Nature, 603, 68-72 (2022).
[7] The works presented here are supported by JST-CREST and ERC MORE-TEM projects.

Kazu Suenaga was born in Osaka in 1966. He got his Ph.D in Materials Science at the University of Tokyo in 1994. He was a postdoctoral fellow at Ecole Nationale Superieure des Mine de Paris (1994-1997) and at the Solid State Physics Laboratory in the University Paris-Sud (1997-1998). Then he joined the Japan Science and Technology Corporation (JST) as a researcher (1998-2001), National Institute of Advanced Industrial Science and Technology (AIST) (2001-2021) as a prime senior researcher, and is now a distinguished professor in Osaka University (since 2021).

Invited Talk: S1-3

Beyond the Static: Unveiling Single-Molecule Dynamics with High-Speed Atomic Force Microscopy

Takayuki Uchihashi
Professor, Department of Physics, Nagoya University

Abstract

Atomic Force Microscopy (AFM) has become an indispensable tool for visualizing biological molecules in liquid environments at nanometer resolution, enabling the observation of a diverse range of specimens from single molecules to cells. One of the most coveted capabilities of AFM was “high-speed imaging,” which held the promise of directly visualizing dynamic processes occurring at solid-liquid interfaces. This dream was realized in 2001 with the advent of high-speed AFM. Since its inception, capable of imaging biomolecules at 80 ms/frame, HS-AFM has overcome the limitations of conventional AFM, enabling the direct visualization of dynamic phenomena at solid-liquid interfaces. Over the past two decades, significant advancements in instrumentation, including reduced invasiveness and expanded functionalities, have propelled HS-AFM to the forefront of dynamic nanoscale investigations across diverse disciplines.

Beyond its initial applications in visualizing biological molecules like proteins at nanometer resolution, HS-AFM has demonstrated remarkable versatility in investigating a wide range of dynamic behaviors in various systems, including synthetic supramolecules and polymers. By capturing real-time changes in these systems, HS-AFM provides crucial insights into the mechanisms underlying molecular interactions, assembly processes, and conformational dynamics. This has led to groundbreaking discoveries in dynamic structural biology and materials science, facilitating unprecedented observations of protein conformational changes, complex interactions, and self-assembly processes.

This presentation will showcase the transformative power of HS-AFM by delving into several recent imaging applications. We will focus on the diverse types of dynamic phenomena observable with HS-AFM, encompassing conformational dynamics of biomolecules, protein-protein interactions, and the dynamic behavior of synthetic supramolecules. I will highlight how HS-AFM is not only deepening our understanding of fundamental biological processes but also paving the way for novel explorations and discoveries across a broad spectrum of scientific disciplines.

Takayuki Uchihashi is a professor of Physics Department at Nagoya University and a visiting professor of Exploratory Research Center on Life and Living Systems, National Institute of Natural Science, Japan. He received his B. Sc., M.Sc. in Physics from Hiroshima University in 1993 and 1995, respectively. In 1998, he obtained Dc. Eng. in Electronics from Osaka University. From 1998 to 2000, he worked at Joint Research Center for Atom Technology (JRCAT) in Tsukuba as a research associate. In 2000, he moved to Department of Electronic Engineering, Himeji Institute of Technology as an assistant professor. After that he moved to Trinity College in Dublin in 2002 and worked as a senior researcher in SFI Nanoscience Institute. In 2004, he joined the Physics Department, Kanazawa University as an assistance professor. He became an associate professor in 2008, and a full professor in Physics Department in 2015. In 2017, he moved to Department of Physics, Nagoya University. His research interests include the instrumentation of scanning probe microscopy and its application to biological science.

NIMS Talk: S1-4

On-surface Synthesis Studied with High-resolution Scanning Probe Microscopy

Shigeki Kawai
Group Leader / Nanoprobe Group / CBRM

Abstract

Since the invention of scanning tunnelling microscopy and atomic force microscopy, it has been explored single atoms and molecules in detail. Particularly, combining with bond-resolved scanning probe microscopy,[1] the field of on-surface synthesis has been rapidly developed.

Here, we present our recent activities about syntheses of nanocarbon structures and tip-induced manipulations of single molecules with low-temperature scanning probe microscopy. We synthesized three-dimensional organometallic compound and graphene nanoribbon by homo-coupling hexabromo substituted-propellane molecules on Au(111) and Ag(111).[2] In the structure, the C-Br bonds distant from the substrate remained intact even after the reaction. The radical species were formed by tip-induced debromination and were subsequently stabilized by either tip-manipulated Br atom or fullerene molecule. Systematic tip-induced isomerization among two chiral dehydroazulene and diradical units was demonstrated as embedding ascii texts of "NIMS" (Figure1).[3] We found that the diradical unit has the spin coupling of 90 meV. For heteroatom substitution, we presented on-surface syntheses of graphene nanoribbon and covalent organic frameworks with silabenzene units (Figure2).[4] The heavier congeners of cyclic aromatic compounds have been studied as an elusive target product for organic synthesis due to their high reactivity at ambient temperature and difficult isolation, but now became achievable.

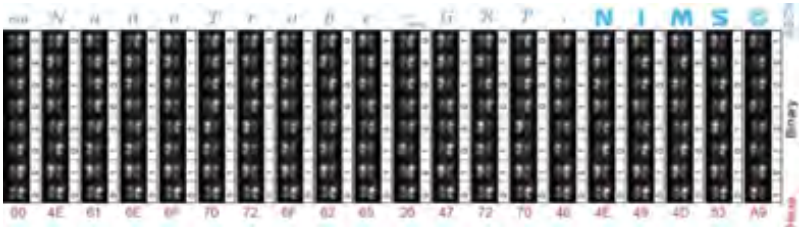


Fig. 1 Systematic local probe isomerization of azulene unit on 3D-OMC. "Nanoprobe GRP. NIMS©" in 8-bit binary ascii code is embedded via sequential 71 isomerization[3].

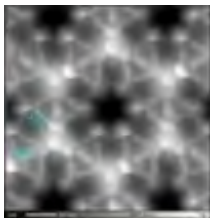


Fig. 2. Bond-resolved image of silabenzene incorporated covalent organic frameworks[4].

[1] Gross, F. Mohn, N. Moll, P. Lilkeroth, G. Meyer, Science 325, 1110 (2009)
[2] S. Kawai, et al Sci. Adv. 6, eaay8913 (2020).
[3] S. Kawai, et al Nat. Commun. 14, 7741 (2023).
[4] K. Sun et al, Nat. Chem. 15, 136 (2023).

Dr. Kawai, a leader of Nanoprobe group, Center for Basic Research on Materials, NIMS is working in the field of scanning probe microscopy, specially focusing on on-surface chemistry with high-resolution imaging. He received a PhD degree from the University of Tokyo in 2005, and worked in EMPA and University of Basel, Switzerland for almost 10 years. He came back to Japan as a NIMS principal researcher in 2016 and was then promoted to be a group leader and also an associate professor in Tsukuba University in 2020. From 2013 to 2017, he conducted JST-PRESTO in a session of Molecular Technology (Chair. Prof. Kato). So far, he has published more than 110 articles, including Science, Science Advances, Nature Chemistry, Nature Synthesis, and Nature Communications. His achievement led to the Awards of the MEXT Young Scientist's Prize, the Kazato Prize, the FY2019 JSPS Prize, and Kao Prize.

Invited Talk: S1-5

Building a New Range of Synchrotron Radiation Facility

Masaki Takata
Professor, Tohoku University

Abstract

It is no exaggeration to say that the emergence of the low-emittance 3GeV synchrotron radiation(SR) facility, NanoTerasu Light Source is being a transformative placemaking in the R&D of materials science. One of the major light source performance of the low-emittance ring, coherence, especially ought to bring be a game changer of facility application. The combination of coherent imaging & X-ray absorption spectroscopy will revolutionize nano-level visualization of materials' function relating to heterogeneous and complex structure. Furthermore, the visualization of NanoTerasu, combined with a computer simulation and/or a data science, is expected to become one of the powerful engines that accelerates Digital Transformation in materials development research, and consequently to play an important role in the problem-solving oriented science & technology.

To reinforce this, it is more effective not only to develop advanced measurement technology, but also to have a needs-pull system in which industry and academia bring issues to the facility, and an organic system that brings together researchers from various fields such as data science, AI science, and manufacturing to take on the challenge of solving problems together.

NanoTerasu is, therefore, entrusted with a mission to involve industrial sector and academia from the planning stage, contribute to science, industrial technologies, and concretize the formation of a research complex. Therefore, a new facility development approach called "Public-Private Regional Partnership" has been introduced. In addition to the nationally promoted "Public Shared Use," a new utilization scheme called "Coalition Use" is being introduced. Industries, universities, and local governments that contribute construction funds will have priority access.

"Coalition" system shall make NanoTerasu a place to take in new seeds from unexplored areas of industry, solve them with science seeds and create new challenges. So far, more than 150 companies, universities, and national research institutes have become members of the coalition through investment, and on April 9th 2024, the coalition system utilization was initiated.

The current status and prospects of facility application at NanoTerasu will be described.

Born in Kure City, Hiroshima Prefecture in 1959. In 1988, he received his PhD from Hiroshima University for studying the grain boundary structure of alloys using electron microscopy. Area of expertise is synchrotron radiation structure science. In 1995, succeeded in determining the structure of metal-encapsulated fullerenes for the first time in the world.After working asan associate professor at Nagoya University, moved to a group leader and division head of the Japan Synchrotron Radiation Research Center (JASRI/SPring-8), a senior researcher and deputy director of the RIKEN Synchrotron Radiation Research Center, assumed current position in 2015. Based on the industry-academia collaboration scheme "Coalition Concept", ushering the plan for NanoTerasu at the new campus of Tohoku University Aobayama new campus..

Invited Talk: S1-6

Real Materials in Action: Studying Structure on Different Length and Time-scales

Simon J. L. Billinge
Professor of Materials Science and of Applied Physics and of Applied Mathematics,
Department of Applied Physics and Applied Mathematics

Abstract

At the heart of materials science studies for next generation materials is an idea that we want to be studying real materials doing real things, often in real devices. In practice, this presents a number of key data analysis and interpretation challenges because it implies we are studying ever more complicated samples, often in complex heterogeneous environments and in time-resolved operando setups, and we are interrogating our data for more and more subtle effects such as microstructures and evolving defects and local structures. Advanced data analysis algorithms and software are essential for the success of this enterprise. Of particular interest is the study of nanomaterials and materials structure on different lengthscales. In this talk I will describe various developments that leverage latest data acquisiont and analysis techniques, sometimes powered by artificial intelligence (AI) and machine learning (ML), that reveal how materials behave on different length-scales and sometimes also timescales. The materials studied include materials for sustainable energy, environmental remediation, and cultural heritage studies, and techniques range from spatially resolved x-ray and electron nanostrucuture studies and neutron diffraction and scattering.

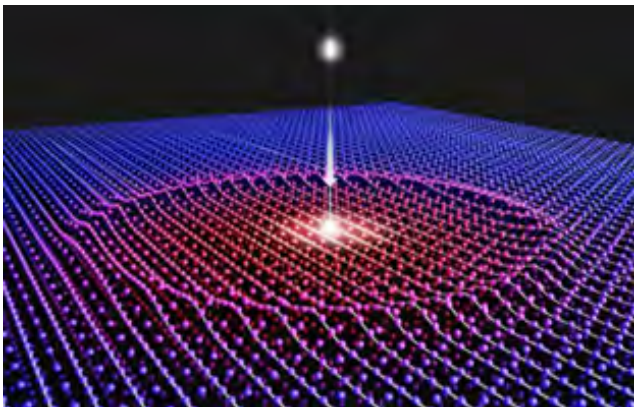


Figure caption: Schematic of a wave of structural reorganization that spreads out from a localized photo excitation even in a quantum material studied with ultrafast PDF.

Prof. Billinge has more than 25 years of experience developing and applying techniques to study local structure in materials using x-ray, neutron and electron diffraction including the development of novel data analysis methods including graph theoretic, artificial intelligence and machine learning approaches. He earned his Ph.D in Materials Science and Engineering from University of Pennsylvania in 1992. After 13 years as a faculty member at Michigan State University, in 2008 he took up his current position as Professor of Materials Science and Applied Physics and Applied Mathematics at Columbia University and held a joint position of Physicist at Brookhaven National Laboratory between 2008 and 2022. Prof. Billinge has published more than 350 papers in scholarly journals. He is a fellow of the American Physical Society and the Neutron Scattering Society of America, a former Fulbright and Sloan fellow and has earned a number of awards including the 2022 Distinguished Powder Diffractionist Prize of the European Powder Diffraction Conference, the 2018 Warren Award of the American Crystallographic Association and being honored in 2011 for contributions to the nation as an immigrant by the Carnegie Corporation of New York.

NIMS Talk: S1-7

Structure and Thermophysical Properties of High-temperature Levitated Liquids

Shinji Kohara

Group Leader, Quantum Beam Diffraction Group,Center for Basic Research on Materials (CBRM), National Institute for Materials Science (NIMS)

Abstract

Determining the liquid structure is the first step in understanding the nature of glass-liquid transitions. High quality diffraction and density data are very important in obtaining a reliable structural model by modeling or simulation. In addition, precise knowledge of viscosity is essential in order for understanding the nature of glasses and liquids. However, it is difficult to obtain these data for oxides with high melting temperatures (Tm) in the liquid state, because the samples are easily contaminated by container materials or nucleated from the heterogeneous interface between the container and the liquid. To overcome such problems, we have developed levitation furnaces that can keep high-temperature liquids in place without any contact (see Fig. 1).

The combination of quantum beam (X-ray and neutron) measurements and levitation techniques is a powerful approach to reveal the structure of high-temperature liquids, as well as of glasses with limited glass forming ability. In particular, the aerodynamic levitation technique is very useful for measuring diffraction data from oxide liquids, and preparing bulk oxide glasses with low glass forming ability. On the other hand, the electrostatic levitation furnace (ELF) is available in the international space station (ISS) KIBO for determining the density and viscosity of oxide liquids. We review scientific investigations of oxide glasses and high-temperature liquids considered by us over the past ten years [1–3].

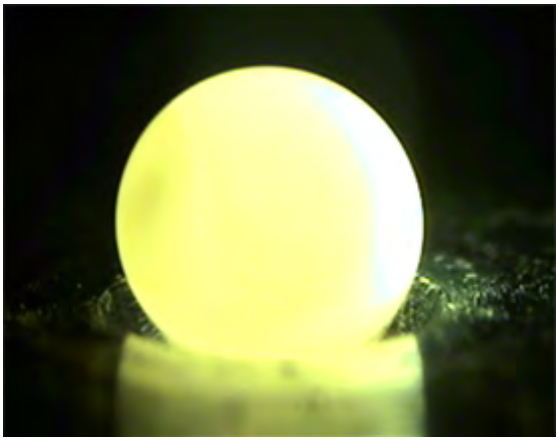


Fig. 1 Aerodynamically levitated La4Ti9O24 liquid (1800 ℃). The sample was levitated by dry air and heated by a CO2 laser.

[1] S. Kohara et al., Nat. Commun. 5, 5892 (2014)

[2] C. Koyama et al., NPG Asia Mater. 12, 43 (2020)

[3] Y. Shuseki et al., J. Phys. Chem. A 128, 716 (2024)

Shinji Kohara is the group leader of the quantum beam diffraction group in the Center for Basic Research on Materials (CBRM) at NIMS. He received his Ph.D. degree in 1998 from the Tokyo University of Science. In 1998, he was involved in the development of a dedicated high-energy X-ray diffractometer for disordered materials at the world's largest synchrotron radiation facility, SPring-8. From 2001 to 2015, he worked there as a beamline scientist. Since 2015, he has been working at NIMS. His current research interests include the inorganic chemistry and materials science of glasses, liquids, and amorphous materials.

Session2: Synchrotron Spectroscopy and Imaging

Invited Talk: S2-1

Manipulation & Detection of Electronic States of Atomically Thin Films of Quantum Materials

Changyoung Kim

Professor, Department of Physics & Astronomy, Seoul National University

Abstract

2D systems can not only have physical properties distinct from those of 3D materials but also allow control/manipulation of their properties. For example, Mott insulating and superconducting states, unavailable in a single layer graphene, are realized in twisted bilayer graphene systems. While these novel 2D systems are mostly obtained through exfoliation of van der Waals materials, a more conventional approach is to achieve it through thin film growth. In this presentation, I wish to introduce our research efforts to measure and manipulate electronic properties of a few unit-cell (uc) thick thin films by using thin film growth and in-situ angle resolved photoemission (ARPES).

We started with ARPES on a few uc thick film of $SrRuO_3$ (SRO), a prototypical metallic ferromagnet with spin-orbit coupling. It was found that nodal lines and quadratic band crossing points are generic features of ultrathin perovskite films. These symmetry-protected nodal lines and quadratic band crossing points are sources of Berry curvature that causes the sign changing anomalous Hall effects [1]. By using additional 'conducting layer', we were able to obtain the electronic structure of 1 uc thick SRO films. Our results show that 1 uc films are not insulators but remain metallic. Dosing experiments reveal that 1 uc films are correlated Hund metals caused by the high density of states near EF from the van Hov singularity [2]. We further controlled the strain and octahedron distortion of 1 uc films by using different substrates with various lattice constants. We demonstrate that the electronic state of 1 uc films can be manipulated from a good metal to a correlated Hund metal, and finally to a Mott insulator [3][4].

Our work on SRO was extended to $SrIrO_3$ (SIO) and a cuprate superconductor $(La,Sr)_2CuO_4$ (LSCO). It is found that SIO 1uc films have the electronic structure of Sr2IrO4, relativistic Mott insulating state with (short) AF order, which is not surprising considering the similarity in their crystal structure. Meanwhile, 0.5 uc LSCO (a single CuO_2 plane) shows a d-wave gap structure, strongly suggesting that superconductivity is retained even in a single CuO_2 plane.

[1] Sohn et al., NAT. MATER. 20, 1643-1649 (2021).

[2] Sohn et al., Nat. Commun. 12, 6171 (2021).

[3] Kim et al., Adv. Mater. (2023).

[4] Ko et al., Nat. Commun. (2023).

Prof. Kim received his Ph.D. in Applied Physics from Stanford University. After working at SSRL as a staff member, he took a faculty position at Yonsei University in the department of Physics. He moved to Seoul National University as a professor in the department of Physics and Astronomy as well as an associate director of the center for correlated electron systems.

His expertise is in angle resolved photoelectron spectroscopy on correlated materials, including high temperature superconductors and topological materials. His recent research interest is focused on investigation of novel electronic phases, via in-situ ARPES, that can be realized in atomically thin films of correlated materials. In addition to the atomically thin film results, his notable accomplishments include observation of spin-charge separation and discovery of the role of orbital angular momentum in solids.

Invited Talk: S2-2

Complex Materials at Device Relevant Time- and Length-scales - A Soft X-ray Spectromicroscopy Study

Hendrik Ohldag
Staff Scientist, Lawrence Berkeley National Laboratory (USA)
Adjunct Professor, Department of Material Science, Stanford University (USA)
Adjunct Professor, Department of Physics, University of California Santa Cruz (USA)

Abstract

X-ray based spectroscopy and microscopy has been shown to be a powerful tool for the characterization of complex materials on the nanoscale. Using polarization dependent effects (dichroism) we are able to learn about magnetic, structural and electronic order, with tens of nanometer spatial resolution. In addition, so called photon-in, photon-out techniques are insensitive to the presence of external stimuli or even changes in ambient conditions, which allows us to study devices in-operando in state-of-the-art x-ray microscopes. Altogether, these features have led to the development of a strong international user community with a focus on e.g. battery devices or magnetic and electric devices. However, the feature that synchrotrons are pulsed sources of x-rays is typically less used by experimentalists. Synchrotrons operate at repetition rates up to 500 Mhz producing x-ray pulses that are less than 100 picosecond long with very little temporal jitter (~10ps). By using point detectors, e.g. Avalanche Photodiodes, and fast electronics with bandwidths of 10 Ghz or more it is then possible to follow reversible processes with about 10 picosecond time resolution.

In this talk I will layout the scientific motivation of time resolved work at synchrotrons and their impact as compared to complementary dynamic studies at free electron lasers. I will then present examples of picosecond dynamics with a special focus on magnetism, e.g. spin waves in artificial nano-structures compared to spin waves in magnetosomes as produced by magnetotactic bacteria.

Dr. Ohldag received his Ph.D. in Experimental Physics from the University of Duesseldorf (Germany) in 2002. He joined SLAC National Accelerator Laboratory in 1999 as a research assistant and became a postdoctoral researcher at SLAC in 2002. In 2005 he joined the lab as a full-time staff scientist until 2018 when he became a staff scientist at the Advanced Light Source at Lawrence Berkeley National Laboratory. His expertise is soft x-ray spectroscopy and microscopy of complex materials and devices. Dr. Ohldag has been awarded the David Shirley prize at LBNL and he is a fellow of the American Vacuum Society and the American Physical Society. In addition, Dr. Ohldag was awarded a Distinguished Lectureship by the IEEE Magnetics Society in 2017. Currently he is an editor for the Nature Partner Journal Spintronics and chair of the lectureship program of the IEEE Magnetics Society.

Invited Talk: S2-3

Visualization of Nanoscale Structures and Chemical States by Coherent X-ray Diffraction Imaging

Yukio Takahashi[1,2]

[1] International Center for Synchrotron Radiation Innovation Smart, Tohoku University, Sendai 980-8577, Japan

[2] RIKEN SPring-8 Center, Sayo-gun, Hyogo 679-5148, Japan

Abstract

Coherent X-ray diffraction imaging (CXDI) is a lensless imaging technique based on the measurement of coherent diffraction patterns and phase retrieval calculation, which can realize high spatial resolution beyond the limitation of lens-based X-ray microscopy. In particular, scanning CXDI, also known as X-ray ptychography, is a technique that is rapidly gaining popularity in synchrotron radiation facilities, allowing micrometer-sized objects to be observed with nanoscale resolution. So far, we have developed a high-resolution and high-sensitivity X-ray ptychography apparatus at SPring-8 [1], and have applied it to nanoscale structural imaging of various samples. X-ray ptychography using multiple energies including the absorption edge of a specific element, which is often referred to as X-ray spectroscopic ptychography, enables us to visualize not only nanoscale structures but also chemical states. So far, we have applied it to the observation of catalysts [2] and battery [3, 4] materials. The 3 GeV high-brilliance synchrotron radiation facility NanoTerasu, which commenced operations in April 2024, provides higher brilliance synchrotron radiation than SPring-8 in both the soft X-ray and tender X-ray regions. We have performed the first experiment of tender X-ray ptychography at NanoTerasu. The coherent diffraction patterns from a micrometer-sized particle of sulfurized polymer were collected, and then the phase image was reconstructed with resolutions of sub-50 nm [5]. In the near future, tender X-ray ptychography with sub-10 nm resolution is anticipated to potentially revolutionize the visualization of nanoscale structures and chemical states in various functional materials composed of light elements.

[1] Y. Takahashi et al., Phys. Rev. B 83, article number 214109 (2011).

[2] M. Hirose et al., Commun. Chem. 2, 50 (2019).

[3] H. Uematsu et al., J. Phys. Chem. Lett. 12, 5781-5788 (2021).

[4] M. Abe et al., J. Phys. Chem. C 126, 14047–14057 (2022).

[5] N. Ishiguro et al., Appl. Phys. Express 17, article number 052006 (2024).

Yukio Takahashi is a professor at International Center for Synchrotron Radiation Innovation Smart (SRIS), Tohoku University. His research interests lie in the development of novel coherent X-ray diffraction imaging techniques for characterization of functional materials. He received his PhD degree in engineering from Tohoku University in 2004. After a two-year postdoctoral researcher at RIKEN SPring-8 Center, he became a lecturer at Osaka University in 2007 and an associate professor in 2011. He became a professor at Tohoku University in 2019. He was awarded the MEXT prize for young scientists in 2011, and the Kohra-Sasaki prize of the Japanese Society for Synchrotron Radiation Research in 2024.

NIMS Talk: S2-4

Synchrotron Radiation Imaging for Magnetic Materials Research

Yuichi Yamasaki

Team Leader, Synchrotron Radiation Imaging Team, Center for Basic Research on Materials (CBRM), National Institute for Materials Science (NIMS)

Abstract

Research on magnetic materials using synchrotron radiation imaging is an advanced technology for precisely analyzing the magnetic properties of materials at the nanoscale. Synchrotron radiation, with its significantly higher energy and brightness compared to in-house X-rays, allows for detailed visualization of the internal structures and properties of materials. When applied to magnetic material research, this technology enables the observation and analysis of fine structures, magnetic domain dynamics, and magnetic anisotropy at the nanoscale.

In magnetic material research using X-ray absorption, X-ray magnetic circular dichroism (XMCD), where the absorption of circularly polarized X-rays varies depending on the direction of the magnetic moment, is utilized to visualize microscopic images of magnetic materials by obtaining spatial distributions of absorption. We have been developed measurement systems such as the scanning X-ray microscopy (SXM) method, which acquires microscopic images by focusing X-rays using a Fresnel zone plate and scanning the sample, and the coherent diffraction imaging (CDI) method, which utilizes the high coherence of synchrotron radiation X-rays. These techniques have advanced research on visualizing magnetic skyrmions and topological materials, contributing to the investigation of emergent physical properties. Recently, it has been demonstrated that not only ferromagnetic materials but also antiferromagnetic materials, where magnetic moments cancel each other out, can be visualized by XMCD [1,2]. In this presentation, I will introduce recent research on magnetic materials using synchrotron radiation imaging.

[1] Y. Yamasaki, H. Nakao, and T. Arima, J. Phys. Soc. Jpn. 89, 083703 (2020)
[2] M. Kimata, Y. Yamasaki et al., Nature Communications 12, 5582 (2021)

Received his Ph.D. in Engineering from the University of Tokyo in 2009. From 2009, he worked as an assistant professor at synchrotron radiation facility, Photon Factory, the High Energy Accelerator Research Organization (KEK), and from 2014, he was a project lecturer at the University of Tokyo. Since 2017, he has been with NIMS. At synchrotron radiation facilities, he has advanced the development of cutting-edge measurement techniques, particularly in resonant X-ray scattering, imaging techniques, and time-resolved measurement methods. By elucidating electronic states through X-ray absorption and scattering, he promotes research on emergent properties in strongly correlated electron oxide systems, magnetic skyrmions, topological materials, and altermagnet materials.

Session3: Scanning Probe Microscopy

Invited Talk: S3-1

From N-alkane to Conjugated Polyene and Their Aromatization via On-surface Chemistry

Lifeng Chi
Institute of Functional Nano & Soft Materials (FUNSOM), Soochow University, Suzhou, China
E-mail: chilf@suda.edu.cn

Abstract

On-surface chemistry is an emerging interdisciplinary discipline developed in recent years, which presents the great potential in breaking through limitations of traditional chemical synthesis and accurately preparing functional molecular nanostructures. After a series of explorations to address the challenging scientific problem of selective C-H bond activation and C-C coupling of saturated alkanes on Au(110) surface [1,2], we further realized the conversion of normal alkanes to conjugated polyenes on the surface of Cu(110) and interpreted the underline mechanisms[3-6]. More recently, we demonstrated the high selective dehydrogenative aromatization of n-alkane on different metal surfaces. Thereby new methods for the on-surface conversion from n-alkane to conjugated polyene and their aromatization are established.

[1] D. Y. Zhong et al., Science 334, 213(2011).
[2] K.W. Sun et al., J. Am. Chem. Soc. 140, 4820(2018).
[3] X.C. Li et al., Nat. Sci. Rev. 8, nwab093 (2021).
[4] Z.M. Hao et al., J. Phys. Chem. Lett. 13, 3276(2022).
[5] Y.N.Tang et. al., Angew. Chem. Int. Ed. 61, e202204123(2022).
[6] L.N. Wang et al., Angew. Chem. Int. Ed. on-line (2024).

Lifeng Chi obtained her PhD in Max-Planck-Institute for Biophysical Chemistry (University of Goettingen) in 1989 and then went to University of Mainz and BASF working as a Postdoc. She became a Group Leader in Physics Institute of Muenster University from 1993 and granted a Lisa Meitner stipendium in 1997. She received National Outstanding Youth Science Foundation (Type B) of China in 1999 and became a professor in physics of Muenster University in 2004. In 2012, She was appointed as a chair professor in Soochow University. She was selected as a Foreign Academician of Academia Europaea, an Academician of Chinese Academy of Sciences and a Fellow of the World Academy of Sciences for the Advancement of science in developing countries (TWAS) respectively in 2020, 2021 and 2023. She obtained the 2016 ACS Nano Lectureship Award and received Distinguished Women in Chemistry/Chemical Engineering Award of IUPAC in 2017. Currently, she is serving as the Associate Editor of ACS Nano and Chemical Research in Chinese Universities. Up to now, she has presided over 20 national-level research grants and published nearly 500 papers.

Invited Talk: S3-2

Optical Imaging of a Single Molecule with Subnanometer Resolution by Photoinduced Force Microscopy

Yasuhiro Sugawara
Professor, Department of Applied Physics, Osaka University, Japan

Abstract

Visualizing the optical response of individual molecules is a long-standing goal in catalysis, molecular nanotechnology and biotechnology. The molecular response is dominated not only by the electronic states in their isolated environment but also by neighboring molecules and the substrate. Information about the transfer of energy and charge in real environments is essential for the design of desired molecular functions. However, visualizing these factors with spatial resolution beyond the molecular scale has been challenging. Recently, a new optical microscopy concept (photoinduced force microscopy: PiFM) [1], which detects the intensity distribution of near-field light localized on a material surface as a force, has attracted much attention as a method to study the local optical response of materials. The dipole–dipole interaction between the dipole induced by the tip and the dipole induced by the sample surface is measured as a photoinduced force. The local optical responses of materials can be visualized with high spatial resolution because the photoinduced force is inversely proportional to the fourth power of the tip–sample distance. Since PiFM is based on atomic force microscopy (AFM), the structure of the sample surface, including insulator surfaces, can be observed, and the charge transfer (or change in the contact potential difference (CPD)) of the sample can be measured by using Kelvin probe force microscopy (KPFM). PiFM is an ideal experimental platform for studying the optical response of materials at the nanoscale, which has not been previously investigated in detail.

Here, by combining PiFM and KPFM, we have mapped the photoinduced force in a pentacene bilayer with a spatial resolution of 0.6 nm and observed its ‘multipole excitation’ for the first time [2]. We identified the excitation as the result of energy and charge transfer between the molecules and to the Ag substrate. These findings can only be achieved by combining microscopy techniques to simultaneously visualize the optical response of the molecules and the charge transfer between the neighboring environments. Our technique and findings open up the possibility of designing molecular functions from the optical response at each step of stacking molecules layer by layer.

[1] J. Yamanishi et al., Nat. Commun.,12, article number 3865 (2021).
[2] T. Yamamoto et al., ACS Nano, 18(2), 1724-1732 (2024).

Yasuhiro Sugawara received his Ph.D. degree from Tohoku University, Japan in 1988. He has been a professor at the Department of Applied Physics, Graduate School of Engineering, Osaka University, Japan. He is a nano-physist working in the interdisciplinary areas on nanoscience and nanotechnology using scanning probe microscopy. His research topics are nanophotonics, charge manipulation, nanomagnetism, the characterization of nanostructures, catalytic reactions on nanostructures, and atom manipulation. He explores the novel physical and chemical phenomena in a nano-meter scale. He is awarded Metal Investigation Encouragement Prize, Andoh-Hiroshi Memorial Prize, and Nanoprobe Technology Prize.

Invited Talk: S3-3

A Qubit Platform Crafted Atom-by-atom

Soo-hyon Phark
Center for Quantum Nanoscience, Institute for Basic Science, Korea
Ewha Womans University, Korea

Abstract

Atom-by-atom addressability, unique in the scanning tunneling microscopy (STM) [1], has enabled control of atomic-scale quantum objects as well as bottom-up design of functional quantum devices. A recent advance in the STM equipped with electron spin resonance (ESR), combining high spatial resolution of STM and high energy resolution of ESR, has enabled magnetic resonance of individual spins on surfaces [2], which raised on-surface single spins as a promising qubit candidate at the atomic scale [3]. In this talk, I first introduce a noble qubit platform using tailored Ti nanostructures on a MgO surface, composed of a sensor and remote spins, where coherent driving and readout of single, two, and three qubits were demonstrated in an all-electrical fashion [4–8]. Second, I discuss the spin dynamics of our qubits, in regard to coupling with environments inherent in a tunnel junction, which shed light on a long-coherent quantum platform on surface.

[1] D. M. Eigler, and E. K. Schweizer, Nature 344, 524–526 (1990).
[2] S. Baumann et al. Science 350, 417-420 (2015).
[3] K. Yang et al. Science 366, 509-512 (2019).
[4] Y. Wang et al. npj Quantum Info. 9, 48 (2023).
[5] S. Phark et al. Adv. Sci. 10, 2302033 (2023).
[6] S. Phark et al. ACS Nano 17, 14144 (2023).
[7] Y. Wang et al. Science 382, 87-92 (2023).
[8] H. Bui et al. ACS Nano 18, 12187–12193 (2024).

Soo-hyon is currently working at Center for Quantum Nanoscience (QNS) of Institute for Basic Science (IBS) in Republic of Korea. He got his PhD in Solid State Physics from Seoul National University (SNU) in 2006. Then, he had worked as postdocs at SNU and Max-Planck-Institute of Microstructure Physics. His major has been studies on surface nanostructures using a UHV low temperature scanning tunneling microscope (STM), in particular, spin-resolved electronic structures in magnetic nanostructures by means of spin-polarized STM. He joined QNS from Oct 2016 and is leading the team “Atomic Scale Qubit Platforms on Surface” using a low-temperature STM equipped with electron spin resonance.

NIMS Talk: S3-4

Imaging Quantum Phenomena with Scanning Tunneling Microscopy

Shunsuke Yoshizawa
Senior Researcher, Nanoprobe Group, Center for Basic Research on Materials (CBRM),
National Institute for Materials Science (NIMS)

Abstract

Scanning tunneling microscopy (STM) measures the electronic density of states near the Fermi energy with atomic-scale spatial resolution. It is also compatible with low temperatures and high magnetic fields, playing an important role in the study of quantum materials. Our cryogenic, high-field STM system features low temperatures down to 0.4 K, high magnetic fields up to 16 T, and ultra-high vacuum chambers to prepare clean surfaces. Here we will briefly present some examples of our STM data and then focus on the result on the transition metal dichalcogenide 2*H*-$NbSe_2$.

2*H*-$NbSe_2$ is a layered compound that exhibits charge density waves (CDWs) below ~30 K. It also undergoes a superconducting transition at ~7 K. The superconducting state coexists with the CDW state, and the interplay between the two states is of increasing interest. With this question in mind, we first investigated the unknown aspects of the CDW structure; previous STM studies reported the existence of two types of lattice-commensurate CDW structures on the same surface, but the spatial distribution of their domains was not clearly resolved. We have developed a numerical method to accurately determine the local CDW structure from our high-resolution STM image and clearly define the spatial distribution of the domains. Our result shows the formation of alternating triangular domains of the two types of structures, which is in good agreement with the predictions of a phenomenological theory proposed before the widespread use of STM [2].

[1] S. Yoshizawa, K. Sagisaka, and H. Sakata, ***Phys. Rev. Lett.* 132,** 056401 (2024).
[2] K. Nakanishi and H. Shiba, ***J. Phys. Soc. Jpn.*, 52,** 1278 (1983).

Shunsuke Yoshizawa has been a senior researcher at NIMS since 2018. He received his Ph.D. degree from the Tokyo Institute of Technology in 2010. He started his career as a project researcher at the Institute for Solid State Physics, the University of Tokyo in 2010. He moved to NIMS as a postdoctoral researcher in 2012 and became an ICYS (International Center for Young Scientists) researcher in 2015. His main research topic is the nanoscale spectroscopic investigation of superconductors and topological materials using low-temperature scanning tunneling microscopy. He is interested in the visualization of physical phenomena by tuning the measurement and analysis methods best suited to the target.

Session4: Advanced Electron Microscopy

Invited Talk: S4-1

Electron Holography Studies on the Charging State of Catalyst Nanoparticles

Yasukazu Murakami
Professor, The Ultramicroscopy Research Center, Kyushu University, Japan

Abstract

Understanding of the charging state in a metallic nanoparticle supported on oxide surface is vitally important in science and engineering of heterogeneous catalysts. Indeed, the charging affects adsorption and/or dissociation of molecules on the catalyst surface via a change in the electronic occupancy of the antibonding state.

As a pioneering study on the charging state in a heterogeneous catalyst, X-ray photoemission spectroscopy revealed the charge amount per nanoparticle [1] although the result was the average from many nanoparticles. The author and his collaborators attempted “particle-by-particle analysis” of the charging state in Pt nanoparticles supported on a TiO2 crystal by using off-axis electron holography [2]. The phase-shift analysis revealed a slight change in the electrostatic potential due to the weak charging of Pt nanoparticle: i.e., only 1–6 electrons per nanoparticle. Importantly, Pt nanoparticles could be charged either positively or negatively depending on the orientation relationship with the TiO2 crysta1 [Fig. 1]. The results could be explained by first-principles calculations, in terms of the charge transfer between Pt and TiO2. The impact of oxygen-gas pressures on the charging state (examinations from another catalyst Au/CeO2) will be also discussed.

[1] Y. Lykhach et al., Nat. Mater., 15, 284-289 (2016).
[2] R. Aso et al., Science, 378, 202-206 (2022).

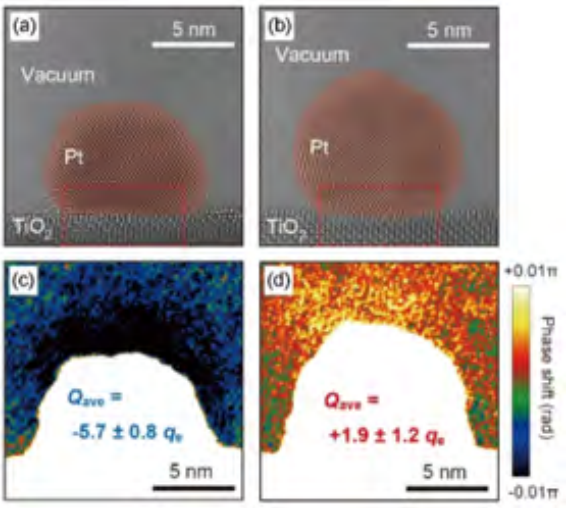


Figure 1. (a),(b) Lattice images of Pt nanoparticles and (c),(d) phase images (outside of nanoparticles) revealed by the amplitude/phase reconstruction using electron holography. The amount of charging (Qave) was presented in the unit of elementary charge (qe). Adopted from [2].

Yasukazu Murakami is a distinguished professor at Kyushu University (department of applied quantum physics and nuclear engineering). Since 2022, he serves as the director of the Ultramicroscopy Research Center, Kyushu University. His research interests include (1) electron holography studies on magnetic nanostructures, (2) precision improvement of electron holography to measure weak electromagnetic field, (3) in situ electron microscopy about phase transformations and pattern formations in crystals, etc. He received several awards, the Gold Medal from the Japanese Society of Microscopy (2010), Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology (2024), and others.

Invited Talk: S4-2

New Dimensions in Phase Contrast Scanning Transmission Electron Microscopy

Colin Ophus
Associate Professor, Materials Science and Engineering, Stanford University, USA
Center Fellow, Precourt Institute, Stanford University, USA

Abstract

Scanning transmission electron microscopy (STEM) has become an essential tool for materials science research, where it has been applied to atomic-scale imaging, diffraction, spectroscopy, and 3D tomography of many materials. The most popular STEM method is annular dark field (ADF) imaging, which provides approximately linear and incoherent contrast. This makes 2D imaging simple and interpretable, and the 3D tomographic reconstructions using ADF straightforward to implement. Atomic electron tomography (AET) of nanostructures performed using ADF STEM can both resolve the 3D positions of every atom and estimate the species of each atomic site. However, ADF-STEM is relatively dose-inefficient, and cannot be used to image beam sensitive materials or resolve light elements such as carbon or oxygen. These limitations prevent AET from being applied to materials such as polymers, lithium-containing battery materials, and biological samples.

To move beyond these limits, we require more sensitive and dose-efficient methods such as phase contrast imaging. High speed direct electron detectors now allow us to record a full 2D image of the diffracted STEM probe over a 2D grid of probe positions, producing a four-dimensional (4D)-STEM dataset. In this talk, I will demonstrate several phase contrast 4D-STEM methods, including center-of-mass differential phase contrast (CoM-DPC), parallax (or tilt-corrected bright field) imaging, and iterative ptychography, applied to inorganic and biological materials at high resolution. I will also show how we have applied ptychographic atomic electron tomography (PAET) to solve the 3D structure of a hybrid material composed of a complex ZrTe nanowire encapsulated in a double-walled carbon nanotube. I will emphasize the important role of developing open-source algorithms, codes, and simulation methods to promote robustness, reusability, and repeatability for scientific studies.

Colin Ophus is an Associate Professor in the Materials Science and Engineering Department and a Center Fellow at the Precourt Institute at Stanford University. He was formerly a Staff Scientist at the National Center for Electron Microscopy (NCEM), part of the Molecular Foundry user facility, at Lawrence Berkeley Lab. His research focuses on experimental methods, reconstruction algorithms, and software codes for simulation, analysis, and instrument design of scanning transmission electron microscopy (STEM). In 2018 he received a DOE Early Career award, and in 2022 he was awarded the Burton medal from the Microscopy Society of America (MSA). He has published over 200 articles and given invited talks around the world. He is project leader for the open-source Prismatic STEM simulation and py4DSTEM analysis codes, and editor-in-chief for the newly launched interactive journal Elemental Microscopy.

NIMS Talk: S4-3

Thermal Transport Measurements Using Thermocouple Probing in Pulsed STEM

Naoyuki Kawamoto
Principal Researcher, Electron Microscopy Group, Center for Basic Research on Materials (CBRM),
National Institute for Materials Science (NIMS)

Abstract

Thermal energy that goes unused, generated by power plants, industrial processes, automobiles, heating and cooling systems, computers, and domestic waste such as sewage heat, is typically released into the atmosphere. To improve energy recovery and conservation, the development of high-performance materials for thermal conductivity, insulation, composites, and thermoelectric conversion, as well as devices for precise thermal control, has become increasingly important. As we strive to create more advanced materials and devices, precise control of thermal behavior at the mesoscopic scale and understanding of thermal transport mechanisms are becoming essential. This demands new techniques capable of evaluating thermal transport phenomena within specific microscopic areas while simultaneously correlating these phenomena with atomic arrangements, defects, compositions, and other material characteristics.

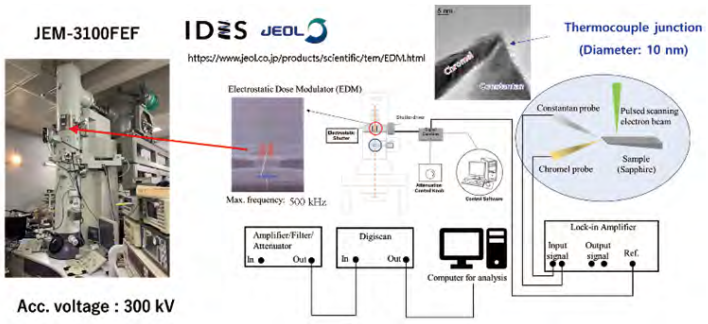


Fig. 1 Pulsed STEM-based thermal analytical microscopy

In response to this need, we have developed a novel method for measuring thermal transport within a transmission electron microscope (TEM). This method utilizes our proprietary nanoscale thermocouple temperature sensor, integrated into a two-probe TEM holder. Initially, by combining this temperature sensor with a nano-heating technique that employs focused electron beam irradiation, we developed the STEM-based thermal analytical microscopy (STAM) method. This technique allows for the evaluation of steady-state thermal transport in TEM specimens. More recently, we have further advanced this method by incorporating an electrostatic dose modulator (EDM) from IDES into TEM, which pulses the electron beam as shown in Fig. 1. This advancement has led to the development of a quantitative thermal diffusivity measurement method (Pulsed-STAM), based on the phase analysis of temperature waves propagating through TEM specimen. Details will be presented during the presentation.

Dr. Kawamoto is a principal researcher and a member of the Center for Basic Research on Materials (CBRM) in National Institute for Materials Science (NIMS). He received his Ph.D. in Engineering from Tohoku University, Sendai, Japan. He joined NIMS as a MANA researcher, Tsukuba, Japan, in 2009. His primary research interests are developing in-situ S/TEM measurement method such as nanoscale thermal and electrical transport measurements using probing techniques in S/TEM.

Poster Presentation

P1-01

Poster Award Nominee

Thickness-dependent Electronic Structures and Transport Properties of K-intercalated Graphene

Tatsuya Nakamura[1], Satoru Ichinokura[1], Kei Tokuda[1], Kiyohisa Tanaka[2], and Toru Hirahara[1]
[1] Department of Physics, Institute of Science Tokyo
[2] UVSOR Facility, Institute for Molecular Science

Recent scanning tunneling spectroscopy measurements have shown that potassium (K)-intercalated bilayer graphene (C_8KC_8) forms an energy gap in its electronic band at 3.6 K [1], suggesting a higher superconducting transition temperature (T_c) than bulk counterpart (C_8K), which has a T_c of 0.13 K [2]. While the potential T_c increase due to reduced dimensionality is intriguing, no follow-up studies have confirmed superconductivity in C_8KC_8. The possibility of the gap being caused by other phenomena, such as charge density waves, cannot be ruled out, and further experimental confirmation is needed.

In this study, we performed low-temperature electrical conductivity and energy band structure measurements on K-intercalated bilayer and multilayer graphene. No superconducting transition was observed above 2.7 K in either sample, in contradiction to Ref. [1]. Furthermore, angle-resolved photoemission spectroscopy revealed similar electronic structures between the bilayer and multilayer, with less than 10% variation in key band parameters related to Tc, such as effective mass and charge transfer rates between carbon and potassium. This result suggests that there are no factors in the band dispersion to significantly enhance the Tc in bilayer form, consistent with the transport measurements.

[1] T. Huempfner, ***Adv. Mater. Interfaces*, 10,** 2300014 (2023).
[2] E. P. Wolski, ***Solid State Commun.*, 57,** 421 (1986).

P1-02

Poster Award Nominee

Operando Study of Graphene Charge Transfer Through Micro-Raman Spectroscopy and Machine Learning

Riku Gotoh[1,2], Asako Yoshinari[1,2], Takuya Iwasaki[2], Seiya Suzuki[3,4], Yasunobu Ando[6], Tarojiro Matsumura[5], Masato Kotsugi[1], and Naoka Nagamura[1,2,4]
[1] Tokyo Univ. of Science, [2]NIMS, [3]JAEA, [4]JST PRESTO, [5]AIST, [6] Science Tokyo

Two-dimensional materials such as graphene have attracted a great interest in recent years as semiconductor device materials. In devices using two-dimensional materials, the surface and interface conditions affect the device properties significantly. Microspectroscopy is useful for obtaining rich information from the spatial distribution of spectral shapes. However, to capture local changes, it requires a lot of spectra with high spatial resolution, and fitting analysis takes a long time.

In order to efficiently extract information from Raman mapping data, we have been applying the machine learning peak fitting package “EMPeaks” [1] to Raman spectroscopic data. In this study, we have performed a spatial distribution analysis of doping levels based on high-spatial resolution peak shift distribution analysis. Microscopic Raman observations near the graphene channel/gold electrode interface in a graphene field-effect transistor (G-FET) structure revealed a localized change in the G-band peak position of graphene as a function of backgate voltage. This observation suggests the existence of a charge transfer region induced by hole doping from the electrode to graphene, as reported by synchrotron radiation micro-XPS observations [2].

[1] T. Matsumura, et al., ***Sci. Tech. Adv. Mat.*, 20,** 733 (2019).
[2] N. Nagamura et al., ***Appl. Phys. Lett.*, 102,** 241604 (2013).; ***Carbon*, 152,** 680 (2019).

P1-03

Poster Award Nominee

Lithium ion Transport Environment in Ion-Conducting Glasses

Koji Ohara[1,2], Satoshi Hiroi[1], and Kentaro Kobayashi[1]
[1] Faculty of Materials for Energy, Shimane University
[2] Research Center for Energy and Environmental Materials, NIMS

Controlling Li ion transport in glasses at atomic levels is key to realising all-solid-state batteries, a promising technology for electric vehicles. In this work, Li_3PS_4 glass, a promising solid electrolyte candidate, exhibits dynamic coupling between the Li^+ cation mobility and the PS_4^{3-} anion libration, which is commonly referred to as the paddlewheel effect [1]. In addition, it exhibits a concerted cation diffusion effect, which is regarded as the essence of high Li ion transport. However, the correlation between the Li^+ ions within the glass structure can only be vaguely determined, due to the limited experimental information. We report that the Li ions present in glasses can be classified by evaluating their valence oscillations via Bader analysis to topologically analyse the chemical bonds. We found that three types of Li ions are present in Li_3PS_4 glass, and that the more mobile Li ions (i.e., the Li3-type ions) exhibit a characteristic correlation at relatively long distances of 4.0–5.0 Å [2].

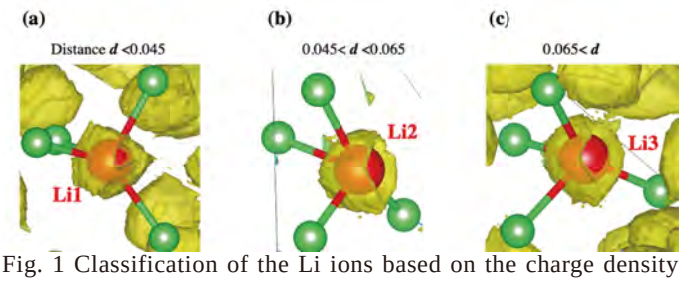


Fig. 1 Classification of the Li ions based on the charge density obtained using the Bader method

[1] J. Smith et al., ***Nat. Commun*, 11(1),** 1483 (2020).
[2] H. Yamada, K. Ohara, S. Hiroi et al., ***Energy & Environ. Mater.***, e12612 (2024).

P1-04

Microstructure of Light-emitting Phosphor of (Sr, Ca)$AlSiN_3$:Eu^{2+}

Hajime Matsumoto[1,2], Kyouta Ueda[1,2], Masahiko Shimizu[1,2], and Tomoyuki Kurushima[1]
Kazutaka Mitsuishi[2] and Naoto Hirosaki[2]
[1] Mitsubishi Chemical Corp.
[2] National Institute for Materials Science

(Sr,Ca)$AlSiN_3$:Eu^{2+} (SCASN) has been well-known as a phosphor for white light-emitting diodes (WLEDs). SCASN has a narrower full width half maximum (FWHM) compared to $CaAlSiN_3$:Eu^{2+} (CASN) [1]. Nevertheless, both have same crystal structure. Using SCASN as a red phosphor, WLEDs are easy to be color tunned, and have an excellent efficacy. Thus we have further investigated into a microstructure of SCASN with TEM.

[1] Kyota Uheda et al, “Luminescence properties of a red phosphor, $CaAlSiN_3$: Eu^{2+} for white light emitting diodes”, ***Electrochemical and Solid-State Letters*, 9 (4),** H22 (2006).

P1-05

Poster Award Nominee

Structural Analysis of Densified SiO_2 Glass Synthesized Under Extreme Conditions Using Quantum Beam

Shuya Sato[1,2], Masashi Miyakawa[3],Takashi Taniguchi[3], Koji Kimoto[2], Yohei Onodera[2], and Shinji Kohara[2,1]
[1] Graduate School of Science and Technology, Tokyo University of Science
[2] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)
[3] Research Center for Materials Nanoarchitectonics, National Institute for Materials Science (NIMS)

Glassy SiO_2 has been applied as a material for optical devices such as optical fibers. In particular, high refractive index and low dispersion glass containing tantalum has been used in camera lenses to achieve high performance such as wide-angle and high-magnification [1]. However, the rising prices of rare metals have created a need for alternate glass materials. In this study, we focused on hot-compressed SiO_2 glass. The higher the temperatures and pressures during synthesis, the glass with high density and structural ordering related to refractive index and dispersion is recovered [2]. However, under these extreme conditions, it is difficult to recover the sample as a glass due to crystallization caused by inhomogeneous nucleation, and there are no reports of synthesis at 7.7 GPa above 1300 °C or higher. In this study, we synthesized densified SiO_2 glass at higher pressures and higher temperatures by removing impurities on the sample surface that cause crystallization using surface treatment with hydrofluoric acid, and investigated the effects on the structure of SiO_2 glass from diffraction and other experimental data.

[1] T. Negishi, K. Yamaguchi, ***NEW GLASS*, 26,** 11 (2011).
[2] Y. Onodera, S. Kohara, P.S. Salmon et al., ***NPG Asia Mater.*, 12,** 85 (2020).

P1-06

Poster Award Nominee

Investigation of the Formation of a Zirconium Oxide Crystal Nucleus in the Initial Nucleation Stage in Aluminosilicate Gdlass

Yohei Onodera[1], Yasuyuki Takimoto[2], Hiroyuki Hijiya[3], Qing Li[3], Hiroo Tajiri[4], Toshiaki Ina[5], and Shinji Kohara[1]
[1] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)
[2] Innovative Technology Laboratories, AGC, Inc
[3] Materials Integration Laboratories, AGC, Inc
[4] Scattering and Imaging Division, Japan Synchrotron Radiation Research Institute (JASRI, SPring-8)
[5] Spectroscopy Division, JASRI, SPring-8

Glass-ceramics are composed of precipitated crystals and a glass matrix and are utilized in many industrial products. We conducted an X-ray multiscale analysis by combining diffraction, small-angle scattering, absorption, and anomalous scattering techniques to observe the structure of a commercially important ZrO_2-doped lithium aluminosilicate glass-ceramic during its initial nucleation stage. Element-specific pair distribution function analysis using anomalous X-ray scattering (AXS) data showed the formation of edge-sharing between ZrO_x polyhedra and $(Si/Al)O_4$ tetrahedra during the initial nucleation stage. Furthermore, AXS data indicated that the local structure of the Zr^{4+} ions, which resembled a cubic or tetragonal ZrO_2 crystalline phase, formed after 2 h of annealing the pristine glass. Therefore, the Zr-centric periodic structure surrounded by the $(Si/Al)O_4$ tetrahedral network was potentially the initial crystal nucleus for the ZrO_2-doped lithium aluminosilicate glass-ceramic[1].

[1] Y. Onodera et al., ***NPG Asia Mater.*, 16,** 22 (2024).

P1-07

Poster Award Nominee

Structural Insights into Thermal Conductivity of Amorphous Germanium Using Topological Data Analysis

Yen-Ju Wu[1], Kazuto Akagi[2], Masahiro Goto[3], and Yibin Xu[1]
[1] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)
[2] Advanced Institute for Materials Research, Tohoku University
[3] Research Center for Materials Nanoarchitectonics (MANA), National Institute for Materials Science (NIMS)

Amorphous materials are gaining industrial attention due to their unique thermal properties. Unlike crystalline materials, they exhibit distinct thermal and lattice vibration characteristics due to their lack of periodic atomic structure. However, analyzing atomic networks in transmission electron microscopy (TEM) images remains challenging. This study utilizes topological data analysis (TDA) and principal component analysis (PCA) on TEM images and molecular dynamics simulations of amorphous germanium (a-Ge) to uncover structural factors influencing thermal conductivity. Results indicate that larger atomic rings, formed at elevated deposition temperatures, improve heat transfer, offering a data-driven approach for designing optimized thermal insulators and thermoelectric materials through atomic network tailoring.

[1] Y. Wu, K. Akagi, M. Goto, and Y. Xu, ***International Journal of Heat and Mass Transfer*, 221,** 125012 (2024).

P1-08

Poster Award Nominee

Structural Properties of Na_2O-SiO_2 Melts Under High Pressure, as Revealed by X-ray Diffraction and Molecular Dynamics Simulation

Shino Hayafune[1], Haruki Ichikawa[1], Yohei Onodera[2], Shinji Kohara[2], Ken-ichi Funakoshi[3], Tatsuya Sakamaki[1], and Akio Suzuki[1]
[1] Department of Earth Science, Graduate School of Science, Tohoku University
[2] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)
[3] Neutron Science and Technology Center, Comprehensive Research Organization for Science and Society (CROSS)

Clarifying the structure of silicate melts under high pressure is crucial for understanding properties such as the density and viscosity of magma in the Earth's interior from a microscopic perspective. The present study aims at investigating the structure of Na_2O–SiO_2 melt under high pressure (2–5.4 GPa) using synchrotron radiation X-ray diffraction (XRD) experiments and classical molecular dynamics (MD) simulations. Energy-dispersive XRD measurements were conducted at the NE5C beamline of the PF-AR at KEK. MD simulations were performed in the NPT ensemble, using the LAMMPS code [1]

The position of the First Sharp Diffraction Peak (FSDP) in the X-ray structure factor S(Q) shifted towards higher Q-values, and the height of the Second Sharp Diffraction Peak (SSDP) becomes more pronounced with increasing pressure. Analysis of the partial structure factors revealed that the contraction of Si–O network structure contribute to the shift of the FSDP. Moreover, it is found that the Na–O coordination number increases from 5.8 (2 GPa, 2000 K) to 7.0 (5 GPa, 2000 K), which is the origin of the evolution of SSDP.

[1] A. P. Thompson et al., ***Comp. Phys. Comm.*, 271,** 108171 (2022).

P1-09

Poster Award Nominee

Phonon Dispersions of Element-doped Fe2VAl Thermoelectric Compounds Studied by Inelastic X-ray Scattering

Koji Kimura[1,2,3], Satoshi Tsutsui[2,4], Hidetoshi Miyazaki[1], Yoichi Nishino[1], and Koichi Hayashi[1,2]
[1] Department of Physical Science and Engineering, Nagoya Institute of Technology
[2] Japan Synchrotron Radiation Research Institute (JASRI), SPring-8
[3] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)
[4] Institute of Quantum Beam Science, Graduate School of Science and Engineering, Ibaraki University

Fe_2VAl has attracted much attention as a high-performance thermoelectric material. To improve its performance, it is necessary to reduce the lattice thermal conductivity, κ_{ph}. It is well-known that κ_{ph} is suppressed by adding forth element. Here, we performed inelastic X-ray scattering (IXS) measurements on Ta- and Ti-doped Fe_2VAl to reveal the mechanism of κ_{ph} reduction through their phonon dispersions [1].

Figures 1(a)(b) show the IXS spectra of Ta- and Ti-doped Fe_2VAl. The spectra are not significantly changed by adding Ta, except for the appearance of a broad peak at ~17 meV. On the other hand, the overall shape of the spectra is largely changed with increasing Ti concentration (Fig. 1(b)). Based on these results, the underlying mechanisms for the reduction of κ_{ph} will be discussed.

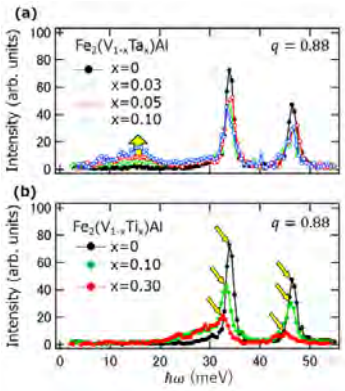


Fig. 1 IXS spectra of (a) Ta and (b) Ti-doped Fe2VAl at Q=(6.88, 0, 0).

[1] K. Kimura et al. ***Acta Mater.*** (in press).

P1-10

Poster Award Nominee

Formation of Ultrathin Oxide Films and Controlled Single-Photon Emitters at SiC Interfaces

Yasuaki Miyakawa, Satoru Ichinokura, and Toru Hirahara
Department of Physics, Institute of Science Tokyo

Defects in wide-bandgap semiconductors can act as single-photon emitters (SPEs), with potential applications in quantum sensors. Generating SPEs near the surface enables the detection of small magnetic fields. SPEs formed at the oxide/SiC interface during thermal oxidation are promising candidates for surface-proximal single-photon sources [1]. However, previous research has struggled with atomic-level control of the interface structure, resulting in SPEs with varying emission wavelengths [2]. This variability may be caused by the formation of native oxide layers during transport before thermal oxidation, leading to non-uniform interfaces.

To address this issue, we developed a method to form ultrathin oxide films and generate uniform SPEs near the surface. Silicon atomic layers were epitaxially grown on 4H-SiC(0001), followed by in-situ oxidization in a molecular beam epitaxy facility, to achieve an atomically flat interface. Scanning probe microscopy confirmed atomically flat step-terrace structures, while X-ray photoelectron spectroscopy revealed increased oxidation components, with oxide film thicknesses measured at 1.3 nm. Photoluminescence measurements showed a sharp emission peak at 740 nm, indicating superior monochromaticity and selective generation of carbon-related defects at the atomically flat interface.

[1] A. Lohrmann, ***Appl. Phys. Lett.*, 108,** 021107 (2016).
[2] S. Castelletto, ***J. Phys.: Photonics*, 2,** 022001 (2020).

P1-11

Poster Award Nominee

Synthesis and Characterization of $BaZrS_3$ Thin Films for Photovoltaic Applications Using a Stacked Elemental Layer Methodology

Sumbal Jamshaid[1,2], Peter J. Wellmann[1], and Koichi Hayashi[2]
[1] Crystal Growth Lab, Materials Department 6, University of Erlangen-Nürnberg, Erlangen, Germany
[2] Department of Physical Science and Engineering, Nagoya Institute of Technology, Nagoya, Japan

The demand for environmentally benign and efficient semiconductors for optoelectronic applications has led to the exploration of non-toxic perovskites, with chalcogenide perovskites emerging as a promising candidate due to their direct bandgaps and high absorption coefficients[1]. This study introduces a novel approach for synthesizing barium zirconium sulfide ($BaZrS_3$) thin films, a chalcogenide perovskite, utilizing a stacked elemental layer methodology. This technique, inspired by methods used in chalcopyrite and kesterite fabrications, involves sputtering elemental Zr on silicon carbide (SiC) substrates, followed by electron beam evaporation of BaS, and culminates in a high-temperature sulfurization annealing process[2,3]. The resultant $BaZrS_3$ thin films were characterized for their structural, optical, and surface properties through X-ray diffraction, UV-Visible spectroscopy, scanning electron microscopy, and energy-dispersive X-ray spectroscopy, revealing polycrystalline structures with an optimal band gap for photovoltaic applications. Comparative analysis of films synthesized on different substrates highlights the versatility and efficacy of this fabrication method, offering insights into substrate influence on film characteristics.

[1] S. Niu, ***arXiv preprint***, arXiv:1804.09362 (2018).
[2] S. Jamshaid, ***Advanced Engineering Materials*****, 26(18),** 2302161 **(**2024).
[3] T. Freund, ***Crystals*****, 14(3),** 267 (2024).

P1-12

Spin-dependent O_2 Chemisorption and Catalytic CO Oxidation on Magnetized PtCo Surface

Mitsunori Kurahashi
Center for Basic Research on Materials, National Institute for Materials Science (NIMS)

The effects of electron spin on surface reactions are attracting attention since many technologically important catalytic reactions involve paramagnetic species and magnetic catalysts. Although spin-dependent chemical processes happening on magnetic atoms have been observed previously, how the magnetic atoms contained in alloy catalysts affect the catalytic activity of neighboring nonmagnetic atoms remains unclear. PtCo alloy has been investigated intensively for its application to fuel cell because it shows higher O_2 reduction reaction efficiency than pure Pt. The Pt atoms in the PtCo alloy is expected to be slightly spin-polarized by neighboring Co, but how such induced spin polarization affects the catalytic activity of Pt is unknown. The present spin-resolved O_2 chemisorption and CO oxidation experiments conducted with a spin-rotational state-selected O_2 beam and a perpendicularly-magnetized Pt/Co(2ML)/Pt(111) film have indicated that the O_2 chemisorption probability and the catalytic CO oxidation rate depend strongly on the spin orientation between O_2 and the Pt surface. The magnitude of the spin orientation dependence was found to be greater than that observed for O_2/Ni [1] even if the magnetic moment of Pt is much smaller than that of Ni. The SPMDS measurement and DFT calculation have indicated that surface Pt has a considerable spin polarization at around the Fermi level, which may cause the spin-dependent chemical activity of Pt/Co/Pt(111).

[1] M. Kurahashi and Y. Yamauchi, ***Phys. Rev. Lett.*****, 114,** 016101 (2015).

P1-13

Adjacent Elemental Analysis of Oxide Fuel Cell Materials by High Field Solid-state NMR

Masataka Tansho[1], Atsushi Goto[1], Shinobu Ohki[1], Yuuki Mogami[1], Yuta Yasui[2], Yuichi Sakuda[2], Kotaro Fujii[2], Takahiro Iijima[3], and Masatomo Yashima[2]
[1] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)
[2] Department of Chemistry, School of Science, Tokyo Institute of Technology
[3] Institute of Arts and Sciences, Yamagata University

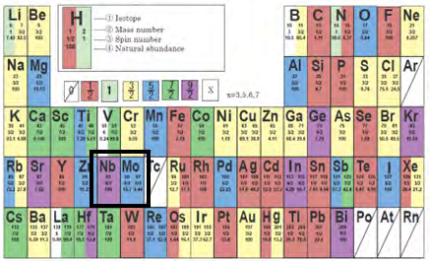


Fig. 1 Separate analysis of adjacent Nb and Mo in the periodic table using 800 MHz NMR of NIMS

$Ba_3MoNbO_{8.5}$ [1], $Ba_7Nb_4MoO_w$ [2], and related materials are gaining attention as materials that can surpass yttria stabilized zirconia (YSZ) for oxide fuel cells. The local structure around niobium (Nb) and molybdenum (Mo) is thought to be important for oxygen (O) ions and proton (H) mobility. Mo and Nb, which are adjacent to each other on the periodic table (Figure 1), have been treated as the same because they are difficult to distinguish by ordinary XRD analysis, but NMR results using the NIMS 800 MHz NMR system show that Nb and Mo are clearly different.

[1] M. Tansho, A. Goto, S. Ohki, Y. Mogami, Y. Sakuda, Y. Yasui, T. Murakami, K. Fujii, T. Iijima, and M. Yashima, ***J. Phys. Chem. C,* 126,** 13284-13290 (2022).
[2] Y. Yasui, M. Tansho, K. Fujii, Y. Sakuda, A. Goto, S. Ohki, Y. Mogami, T. Iijima, S. Kobayashi, S. Kawaguchi, K. Osaka, K. Ikeda, T. Otomo, and M. Yashima, ***Nat. Commun.,* 14**, 2337 (2023).

P1-14

NMR Techniques for the Detection of Photo-induced Effects in Solids

Atsushi Goto[1], Kenjiro Hashi[1], and Shinobu Ohki[2]
[1] Center for Basic Research on Materials, National Institute for Materials Science (NIMS).
[2] Research Network & Facility Service Division, National Institute for Materials Science (NIMS).

The photo-induced effects in solids play useful roles in our lives through optoelectronics, photocatalysts, etc. The mechanisms of these effects can be well understood by in-situ detection of changes in the states caused by light illumination. For this purpose, we have been developing nuclear magnetic resonance (NMR) systems that operate under light illumination [1]. These systems have been successfully applied to investigations of optical effects in semiconductors [2].

One of the challenges in the development is the stable control of sample temperature under light illumination. In our previous systems, samples were cooled through thermal conduction to the GM refrigerator in a vacuum environment, and the absence of exchange gas resulted in insufficient cooling efficiency. To address this issue, we have developed a “sample chamber” that encapsulates the sample and detection coil in exchange gas, enabling efficient removal of heat generated by light irradiation.

In this presentation, the details of the system under development, including the sample chamber, will be reported. This work has been partly supported by JSPS KAKENHI Grant Nos. JP21K18897; JP23H01131; and JP23K25828.

[1] A. Goto et al., Rev. Sci. Instrum. 77, 93904 (2006); ***Jpn. J. Appl. Phys.,* 50,** 126701 (2011).
[2] A. Goto, S. Ohki, K. Hashi, and T. Shimizu, ***Nat. Commun.,* 2,** 378 (2011); ***npj Quant. Inform.,* 8,** 59 (2022); JPS Conf. Proc. 38, 011185 (2023).

P1-15

Development and Application of High-temperature NMR

Kenjiro Hashi
Center for Basic Research on Materials, National Institute for Materials Science (NIMS)

Understanding the diffusion property of Li ions is crucial for improving the performance of Li-ion batteries. NMR is one of the most important techniques for characterizing the Li-ion mobility from microscopic points of view. However, the Li-ion mobility of solid electrolyte is too slow to explore with NMR around room temperature. To investigate the ion diffusion at high temperatures, we constructed a high-temperature pulsed-field-gradient (PFG) NMR probe capable of measurements at temperatures > 700K.

Fig. 1 Picture of the high-temperature NMR probe.

The temperature of the sample was varied from 296 to 724 K by a flow of heated nitrogen gas. The temperature of the nitrogen gas was monitored by a thermocouple. The accuracy of the temperature calibration was confirmed by 79Br NMR measurements of KBr.[1]

The high-temperature NMR probe was applied for the measurement of the Li-ion diffusion in Perovskyte-type solid electrolyte. Non-Arrehenius behavior of the diffusion coefficients was revealed by the measurement. [2]

[1] K. Hashi, et al., ***Analytical Sciences*, 37,** 1477 (2021).
[2] G. Hasegawa, et al., ***Chemistry of Materials*, 35,** 3815 (2023).

P1-16

Poster Award Nominee

Characterization of the Tensile Properties of GAN-generated 3D Microstructures in Dual-Phase Steels

Ta-Te Chen[1], Ikumu Watanabe[2], Keiya Sugiura[1], Toshio Ogawa[3], and Yoshitaka Adachi[1]
[1] Graduate School of Engineering, Nagoya University
[2] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)
[3] Department of Mechanical Engineering, Faculty of Engineering, Aichi Institute of Technology

This study examines the validity of 3D microstructures generated by Generative Adversarial Networks (GANs) for dual-phase steels [1]. We compared GAN-generated structures with experimentally observed 3D microstructures for two types of ferrite-martensite dual-phase steels. Mechanical behaviors were analyzed using finite element analysis on representative volume elements, employing an image-based modeling approach with voxel coarsening. Results showed that the GAN algorithm successfully captured anisotropic responses caused by microscopic morphology, particularly in steel with higher martensite content. However, quantitative alignment with observed microstructures was limited due to inaccuracies in reproducing phase volume fractions. In the steel with lower martensite content, the algorithm struggled to replicate the connectivity of the martensite phase. This study highlights both the potential and limitations of GAN-based 3D microstructure generation, contributing to the development of computational methods for materials characterization and design.

[1] I. Watanabe, K. Sugiura, T. Chen, T. Ogawa, and Y. Adachi, ***Science and Technology of Advanced Materials*, 25,** 2388501 (2024).

P1-17

Poster Award Nominee

Characterization of Mechanical Properties of Alloys Using Neighboring Indentation Test

Dayuan Liu[1, 2] and Ikumu Watanabe[1, 2]
[1] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)
[2] Graduate School of Science and Technology, University of Tsukuba

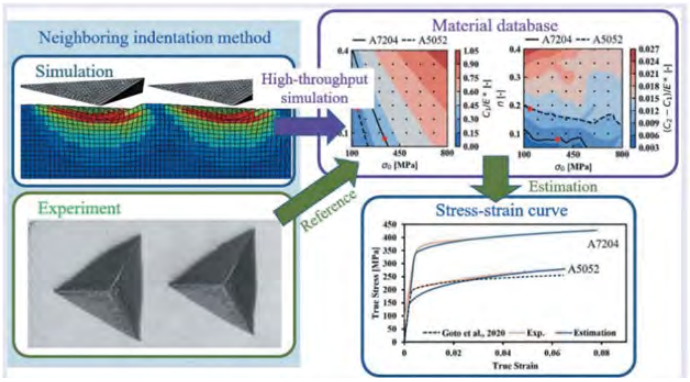


Fig. 1 A schematic illustration of the proposed neighboring indentation method

Instrumented indentation test is an efficient approach to measure mechanical properties such as equivalent elastic modulus and hardness. In this study, we focus on the interaction between the existing and subsequent indentation tests to extract the plastic properties from the result of two indentation tests performed at neighboring positions. With this view, finite element simulations are performed to design suitable indentation condition and draw the response surfaces of the indentation results to determine the material constants of the plastic constitutive model. Eventually, the proposed approach is validated in applications to aluminum alloys and stainless steel, in which the material constants are read from the response surfaces.

[1] K. Goto et al., Int. ***J. Plas.*, 116,** 81-90 (2019).
[2] T. Chen et al., ***STAM: M*, 2,** 416-424 (2022).

P1-18

Poster Award Nominee

Pt_5Ce Single Crystal Ingot: Nanophase Separation from Synthesis to Characterization

Sherjeel Mahmood Baig[1,2], Ayako Hashimoto[1,3], and Hideki Abe[1,2]
[1] Research Center for Energy and Environmental materials, National Institute for Materials Science (NIMS)
[2] Graduate School of Science and Engineering, Saitama University
[3] Graduate School of Science and Technology, University of Tsukuba

Lithographic technique is of pivotal importance in designing nanoscale patterns, yet it is too artificial and not suitable for large scale productions. We have developed an approach to design patterned nanomaterials w/ o lithography by taking advantage of the nanophase separation that occurs during the oxidation of intermetallic compound [1,2]. To investigate the impact of nanophase separation on the developed facets, atomic scale analysis of the nanocomposite is also required. Hence, this study depicts atomic scale investigation of phase separation phenomenon. In this study we synthesized single-crystal Pt_5Ce alloy ingots and studied their subsequent controlled nanophase separation. Utilizing a mono-arc furnace, we developed a more efficient and time-saving method than conventional techniques, such as the Bridgman method. Nanophase separation was induced through atmosphere treatment, resulting in well-defined Pt and CeO_2 nanostructures. Characterization techniques confirmed the nanophase separation occurred in a highly controlled manner along the 0001 plane, a significant advancement in understanding the behavior of Pt_5Ce alloys.

[1] S. M. Baig, S. Ishi, & H. Abe, ***Nanoscale Advances*, 6,** 6 (2024).
[2] Y. Wen, H. Abe, K. Mitsuishi, & A. Hashimoto, ***Nanoscale*, 13,** 2096-2098 (2021).

P1-19

Poster Award Nominee

Automatic Identification of Crystalline Phases Using Bayesian Estimation in XRD

Ryo Murakami[1], Yoshitaka Matsushita[1], Kenji Nagata[1], Hayaru Shouno[2], and Hideki Yoshikawa[2]
[1] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)
[2] Research Network and Facility Services Division, National Institute for Materials Science (NIMS)
[3] School of Informatics and Engineering, The University of Electro-Communications

We developed the method to identify the crystalline phase structure from X-ray diffraction pattern. Traditionally, narrowing down the correct crystalline phase from multiple candidates has relied on the expertise and judgement of an experienced researcher. However, this conventional approach is heavily dependent on the analyst and lacks objectivity. Moreover, there is no established method to discuss the confidence intervals of the results. In this study, we aimed to develop a method for automatically estimating crystalline phases from diffraction patterns using Bayesian estimation (Fig. 1) [1]. Our method successfully identified the true crystalline phase with high probability from among 50 phase candidates.

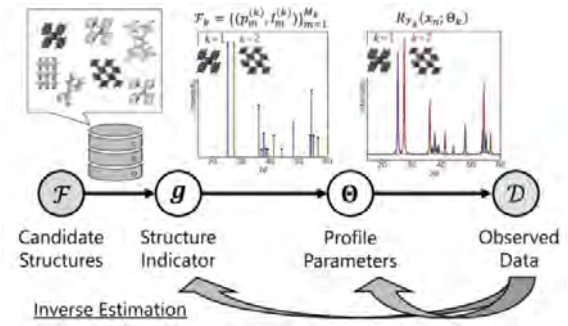


Fig. 1 Overview of our method [1] ©STAM-methods

[1] Ryo Murakami, et. al., ***STAM-methods*, 4** (2024) 1.

P1-20

Poster Award Nominee

Revealing the Surface Adsorbates of Diamond Using MEMS Resonators

Keyun Gu, Zilong Zhang, Wen Zhao, Guo Chen, Yasuo Koide, Satoshi Koizumi, and Meiyong Liao
Research Center for Electronic and Optical Materials, National Institute for Materials Science (NIMS)

Surface states of semiconductors determine the ultimate electronic properties of semiconductor devices. The in-situ realization of the surface properties of semiconductors in atomic scale relies on ultra-high vacuum and sophisticated techniques. In the work, we propose the utilization of diamond microelectromechanical system (MEMS) resonators to reveal the surface properties of adsorption/desorption of oxygen (O)- and hydrogen (H)-terminated diamonds [1,2]. Our strategy is to measure the mechanical resonance frequency shift of diamond cantilevers by in-situ heating and cooling the cantilevers. Based on the frequency shift, the equivalent thickness of the adsorption layer the O- and H-terminated diamond is ~0.4 nm and ~0.9 nm, respectively. This work discloses that MEMS provides a precise insight into the surface nature of the semiconductor surface.

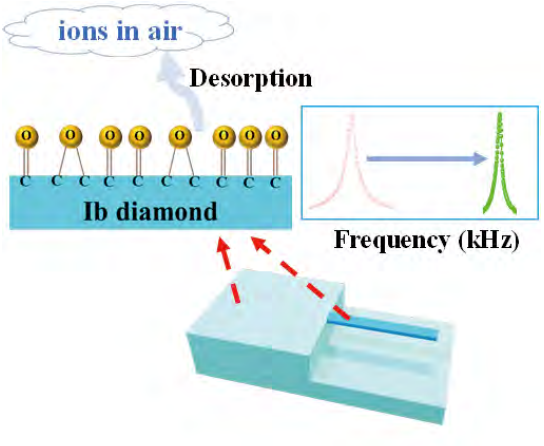


Fig. 1 Frequency shift of the diamond cantilevers of O-terminated diamond.

[1] Meiyong Liao, ***Advanced Materials*, 22(47),** 5393-5397 (2010).
[2] Keyun Gu, ***Carbon*, 225,** 119159 (2024).

P1-21

Poster Award Nominee

Nitrogen-Doped Cobalt/Carbon Composite from Metal Organic Framework on Fullerene Self Assemblies (MOFOF) for Energy Conversion Application

Rabindra Nath Acharyya[1,2], Katsuhiko Ariga[1,3], and Lok Kumar Shrestha[1,2,*]
[1] Research Center for Materials Nanoarchitectonics, National Institute for Materials Science (NIMS)
[2] Graduated School of Pure and Applied Sciences, University of Tsukuba
[3] Department of Advanced Materials Science, School of Frontier Sciences, The University of Tokyo

Fullerenes is a spherical zero-dimensional molecule composed of hexagonal and pentagonal rings with a network of sp^2-hybridized carbon atoms [1]. It can be assembled into various nanostructures with unique shapes and distinct properties. Metal-organic frameworks (MOFs) are highly porous materials with a large surface area and tunable porosity, which are useful in gas/energy storage and catalysis [2]. In this contribution, we report a simple (layer-by-layer (LBL)) yet novel method to prepare MOFOF and its conversion into novel nitrogen-doped cobalt/carbon composite by high temperature carbonization. Fullerene nanotube (FNT) was synthesized by using a dynamic liquid–liquid interfacial precipitation (DLLIP) method. The surface of the FNTs was oxidized by strong acids (H_2SO_4:HNO_3) treatment and MOF (ZIF-67) crystals were grown on the oxidized surface of FNT using LBL technique. The MOFOF was calcinated at high temperature followed by nitrogen-doping under ammonia furnace. Owing to a high specific surface area (1260 m^2/g) and unique microstructure, nitrogen-doped cobalt/carbon composite derived from the MOFOF is expected to show high activity in energy conversion (ORR activity).

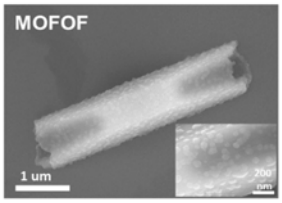


Fig. SEM images of MOFOF

[1] K. Ariga, L. K. Shrestha, ***Mater Adv.,* 2(2),** 582-597 (2021).
[2] B.N. Bhadra, L.K. Shrestha, Y. Yamauchi, K. Ariga, ***ACS Appl Mater Inter.,* 16,** 41363−41370 (2024).

P1-22

Magneto-optical Studies in 2D Carrier Systems of Semiconductor and Semimetal Under High Magnetic Field

Yasutaka Imanaka
Center for Basic Research on Materials, National Institute for Materials Science (NIMS)

Magneto-optical measurements (Cyclotron resonance, Magneto-PL) are essential for studying not only the optical transition between the Landau levels, but the band parameters in semiconductors and semimetals under high magnetic fields [1].

We have investigated the quantum Hall systems of various compound semiconductors with extremely high mobility. Recent progress of the MOCVD growth technique enables us to study the cyclotron resonance (CR) with the magneto-transport measurements even for InGaN heterostructures. Figure 1 shows typical CR spectra in two-dimensional electron systems in InGaN heterostructures. The electron effective mass has just determined accurately through these experiments for the first time.

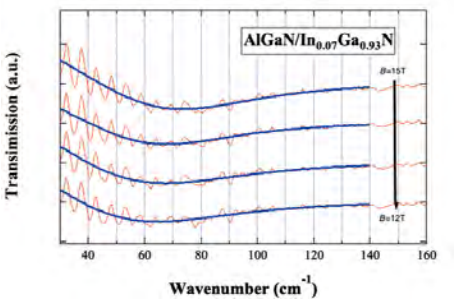


Fig. 1 CR spectra in InGaN

The CR experiment is also applied for semimetal, such as $Bi_{1-x}Sb_x$ thin films recently. The CR and interband transition have been observed clearly at the wide range of the magnetic field with anomalous broad absorption. The third contribution except the bulk electron and hole could be assumed for explaining the origin of the absorption. In this presentation, we will also discuss the possibility of the contribution from the surface carrier to the CR absorption in $Bi_{1-x}Sb_x$ thin films.

[1] Y. Imanaka et. al., ***J. Low Temp. Phys.,* 170,** 389 (2013).

P2-01

Poster Award Nominee

Electronic State Analysis of Ultra-thin Cu Film on FeCo/MgO(100)

Shingo Takezawa[1,2], S. Takase[1,2], D. Ishikawa[1,2], T. Osawa[1,2], R. Goto[1,2], Y. Sakuraba[2], S. Tsuda[2], K. Yaji[2,3], K. Fuku[1,2], M. Imamura[4], M. Kotsugi[1], and N. Nagamura[1,2]
[1] Tokyo University of Science, [2] National Institute for Materials Science, [3]Tohoku University, [4] Saga University

The structures and electronic states of magnetic multilayers are important research topics in spintronics. FeCo/bcc-Cu/FeCo trilayers have been reported to achieve a good magnetoresistance ratio (42%)[1], but its electronic states remain unknown because of the difficulty to synthesize metastable bcc-Cu.

In this study, we prepared Cu/FeCo/MgO by molecular beam epitaxy (MBE) and evaluated its band dispersions by ARPES with synchrotron radiation.

The Cu/FeCo thin films were grown on MgO(100) substrates by MBE in UHV chamber connected with the APRES measurement setup. The ARPES measurements were performed at Saga University Beamline (BL13) in SAGA-LS. Low-energy electron diffraction (LEED) was used for in-situ structural evaluation. X-Ray diffraction (XRD) was used for ex-situ structural evaluation.

Fig.1 is the energy distribution curve of Cu(2 nm)/FeCo(20 nm)/MgO(100) at normal emission angle as a function of photon energy from hν = 45 eV to 180 eV. The bands between initial state energy 2 and 5 eV exhibit d-like bulk bands. The bands marked as bold lines in Fig.1 is suggested to be derived from bulk band structures specific to bcc-Cu and bcc-FeCo, instead of fcc-Cu, which are predicted from calculations[4-5].

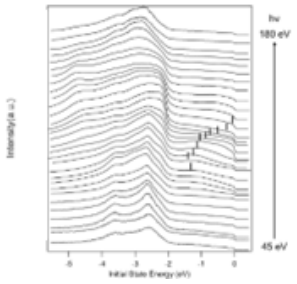


Fig.1 Photoemission spectra at normal emission angle of Cu/FeCo/MgO(100)

[1] K. B. Fathoni et al., ***APL Mater.,* 7,** 111106 (2019). [2] J. L. Alfke et al., ***Phys. Chem. Chem. Phys.*, 24,** 24429 (2022). [3] H. Li et al., ***Phys. Rev. B,* 43,** 6342, (1991). [4] Z. Tang et al., ***Phys. Rev. B,* 65,** 195108 (2002). [5] V. T, Tran et al., ***Computational Materials Science,* 172,** 109344, (2022).

P2-02

Poster Award Nominee

Electronic Properties of Chemical Vapor Deposition-grown Graphene on Ni (111) Investigated by Spin- and Angle-resolved Photoemission Spectroscopy

Thang Dinh Phan[1], S. Tsuda[1], R. Goto[1,2], N. Nagamura[1,2], F. Komor[i1], Y. Tanimoto[3], H. Sato[4], Y. Fukushima[5], K. Kawaguchi[5], R. Mori[5], T. Kondo[5], Y. Yamaji[6], and K. Yaji[1,7]
[1] Center for Basic Research on Materials, NIMS, [2] Faculty of Advanced Engineering, Tokyo Uni. of Science, [3] Graduate School of Advanced Science and Engineering, Hiroshima Uni., [4] HiSOR, [5] Institute for Solid State Physics, The Uni. of Tokyo, [6] Research Center for Materials Nanoarchitectonics, NIMS, [7] UDAC, Tohoku Uni.

Graphene-based spintronics utilizes the spin degree freedom of graphene's electrons at the Dirac points near the Fermi level for novel information storage and logic devices. Shifted Dirac-band in previous studies [1] can be improved by using the chemical vapor deposition (CVD)-grown graphene on the Ni (111) substrate. The electronic property of a CVD-grown graphene/Ni (111) has been studied with (spin-) and angle-resolved photoemission spectroscopy ((S)ARPES) measurements [2,3]. We find that the Dirac point of a single dispersive linear π-band nearly the Fermi level. The spin-polarized π-band around the K-point has been confirmed by SARPES, providing a significant advantage for spin transport. In addition, we find other bands with a two-dimensional nature near the Fermi level.

[1] A. Varykhalov et al., ***Phys. Rev. X,* 2,** 041017 (2012).
[2] K. Yaji et al., ***Sci. Technol. Adv. Mater. Meth.*, 4,** 2328206 (2024).
[3] K. Yaji et al., ***e-J. Surf. Sci. Nanotechnol.*, 22,** 46 (2024).

P2-03

Visualization of Spin-polarized Electronic States by Imaging-type Spin-resolved Photoemission microscopy

Koichiro Yaji[1,2] and Shunsuke Tsuda[1]
[1] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)
[2] Unprecedented-scale Data Analytics Center, Tohoku University

We have developed an imaging-type spin-resolved photoemission microscopy (iSPEM) machine equipped with a multi-channel spin detector developed at the National Institute for Materials Science (NIMS) [1-3]. Thanks to the multi-channel spin detector, the iSPEM machine quickly visualizes the spin-polarized electronic states of materials. Besides, spin-resolved photoemission spectroscopy in real space achieves a spatial resolution of 400 nm. We demonstrate the spin polarization imaging of polycrystalline iron with the real space mode and spin-resolved Fermi-surface imaging of Bi(111) in the momentum space mode.

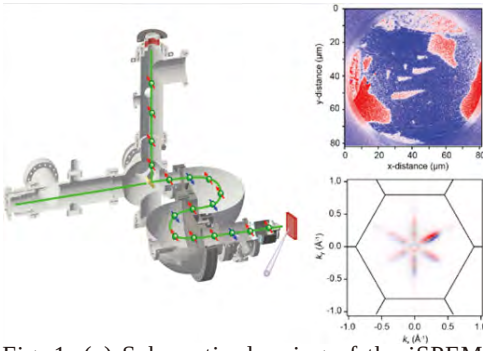


Fig. 1: (a) Schematic drawing of the iSPEM machine. Spin-polarized electronic state images in real (a) and momentum (b) spaces [3].

[1] K. Yaji, S. Tsuda, ***e-JSSNT*, 22,** 46 (2024).
[2] S. Tsuda, K. Yaji, ***e-JSSNT*, 22,** 170 (2024).
[3] K. Yaji, S. Tsuda, ***STAM-M*, 4,** 2328206 (2024).

P2-04

Angle-resolved Photoemission Spectroscopy of Polycrystalline Materials Using an Imaging-type Photoemission Microscope

Shunsuke Tsuda[1], Yohei Yamaji[2], and Koichiro Yaji[1,3]
[1] Research Center for Basic Research on Materials, National Institute for Materials Science (NIMS)
[2] Research Center for Materials Nanoarchitectonics, National Institute for Materials Science (NIMS)
[3] UDAC, Tohoku University

Angle resolved photoemission spectroscopy (ARPES) directly reveals electronic structure of a material. To apply ARPES, the sample surface must be atomically flat. In the case of bulk samples, the sample surface is prepared by cleaving in-situ, or optical polish in air and sputtering and annealing in ultrahigh vacuum. Therefore, the actual target of ARPES is limited. If ARPES could be applied to polycrystalline samples, ARPES would become a more useful technique.

To overcome this problem, we are working on the development of a new analysis method. We have obtained ARPES data from an area of approximately 10 mm × 2 mm area for various locations in polycrystalline silver using imaging-type photoemission microscopy [1-3]. Different spectra reflecting different crystal orientations is obtained for different locations.

In this presentation, we will report on the current status of our method.

[1] K. Yaji and S. Tsuda, ***e-J. Surf. Sci. Nanotechnol.*, 22,** 46 (2024).
[2] K. Yaji and S. Tsuda, ***STAM method*, 4,** 2328206 (2024).
[3] S. Tsuda and K. Yaji, ***e-J. Surf. Sci. Nanotechnol.*, 22,** 170 (2024).

P2-05

Poster Award Nominee

Calibrating Binding Energy for Insulating/Semi-Insulating Carbon-Related Materials in X-Ray Photoelectron Spectroscopy Measurements

Jiangwei Liu[1], Tokuyuki Teraji[1], Bo Da[2], and Yasuo Koide[1]
[1] Research Center for Electronic and Optical Materials, National Institute for Materials Science (NIMS)
[2] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)

Due to the presence of an intrinsic C 1s peak in carbon-related materials, it is impossible to calibrate its binding energies using the adventitious C 1s peak (284.8 eV) during X-ray photoelectron spectroscopy measurement. The absence of accurate binding energy measurement makes it challenging to determine the interfacial band bending for the carbon-related material-based heterojunctions. To overcome this issue, a net-patterned gold (Au) mask is applied to the semi-insulating boron-doped diamond (B-diamond) to suppress the charge-up effect and calibrate the binding energy using the standard Au 4f peak (83.96 eV) [Image shown in Fig. 1]. The B-diamond shows downward band bending towards the surface with valence band maximum of 0.85 eV. Upon the formation of Al_2O_3 using the atomic layer deposition technique, the interfacial band bending for the Al_2O_3/B-diamond has been clarified [1].

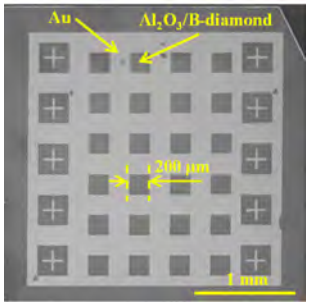


Fig. 1 Net-patterned Au mask on B-diamond for binding energy calibration

[1] J. W. Liu, T. Teraji, B. Da, Y. Koide, ***Applied Physics Letters*, 125 [10]** 101601 (2024).

P2-06

Poster Award Nominee

Time- and Space-resolved Soft X-ray Microscopy for Magnetic Materials

Yuta Ishii[1], Yusuke Kozuka[2], Hironori Nakao[3], and Yuichi Yamasaki[1]
[1] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)
[2] Research Center for Materials Nanoarchitectonics, National Institute for Materials Science (NIMS)
[3] Institue of Materials Structure Science, High Energy Accelerator Research Organization (KEK)

The behaviors of magnetic moments in materials are promising for the advancement of spintronic devices. To facilitate the development of magnonic technologies, the direct detection of magnetic behaviors in real time and space is essential for comprehending the fundamental mechanisms underlying various magnetic phenomena. We have recently developed soft X-ray microscopy (as shown in Fig. 1) which is capable of several imaging measurements, including the visualization of magnetic textures [1], observation of the dynamics of magnetic moments [2], and detection of the spiral phase of X-ray beams [3]. Especially, we have successfully visualized spin waves in Py (Fe-Ni) thin films using time- and space-resolved measurements, where we identified non-reciprocal spin waves in amplitude and wave number. I would like to present the current techniques and our experimental results in my presentation.

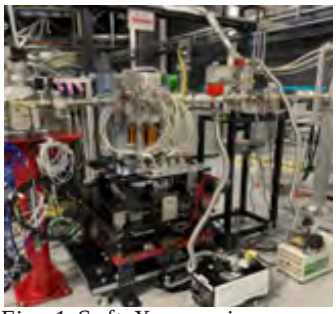


Fig. 1 Soft X-ray microscopy located in NanoTerasu.

[1] Y. Ishii, et al., ***JPS Conf. Proc.*, 38,** 011190 (2023).
[2] Y. Ishii, et al., ***Sci. Rep.*, 14,** 15504 (2024).
[3] Y. Ishii, et al., ***PRApplied.*, 14,** 064069 (2020).; Y. Ishii, et al., ***Sci. Rep.*, 12,** 1044 (2022).

P2-07

Machine-Learning Based Analysis for Synchrotron X-ray Spectral Imaging

Naoka Nagamura[1,2,3], Tarojiro Matsumura[4], Yasunobu Ando[5], Kenji Nagata[1], and Shotaro Akaho[4]
[1] National Institute for Materials Science (NIMS), [2] Tokyo University of Science, [3] Tohoku University,
[4] National Institute of Advanced Industrial Science and Technology, [5] Institute of Science Tokyo

High brilliance synchrotron radiation (SR) X-rays realize multi-dimensional, multi-scale, and extremely high-resolution analysis. Advanced SR spectromicroscopy potentially produce huge number of datasets. Efficient interpretation of spectral big data beyond manual peak assignment is an urgent issue. Here we propose a high-throughput and low-computational-cost spectral peak fitting analysis method assisted by machine learning.

We have developed “spectrum-adapted” expectation-maximization (EM) algorithm for maximum likelihood estimation of parameters at each peak component[1]. We adopted this technique for peak shift detection in spectral imaging data of X-ray photoemission spectroscopy (XPS) taken by a SR soft X-ray operando scanning photoelectron microscopy system. Drastic acceleration of peak fitting analysis was achieved in comparison to the conventional approach. Moreover, we succeeded to clarify the local carrier doping in the atomic layer device microstructures, which had been overlooked by conventional analyses[2,3]. Our analysis methods can be applied to several kinds of spectral data and peak structures, such as X-ray absorption spectra, Raman spectra, fluorescence spectra, luminescence histograms, and so on.

[1] T. Matsumura et al., ***Sci. Tech. Adv. Mat.,* 20,** 733 (2019).
[2] T. Matsumura et al., ***Sci. Tech. Adv. Mat Methods.,* 4,** 2373046 (2024).
[3] M. Okada et al., ***APL Materials,* 9,** 121115 (2021).

P2-08

Poster Award Nominee

XANES spectral analysis of Ni complexes using machine learning

Kentaro Fuku[1], Takefumi Yoshida[2], Tetsu Sato[3], Hiroaki Iguchi[4], Shinya Takaishi[5], Ryota Sakamoto[5], Hitoshi Abe[6,7,8]
[1] Tokyo Univ. of Science, [2] Wakayama Univ., [3] IMRAM, Tohoku Univ., [4] Nagoya University, [5] Tohoku University, [6] KEK-IMSS, [7] SOKENDAI, [8] Ibaraki Univ.

In coordination chemistry, the only methods for structure estimation have been single crystal X-ray structure analysis or DFT calculations. Recently, X-ray absorption fine structure (XAFS) has been attracting attention as a method for estimating coordination environments. However, the use of XAFS (especially XANES) in coordination chemistry is not common technique, and the most of its use are limited to “fingerprint matching” such as comparison with reference samples. In this study, we measured the XAFS spectra of Ni complexes, and aimed to estimate the coordination environment conveniently by spectral clustering using machine learning. As a result of our experiments, we succeeded in cluster partitioning by the number of coordination and the chemical environment of the coordinating atoms. And the clusters to which they belonged were changed following the ligand exchange reaction by adding ligands. These results suggest that the combination of XANES and machine learning will make it possible to estimate the coordination environment more easily.

P2-09

Poster Award Nominee

Sparse Coding-Based Multiframe Superresolution for Efficient Synchrotron Radiation Microspectroscopy

Yasuhiko Igarashi[1,2], Naoka Nagamura[2,3,4], Masahiro Sekine[1], Hirokazu Fukidome[4], Hideitsu Hino[5], and Masato Okada[2,6]
[1] University of Tsukuba, [2] Photoemission Group, National Institute for Materials Science, [3] Tokyo University of Science, [4] Tohoku University, [5] The Institute of Statistical Mathematics, [6] The University of Tokyo

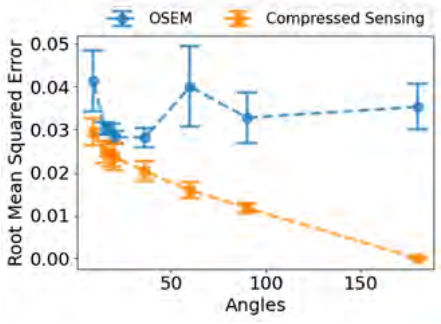
In nanostructure extraction, advanced techniques like synchrotron radiation and electron microscopy are often hindered by radiation damage and charging artifacts from long exposure times. This study presents a multiframe superresolution method using sparse coding to enhance synchrotron radiation microspectroscopy images. By reconstructing high-resolution images from multiple low-resolution ones, exposure time is minimized, reducing radiation effects, thermal drift, and sample degradation while preserving spatial resolution. Unlike deep learning-based superresolution methods, which overlook positional misalignment, our approach treats positional shifts as known control parameters, enhancing superresolution accuracy with a small, noisy dataset. Unlike state-of-the-art deep learning techniques that require large datasets, our method excels with limited data, making it ideal for real-world scenarios with constrained sample sizes. This approach offers enhanced image quality, reduced exposure times, and improved interpretability of scientific data, making it a versatile tool for overcoming the challenges associated with radiation damage and sample degradation in nanoscale imaging.

P2-10

Poster Award Nominee

High-speed measurement of MOF using sparse-view XAFS-CT reconstruction with compressed sensing

Naoki Yamane[1], Hirosuke Matsui[2], Mizuki Tada[2], and Yasuhiko Igarashi[3,4]
[1] Graduate School of Science and Technology, University of Tsukuba
[2] Graduate School of Science, Nagoya University
[3] Institute of Systems and Information Engineering, University of Tsukuba
[4] Photoemission Group, National Institute for Materials Science (NIMS)



XAFS-CT (X-ray Absorption Fine Structure Computed Tomography) is a technique that measures the internal structure and chemical states of materials by varying the projection direction and energy of X-rays. Faster measurements using a limited number of projections, namely sparse-view CT, are necessary. This can be addressed by assuming that CT images are sparse, a principle known as compressed sensing [1]. In this study, we investigated the applicability of sparse-view CT for the reconstruction of multiple coefficient data in XAFS-CT, targeting MOF (Metal-Organic Framework) materials, which are expected to have societal applications as adsorbents [2]. As a result, the compressed sensing method (FISTA) achieved higher reconstruction accuracy with fewer projections than the conventional OSEM (Ordered Subset Expectation Maximization) (Figure 1).

[1] H.Kudo et al., ***QIMS.*, 3,** 14761–14161 (2013).
[2] E.Yamada et al., **J. Am. Chem. Soc., 146,** 9181–9190(2024).

P2-11

Implementation of an Ontology Framework for Integrating Synchrotron Radiation Data

Masashi Ishii[1] and Asahiko Matsuda[2]
[1] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)
[2] Materials Data Platform, National Institute for Materials Science (NIMS)

X-ray absorption fine structure (XAFS) is a typical synchrotron radiation experimental method, and since the interpretation of data is deepened by cross-referencing the spectra, there are many spectral databases around the world. We developed and implemented an ontology framework to make XAFS spectra around the world findable.

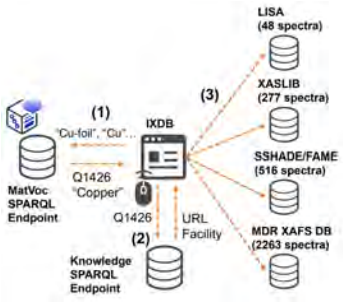


Fig. 1 IXDB search flow

Since the databases of each country have different terminology and table structures, we carried out “unification of vocabulary” and “unification of knowledge” to achieve cross-national searches; we normalized the material names and absorption edge names using the NIMS vocabulary management system MatVoc [1], and also made the XAFS concept, which is common to the target databases, ontologically machine-readable. The International XAFS Database Portal (IXDB [2], Fig. 1) based on this framework has been implemented on the website of the Japanese XAFS Society, and it is now possible to perform cross-searches of more than 3000 spectra recorded in four databases around the world.

[1] NIMS Materials Vocabulary, MatVoc, https://matvoc.nims.go.jp/wiki/Main_Page.
[2] Japanese XAFS society, International XAFS DB portal, https://ixdb.jxafs.org/.

P3-01

Defect Identification at Confined CO_2 Islands Using SPM

Oscar Custance[1], Emiliano Ventura-Macias[2], Hironobu Hayashi[1], Tadakatsu Ohkubo[1], Shigeki Kawai[1], and Ruben Perez[2]

[1] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)
[2] Department of Condensed Matter Theoretical Physics, Universidad Autonoma de Madrid, Spain

Understanding how carbon dioxide (CO_2) behaves and interacts with surfaces is paramount for the development of sensors and materials to attempt CO_2 mitigation and catalysis. Here, we combine simultaneous AFM and STM to resolve the molecular structure of CO_2 islands confined between one-dimensional metal–organic chains grown on a gold (111) surface and formed by PDI molecules linked by gold adatoms (Fig. 1). We have identified a chiral arrangement of flat CO_2 molecules in a windmill structure that populates these islands and enclose standing CO_2 molecules, CO molecules, and Au adatoms. Some of these defects are invisible to the STM and others are undetected by the AFM; only by simultaneously combining these two techniques it is possible to locate and identify all these defects. Our results show the complementarity of AFM and STM and their potential to explore greenhouse gas molecules at surface-supported model systems [1].

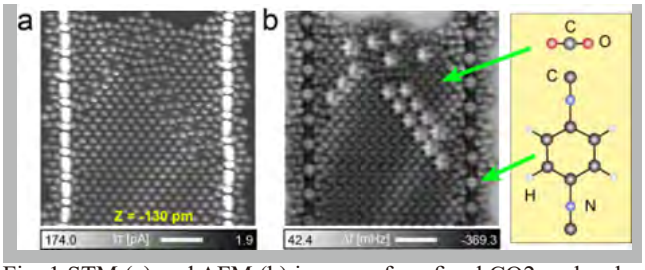


Fig. 1 STM (a) and AFM (b) images of confined CO2 molecules between two PDI-Au chains.

[1] O. Custance et al., ***ACS Nano*, 18,** 26759-26769 (2024).

P3-02

Poster Award Nominee

Water Adsorption on the Magnetite Surface Studied by Scanning Tunneling Microscopy

Tatsuhiro Hirai[1], Keisuke Sagisaka[2], and Tomoko K. Shimizu[1]
[1] Department of Applied Physics and Physico-Informatics, Keio University
[2] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)

The study of gas adsorption on the magnetite (Fe_3O_4) surface is a key to understanding the mechanism of catalytic reactions. Scanning tunneling microscopy (STM) provides atomic-scale insights into surface phenomena involving adsorbed gas species. In this study, we investigate the Fe_3O_4(111) surface after exposure to water using ultrahigh-vacuum (UHV) STM at 79 K (LT).

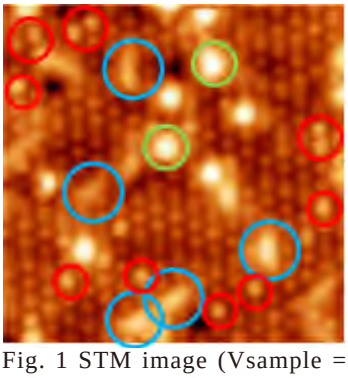


Fig. 1 STM image (Vsample = +2.0 V, Itunnel= 50 nA, scan area: 10 nm × 10 nm) of Fe_3O_4(111) exposed to water.

After annealing the single crystal of Fe_3O_4(111) at 950 K and subsequently cooling it to room temperature, the water-exposed surface exhibited one type of bright spots, which can be attributed to dissociated water species. In contrast, when water exposure was performed while the surface was kept at room temperature for 1 hour after removal from the STM head at 79 K, three types of water-related species were observed (Fig. 1). One of these species (indicated by blue circles) represents a newly discovered type that has not been described in previous studies [1]. It is possible that the three types of bright spots include adsorbed species related not only to dissociated water but also to molecularly adsorbed water.

[1] A. Kiuchi et al., ***Surf. Sci.*, 750,** 122582 (2024).

P3-03

Poster Award Nominee

On-Surface Synthesis of Silicon Incorporated Carbon Nanostructures

Kewei Sun[1] and Shigeki Kawai[2,3]
[1] International Center for Young Scientists (ICYS), National Institute for Materials Science (NIMS)
[2] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)
[3] Graduate School of Pure and Applied Sciences, University of Tsukuba, Tsukuba 305-8571, Japan

Substituting carbon with silicon in organic molecules and materials has long been an attractive way to modify their electronic structure and properties. Silicon-doped graphene-based materials are known to exhibit exotic properties, yet conjugated organic materials with atomically precise Si substitution have remained difficult to prepare. Here we present the on-surface synthesis of two-dimensional covalent organic frameworks (COFs) and one-dimensional graphene nanoribbons (GNRs), both incorporating 1,4-disilabenzene (C_4Si_2) units in their backbones. Silicon atoms were first deposited on a Au(111) surface, forming a AuSiX film on annealing. The subsequent deposition and annealing of a bromo-substituted polyaromatic hydrocarbon precursor (triphenylene or pyrene) on this surface led to the formation of the C_4Si_2-bridged networks, which were characterized by a combination of high-resolution scanning tunnelling microscopy (STM) and photoelectron spectroscopy supported by density functional theory calculations.

[1] Kewei Sun, Orlando J. Silveira, Yujing Ma, Yuri Hasegawa, Michio Matsumoto, Satoshi Kera, Ondřej Krejčí, Adam S. Foster, Shigeki Kawai. ***Nature Chemistry*, 15,** 136–142 (2023).

P3-04

Poster Award Nominee

On-surface Synthesis of Triaza[5]triangulene and its Magnetism

Donglin Li[1], O. J. Silveira[2], H. Hayashi[1], H. Maeda[3], A. S. Foster[2*], and S. Kawai[1,4*]
1 Center for Basic Research on Materials, National Institute for Materials Science (NIMS)
2 Dep. Applied Physics, Aalto University, Espoo, Finland.
3 Dep. Applied Chemistry, College of Life Sciences, Ritsumeikan University, Kusatsu 525-8577 Japan.
4 Graduate School of Pure and Applied Sciences, University of Tsukuba, Tsukuba 305-8571 Japan.

Triangulenes as neutral radicals are becoming promising candidates for future applications such as spintronics and quantum technologies. Doping nitrogen atoms to the carbon structures tunes their electronic and magnetic properties, resulting in higher polyradicals. Here, we synthesize triaza[5]triangulene on Au(111) by cyclodehydrogenation, and its derivatives by cleaving C–N bonds.[1] Bond-resolved scanning tunneling microscopy and scanning tunneling spectroscopy provided detailed structural information and evidence for open-shell singlet ground state. The antiferromagnetic arrangement of the spins in positively doped triaza[5] triangulene was further confirmed by density function theory calculations. Our findings pave the way for the exploration of exotic low-dimensional quantum phases of matter in heteroatom doped organic systems.

Figure: Triaza[5]triangulene, containing three graphitic nitrogen atoms synthesized on Au(111) through cyclodehydrogenation.

[1] D. Li, et al., ***Angew. Chem. Int. Ed.***, e202411893 (2024).

P3-05

Synthesis and Characterization of Oligoacenes

Hironobu Hayashi[1] and Hiroko Yamada[2]
[1] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)
[2] Institute for Chemical Research (ICR), Kyoto University

Oligoacenes are an important class of polycyclic aromatic hydrocarbons that have recently gained exceptional attention as promising materials for organic electronic devices. The nature of the ground state of oligoacenes has been widely debated so far, and remains controversial. One of the main reasons is the difficulty in synthesizing oligomacenes because of their low solubility and stability. To address thes issues, in this study, we utilize “thermal and photochemical precursor methods”. Briefly, bicyclo[2.2.2]octadiene(BCOD)-fused oligoacenes can be converted to the corresponding oligoacenes by the thermally induced retro-Diels-Alder reactions, while a-diketone-type precursors can be converted simply by photoirradiation. Here, we report the synthesis of oligoacene precursors and their on-surface conversion to oligoacenes on Au(111) under ultra-high vacuum conditions. For example, we demonstrate the on-surface generation of nonacene via visible-light-induced photodecarbonylation of a-diketone-type precursors. STM and nc-AFM analyses unambiguously confirmed the chemical structure. In addition, STS measurements coupled with theoretical calculations indicated the open-shell character of nonacene.[1]

[1] J. I. Urgel, S. Mishra, H. Hayashi, J. Wilhelm, C. A. Pignedoli, M. D. Giovannantonio, R. Widmer, M. Yamashita, N. Hieda, P. Ruffieux, H. Yamada, R. Fasel, ***Nat. Commun.*, 10,** 861 (2019).

P3-06

Poster Award Nominee

On-surface Synthesis of Azobenzene-linked Porphyrin

Y. Isshiki[1], D. Li[1], S. Vijayaraghavan[2], K. Sun[1], T. H. Ngo[3], Y. Matsushita[4], E. A. Neal[3], J. P. Hill[3], and S. Kawai[1,5]
[1] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)
[2] CSIR-Central Electrochemical Research Institute
[3] Research Center for Materials Nanoarchitectonics, National Institute for Materials Science (NIMS)
[4] Research Network and Facility Services Division, National Institute for Materials Science (NIMS)
[5] Graduate School of Pure and Applied Sciences, University of Tsukuba

Porphyrins are useful materials in the fields of photonics and organic electronics [1]. In this study, azobenzene-linked porphyrins were synthesized on Au(111) surface from Pt porphyrin with tri-Methyl (tMe-Por) and tert-Butyl (tBu-Por) via diazo coupling reaction between nitro groups. Scanning tunneling spectroscopy revealed that tMe-Por forms self-assembled structures with different chirality molecules, while tBu-Por involves same chirality. Azobenzene-linked porphyrins with mixed chirality were formed after annealing for both precursors, with a significantly higher yield from tMe-Por, indicating that its assembly with different chiralities promotes diazo coupling more efficiently. We clarified that the diazo coupling in tBu-Por goes through multiple reaction steps by the change of chirality.

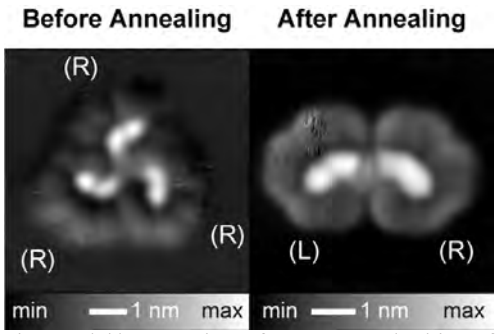


Figure: dI/dV mapping of tBu-Por at the bias of -0.2 V before and after annealing.

[1] J. Chen, et al., ***Angew. Chem. Int. Ed.*, 60,** 5010-5035 (2021).

P3-07

Studying Adsorbates on Rutile TiO_2(110) – (1×2) Surface Using Tip-enhanced Raman Spectroscopy

Kyungmin Kim[1,2], Daiki Katsube[3], Youngwook Park[2], Martin Wolf[2], Masayuki Abe[1], and Akitoshi Shitoari[2]
[1] Osaka University
[2] Fritz Haber Institute
[3] Japan Fine Ceramics Center

We report a microspectroscopic study on the rutile TiO_2(110) – (1×2) surface using low-temperature STM-based tip-enhanced Raman spectroscopy (TERS). As shown in Fig. 1, a high-resolution STM image shows a stripe pattern as reported in the literature [1]. While a far-field Raman spectrum of the sample (black curve in Fig. 1) has bulk phonon mode peaks, the near-field spectrum (red curve) acquired with a STM tip closely located over the stripe in the STM image shows additional peaks at ~700–900 and ~2400 cm^{-1}, indicating local vibrational properties at the site. We also found variations in Raman signals at different sites on the surface, indicating that TERS would be a powerful tool to characterize local chemical composition and bonding environments on TiO_2 surfaces.

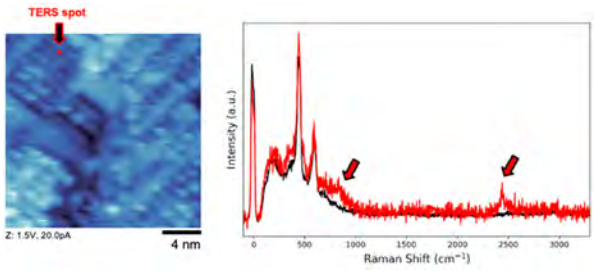


Fig. 1: (Left) STM image of the TiO_2(110) – (1×2) surface. (Right) Far- (black) and near- (red) field Raman spectra of the surface.

[1] C. M. Yim, C. L. Pang, G. Thornton, ***Surf. Sci.*, 650,** 71-75 (2016).

P3-08

Poster Award Nominee

Unveiling the Nanomechanical Phenomena in Silicon Thin Film Electrodes by Real-time Bimodal Atomic Force Microscopy Imaging

Ridwan Putraz[1,2], Kyosuke Matsushita[2], Tsuyoshi Ohnishi[2], and Takuya Masuda[1,2]
[1] Graduate School of Chemical Sciences and Engineering, Hokkaido University
[2] Research Center for Energy and Environmental Materials (GREEN), NIMS

Bimodal atomic force microscopy (AFM) offers nondestructive quantitative nanomechanical mapping of various battery materials, simultaneously with topography imaging, by detecting the changes in the amplitude and frequency shift of the first and higher eigen-modes of the cantilever [1]. In this presentation, we will introduce our newly developed *operando* bimodal AFM system which enables real-time monitoring of nanomechanical phenomena in an amorphous silicon thin film electrode throughout the first electrochemical lithiation/delithiation [2]. The evolution in the topography images and Young's modulus maps of the Si electrode were successfully acquired as a function of apparent Li content x in lithium silicide (Li_xSi), as shown in Fig. 1. In the first lithiation, the elastic modulus dramatically decreased due to the formation of Li_xSi from pristine Si, followed by a moderate modulus reduction with further lithiation up to x = 3.46. In the following delithiation, the elastic modulus gradually recovered up to x = 1.54.

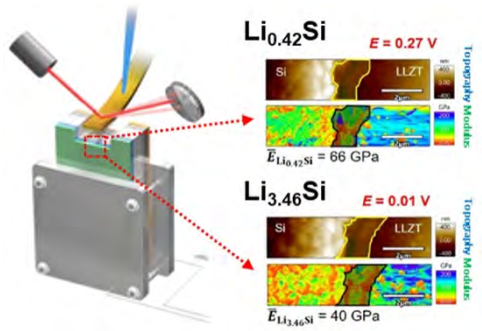


Fig. 1 Real-time nanomechanical mapping of Si electrode. Adapted from [2].

[1] H. Sakai, Y. Taniguchi, K. Uosaki, T. Masuda, ***J. Power Sources*, 413 (15),** 29-33 (2019).
[2] R.P. Putra, K. Matsushita, T. Ohnishi, T. Masuda, ***J. Phys. Chem. Lett.*, 15 (2),** 490 (2024).

P3-09

Poster Award Nominee

Mechanism of Triboelectric Charging in Fluorine-containing Monolayers Using Amplitude-feedback Frequency Modulated Scanning Force Microscopy

Masahiro Nakayama, Tomoki Misaka, Hiroshi Ohoyama, and Takuya Matsumoto
Department of Chemistry, Graduate School of Science, Osaka University

Triboelectric charging is one of the oldest known charging phenomena. Recently, flexoelectric effect was proposed as the origin of triboelectric charging. The flexoelectric effect is a property of a dielectric material that exhibits a spontaneous electrical polarization induced by a strain gradient and generates strong surface voltage. In this study, we focused on the nanoscale flexoelectric charging in fluorine-containing SAMs (F-DT) due to the strain gradient induced by tip-tapping which was measured as a jump in frequency shift caused by electron transfer due to flexoelectric charging. The frequency shifts of these samples were measured under medium vacuum and room temperature conditions using amplitude-feedback frequency-modulated scanning force microscopy (AM-FM SFM). When the frequency shift was measured, intermittent spikes were observed for F-DT. The spike phenomena were highly dependent on the loading force of cantilevers, and good agreement with the predictions from the flexoelectric charging model. These results strongly suggest that the jump in frequency shift is attributed to the nanoscale flexoelectric effect: the instantaneous surface potential change due to the electron transfer between tip and SAM film induced by flexoelectric effect (Fig. 1).

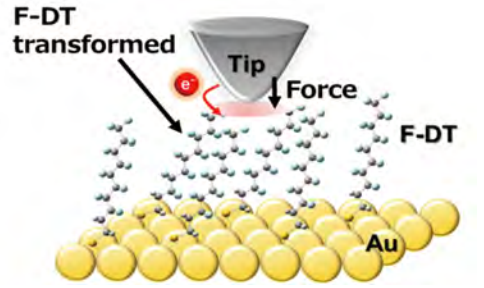


Fig. 1 Mechanism of electron transfer associated with triboelectric charging

P3-10

Quantitative Characterization of Built-in Potential Profile Across GaAs p–n Junctions Using Kelvin Probe Force Microscopy

Nobuyuki Ishida and Takaaki Mano
Center for Basic Research on Materials, National Institute for Materials Science (NIMS)

Kelvin probe force microscopy (KPFM) is a pivotal technique for measuring the electrostatic potential distribution on a sample surface. It has been extensively used to evaluate semiconductor devices, particularly to observe potential distribution across p-n junctions [1]. However, the magnitudes of the built-in potentials have consistently been smaller than those expected from the actual band structure, primarily due to surface band bending and tip-averaging effect.

In this study, we evaluated the quantitative reliability of KPFM by employing an atomic force microscope (AFM) with a qPlus sensor, which is expected to have less tip-averaging effect compared to a cantilever-type AFM and by using a GaAs(110) surface, known for its flat band from the bulk to the surface due to the absence of surface states within the bandgap. KPFM was conducted on the cross section of a GaAs p–n junction, and we demonstrated that using higher-order polynomials instead of a 2nd-order polynomial (quadratic function) in the fitting procedure during CPD derivation improves the accuracy of the CPD measurements [2]. The CPD profiles obtained from these fittings matched well with the line shape of the simulated potential distribution.

[1] T. Glatzel et al., ***Mater. Sci. Eng. B*, 102,** 138 (2003).
[2] N. Ishida and T. Mano, ***Nanotechnology*, 35,** 065708 (2024).

P3-11

Poster Award Nominee

EFM, KPFM Measurement of Photo-induced Charge Separation on F8T2 Monolayer/ TiO_2 Interface

Tomoki Misaka[1], Naoki Hara[2], Hiroshi Ohoyama[1], Shusaku Nagano[2], and Takuya Matsumoto[1]
[1] Department of Chemistry Graduate school of Science, Osaka University
[2] Department of Chemistry, College of Science, Rikkyo University

Charge separation at interfaces plays a crucial role in various devices. In the case of nanoparticle or thin organic molecular layer interfaces, it is essential to consider the overall system charge involved in charge separation and recombination, which differs from bulk materials due to the limited number and mobility of carriers. Our goal is to observe charge transfer dynamics and discuss the energy level alignment at interfaces composed of a small number of molecules. In this study, we fabricated a monolayer of the conducting polymer Poly(9,9-dioctylfluorenyl-alt-bithiophene) (F8T2) on a TiO_2 substrate, focusing on an interface with a minimal number of molecules. We investigated the photoexcited charge separation dynamics at the interface using Kelvin Probe Force Microscopy (KPFM) and Electrostatic Force Microscopy (EFM). EFM measurements at various applied DC voltages demonstrated a voltage-dependent optical response in the time evolution of charge separation. We analyzed the time evolution of charge separation using a model based on the energy alignment of the interface, taking into account the limited number of molecules involved in the charge separation reaction.

P3-12

Surface Resistivity Measurements Using Frequency Modulation Atomic Force Microscopy in Ultrahigh Vacuum

Naoki Shima[1], Takahiro Kato[1], Masahiko Tomitori[2], and Toyoko Arai[1]
[1] Kanazawa University,
[2] Japan Advanced Institute of Science and Technology

The conservative and non-conservative forces between a tip and a sample can be simultaneously estimated by frequency modulation atomic force microscopy (FM-AFM). The conservative forces are derived from the resonance frequency shift (Δf) of an oscillating AFM cantilever; f is the cantilever's resonance frequency. The non-conservative forces are detected as the dissipation energy (D), derived from the change in the amplitude of the excitation signal to maintain a constant amplitude (A) of the cantilever oscillation. Previously, we reported that the dissipation energy (D_J) due to Joule heat was proportional to Δf_{ele} due to the long-range electrostatic force under a bias voltage (V) between the tip and sample, as the following equation, notably excluding V and the tip-sample separation: [1]

$$D_J = -16\pi^3 \varepsilon_0 k A^2 r_{\mathrm{tip}} \times R_{\mathrm{J}} \times \Delta f_{\mathrm{ele}}$$

where ε_0 is the permittivity of vacuum, k is the spring constant of the cantilever, r_{tip} is the tip radius, and R_J is the resistance responsible for Joule heat. The value of R_J can be evaluated from the proportional coefficient in the relationship between D_J and Δf_{ele}. In this study, we evaluate the surface resistance of a gold (Au) film on mica in an ultrahigh vacuum (UHV) with a tungsten (W) tip sharpened by high-temperature flame-etching; r_{tip} was estimated by field electron emission in the UHV. The W tip is on a quartz-tuning-based retuned force sensor with a high Q. We will discuss the validity of the equation.

[1] T. Arai, D. Kura, R. Inamura & M. Tomitori, ***Jpn. J. Appl. Phys.*, 57,** 08NB04 (2018).

P3-13

Poster Award Nominee

Measuring Electronic Structure of Thermoelectric Materials by Scanning Tunneling Microscopy

Yuya Hattori[1], Shunsuke Yoshizawa[1], Keisuke Sagisaka[1], Yuki Tokumoto[2], Keiichi Edagawa[2], Takako Konoike[3], Shinya Uji[3], and Taichi Terashima[3]
[1] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)
[2] Institute of Industrial Science, The University of Tokyo
[3] Research center for Materials Nanoarchitectonics, National Institute for Materials Science (NIMS)

The dimensionless figure of merit (zT) of thermoelectric (TE) materials has been increasing rapidly in recent years. In the 1990s, the zT values of bulk thermoelectric materials are around zT~1.0, but high performance materials with zT>2.5 with doubled conversion efficiency are reported in many classes after 2010s. The drastic leap in performance stems from the band engineering. By adding dopants, it is possible to control the bandgap and to change the energy of the band edge, which is crucial for the TE performance. However, there was no experimental verification of the modification of the band structure by doping. Here, we use scanning tunneling microscopy (STM) to verify the band modification of Sr/Na doped PbTe [1], which is reported to have zT=2.5. By measuring the dI/dV values, which are proportional to the local density of states, we show that the band gap of Sr/Na doped PbTe becomes larger (350 meV) than the pristine PbTe (200 meV). We also find other band modifications, and the details will be discussed in the poster presentation.

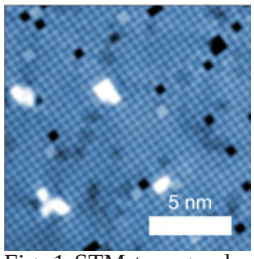


Fig. 1 STM topography of Sr/Na doped PbTe

[1] Y. Hattori et al., ***Phys. Rev. B*, 108,** 125119 (2023).

P3-14

Poster Award Nominee

Structures and Surface Conductivity on Dense Pb Monolayers Formed on Si(111) Studied by Low Temperature Scanning Tunneling Microscopy/Potentiometry

Junya Okazaki[1], Masahiro Haze[1], Masayuki Hamada[1], Yudai Sato[2], and Yukio Hasegawa[1]
[1] The Institute for Solid State Physics, The University of Tokyo, Japan
[2] Leiden Institute of Physics, Leiden University, the Netherlands

In two-dimensional superconductors, superconducting properties are sensitive to the presence of disorder. In the case of monolayer superconductors, atomic steps on the substrate are known to behave as disorders [1]. Because the manner in which the steps disturb the superconductivity depends on the monolayer structure, we investigated the resistivity of the atomic steps of various monolayers using low-temperature scanning tunneling microscopy/potentiometry (LT-STM/P). This method allows us to obtain surface images with atomic-scale spatial resolution and electrochemical potential images with μV resolution, providing information about the local surface transport properties. In this study, LT-STM/P measurements were performed on dense Pb atomic layers formed on Si(111) and revealed that the atomic step in the 1.2 monolayer (ML)-$\sqrt{3} \times \sqrt{7}$ phase works as a stronger disorder than that in the 1.33 ML-striped incommensurate (SIC) phase. In this presentation, we discuss the differences in the surface electrical resistance between the two phases.

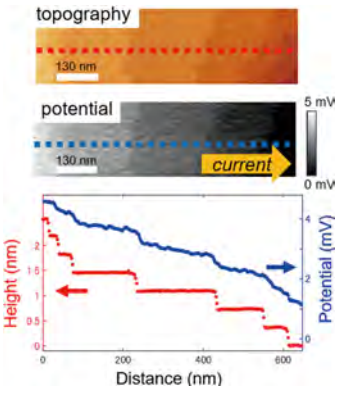


Figure: STP results for the $\sqrt{3} \times \sqrt{7}$ phase. (upper) Topographic image (middle) Electrochemical potential image (bottom) Line profiles showing the distribution of potential over terraces and steps.

[1] Y. Sato et al., ***PRL*, 130,** 106002 (2023).

P3-15

Poster Award Nominee

High-speed Subnanoscale-resolution 2D/3D-AFM Imaging of Calcite Dissolution Process

Kazuki Miyata[1], A. S. Foster[1,2], and T. Fukuma[1]
[1] Nano Life Science Institute (WPI-NanoLSI), Kanazawa University
[2] Department of Applied Physics, Aalto University

Recent progress in liquid-environment frequency modulation AFM (FM-AFM) has enabled to visualize atomic-scale 2D height images and 3D force distributions at solid/liquid interfaces. However, its imaging speed (typically ~1 min/frame) has often been too slow to visualize dynamic processes. So far, we have made effort to enhance the measurement bandwidth by improving several key FM-AFM elements, including ultrasmall cantilevers with a megahertz-order resonance frequency in liquid, a low noise wide-band frequency shift detector, a cantilever deflection sensor, a cantilever photothermal excitation system, and Z-tip and XY-sample scanners.[1] With these improvements, we have succeeded in subnanoscale-resolution 2D and 3D imaging of calcite ($CaCO_3$) crystal dissolution processes in water at ~1 s/frame.[2,3] The obtained images revealed the formation of a characteristic transition region (TR) along the step edges. Our simulations suggested that the TR is most likely to be a $Ca(OH)_2$ monolayer formed as an intermediate state in calcite dissolution. Based on this finding, we proposed major improvements in the atomistic calcite dissolution model.

[1] K. Miyata et al., ***Jpn. J. Appl. Phys.*, 54,** 08LA03 (2015).
[2] K. Miyata et al., ***Nano Lett.*, 17,** 4083-4089 (2017).
[3] K. Miyata et al., ***Nano Lett.*, 24,** 10842-10849 (2024).

P3-16

Poster Award Nominee

Role of Steps on Transport Measurements Studied by Scanning Tunneling Potentiometry

Masahiro Haze, Junya Okazaki, Masayuki Hamada, and Yukio Hasegawa
Institute for solid state physics, The University of Tokyo

Transport property is one of the fundamental information to characterize materials. The transport measurements in nanometer scale are, however, still challenging. By using scanning tunneling potentiometry one can investigate surface conductivity in atomic scales. While most of the works related to STP have been performed at room temperature, to investigate the ground state properties, it is necessary to perform measurements at low temperature. Here, we have demonstrated low temperature STP measurements along with scanning tunneling microscopy/spectroscopy (STM/S) on Pb atomic layer formed on Si(111) to investigate structures, local density of states (LDOS), and transport properties, simultaneously.

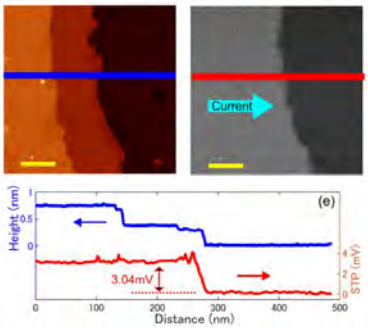


Figure: (Upper right) Topographic image (Upper left) STP image (lower) Line profiles

Our STP measurements reveal that the total resistance is dominated by the steps, when the coverage is 1.0 monolayers (ML). This result is well explained by our STM/S measurements, revealing that semiconducting regions are formed in the vicinity of step edges.

P3-17

Preparation and Evaluation of a High-temperature Flame-etched Tungsten Tip for Scanning Probe Microscopy

Yuta Okabe[1], Nobuhiko Utsunomiya[2], Yuki Araki[2], Masahiko Tomitori[3], and Toyoko Arai[1,2]
[1] School of Mathematics and Physics, Kanazawa University
[2] Graduate School of Natural Science and Technology, Kanazawa University
[3] Japan Advanced Institute of Science and Technology (JAIST)

The sharpness and physical-chemical states of a tip for scanning probe microscopy (SPM) are of central concern to obtaining high-resolution SPM images without artifacts, in particular, toward nanoscale materials characterization regarding their electronic properties, because the SPM images stem from a complex interaction occurring between the tip and the sample at the close separations. The atomic arrangements of the tip chiefly govern the mechanical and electronic properties of the tip. Therefore, a single crystalline tip, whose apex is surrounded by stable crystallographic planes, is attractive. Conventional high-temperature (> 2000 °C) flame-etching of a polycrystalline W wire using a $2H_2+O_2$ mixed gas, electrolyzed from pure water, can produce a sharp tungsten (W) tip quickly in less than 1 sec, whose apex is of a few-tens micrometer single crystal domain. However, the surface is covered with tungsten oxides (WO_x) after the flame etching. In the present study, we develop a method to remove the oxides while making the tip sharper by following a short-time electrochemical etching at low bias voltages. Furthermore, we also heat the W tip with a high-power blue laser in a vacuum. The tip shape and chemical compositions are analyzed using scanning electron microscopy with Auger electron spectroscopy and transmission electron microscopy with electron diffraction.

P4-01

Poster Award Nominee

Visualization of Magnetic Soliton Using Aberration-Corrected Lorentz Microscopy

Takuro Nagai
Research Network and Facility Services Division, National Institute for Materials Science (NIMS)

Lorentz microscopy is a modern TEM-based technique for magnetic imaging. However, the spatial resolution of Lorentz images is considerably reduced by the spherical aberration (C_s) and chromatic aberration (C_c) of the weakly excited Lorentz lens. We have therefore used an image C_s corrector and a monochromator simultaneously to reduce both aberrations for sake of the drastic improvement of the resolution, leading real-space observation of the magnetic phase separation in a single crystal of dysprosium (Dy) [1]. Figure 1 shows the in-plane magnetization distribution for Dy at 127K, obtained by the aberration-corrected Lorentz microscopy combined with the transport-of-intensity equation (TIE) method. Coexistence of magnetic soliton, an isolated single domain of the ferromagnetic phase, and the helical antiferromagnetic (AFM) phase is successfully visualized.

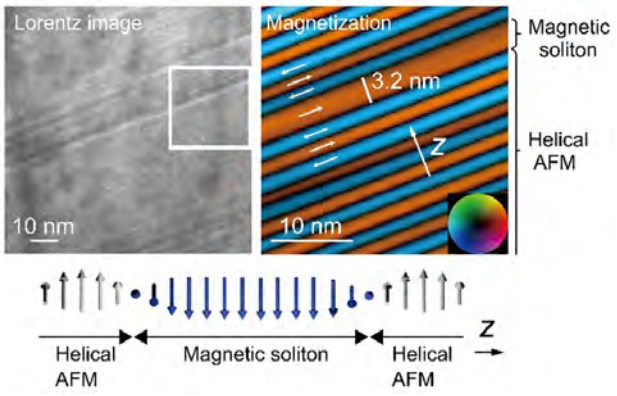


Fig.1 Aberration-corrected Lorentz image (left) and in-plane magnetization (right) for Dy at 127K, showing coexistence of magnetic soliton and the helical AFM phase.

[1] T. Nagai et al., ***Phys. Rev. B*, 96,** 100405(R) (2017).

P4-02

In-situ TEM Observation of Ni-based Catalysts for DRM

Ayako Hashimoto[1,2] and Hideki Abe[1,3]
[1] Research Center for Energy and Environmental Materials, National Institute for Materials Science (NIMS)
[2] Degree Programs in Pure and Applied Sciences, University of Tsukuba
[3] Graduate School of Science and Engineering, Saitama University

Dry reforming of methane (DRM, $CH_4 + CO_2 \rightarrow 2H_2 + 2CO$) is a powerful reaction utilizing the two greenhouse gases for a global warming issue. Ni-based catalysts are useful owing to their high catalytic activities and lower cost. But they are easily deactivated by carbon deposition (coking) during DRM reactions. In this work, structural and chemical changes of Ni nanoparticles on Al_2O_3 support during DRM process were investigated through in-situ scanning transmission electron microscopy (STEM) with electron energy-loss spectroscopy (EELS) analysis, which were performed by using a developed gas environment heating specimen holder system [1]. While the Ni nanoparticles were mainly metallic Ni before the DRM gas flowing, most of the nanoparticles changed from Ni to oxidized Ni or from oxidized Ni to reduced Ni depending on temperature after the gas flowing. In addition, structural changes of the Ni nanoparticles were observed with the oxidation and reduction.

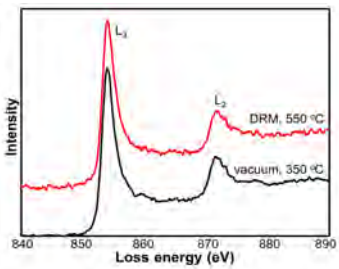


Fig. 1 In situ EELS spectra for Ni L edge under different conditions.

[1] A. Hashimoto et al., ***Microscopy*, 70,** 545-549 (2021).

P4-03

Poster Award Nominee

In-situ Observation of Post-nucleation Process of NaCl Nanocrystals in an Aqueous Environment Using Liquid-cell Transmission Electron Microscopy

Toshiki Shimizu[1,2], Ryoga Numazaki[1], Natsuki Nakasone[2], and Hiroki Minoda[1,2]
[1] Department of Applied Physics, Tokyo University of Agriculture and Technology
[2] Department of Applied Physics and Chemical Engineering, Tokyo University of Agriculture and Technology

Understanding the mechanism of crystal growth is one of the key factors in developing innovative materials with crystalline properties. Crystalline materials are essential to our daily lives and are closely involved in the production of foods such as salt and the development of new medicines or devices. The crystal growth is the post-nucleation process in which molecules or clusters are attaching to a host crystal. However, due to its stochasticity, complexity and diversity, the research in aqueous environment has been a great experimental challenge. In this work, by using liquid-cell transmission electron microscopy (LC-TEM), we observed the post-nucleation processes of a NaCl nanocrystal in a liquid cell made by amorphous carbon films that enabled stable observation under an electron beam. We succeeded in capturing the same NaCl nanocrystal grew through multiple post-nucleation processes which occurred simultaneously in different planes. The sub-nano level analysis confirmed that NaCl nanocrystal growth occurred via the stepwise attachment of sodium and chlorine ions or the orientated attachment of a cluster. We believe that our LC-TEM methodology will be one of the state-of-the-art materials characterization techniques for observing and analyzing samples in a liquid environment.

This study got support from the Precise Measurement Technology Promotion Foundation (PMTP-F), JSPS KAKENHI (JP23K13628) and JKA (KEIRIN RACE).

P4-04

Poster Award Nominee

In Situ Scanning Transmission Electron Microscopy of the MoS_2 Lithiation Process

Kei Nakayama and Shunsuke Kobayashi
Nanostructures Research Laboratory, Japan Fine Ceramics Center (JFCC)

Lithiation reactions are crucial, particularly for Li-ion batteries. In many instances, the migration of Li ions into electrode materials is accompanied by atomic-scale and nanoscale structural changes. Therefore, in situ observation is necessary to comprehensively understand the dynamic processes involved in lithiation reactions, which has commonly been achieved through high-resolution transmission electron microscopy (HRTEM). However, the image contrast produced by HRTEM is not always directly interpretable, necessitating the investigation of alternative techniques.

In this study, we used annular dark-field (ADF) scanning transmission electron microscopy (STEM), which is expected to provide more directly interpretable image contrast, to perform in situ observation of the MoS_2 lithiation process. A tungsten probe equipped in a sample holder was used to bring air-exposed lithium (Li_2CO_3, etc.) into contact with single-crystalline MoS_2 within an electron microscope. In situ ADF STEM at low magnification and following electron energy-loss spectroscopy confirmed the occurrence of a lithiation reaction. High-magnification in situ ADF STEM revealed contrast changes at subnanometer resolution. Although the visibility of the contrast in the raw data was very low due to a low signal-to-noise ratio, applying a threshold filter in Fourier space and a moving average filter improved clarity. As a result, a stepwise formation of a nanoscale domain structure was observed, likely serving to relieve internal stress during the lithiation process.

This work was supported by JST PRESTO (JPMJPR23J9), JSPS KAKENHI (JP23K13567, JP23H00241), ISTF (0341198-A), NSGF (no grant number), and ATLA (JPJ004596) in Japan.

P4-05

Real-Time Electron Microscopic Imaging and Analysis for Single Molecules and Atomically-Precise Nanomaterials

Koji Harano, Jun Kikkawa, and Koji Kimoto
Center for Basic Research on Materials, National Institute for Materials Science (NIMS)

In high-resolution electron microscopy of molecular materials and nanomaterials, sample damage caused by electron irradiation hinders atomically precise imaging and electron beam analysis. In this study, based on new sample preparation methods for TEM and high-speed TEM/STEM imaging and analysis technologies, we have achieved structural and elemental mapping of single molecules, molecular assemblies, and nanomaterials by minimizing sample damage from electron beams. For example, using single-walled carbon nanotubes as single-molecule specimen support, we succeeded in tracking structural changes of a single polymer chain during heating of carbon fibers produced by the heat treatment of polyacrylonitrile, capturing the conversion process in atomic resolution images. In another example, utilizing STEM-EDS analysis, we characterized a single atomic silver shell formed on the surface of ultra-thin gold nanorods synthesized via a wet process, revealing a hierarchical structure at nanoscale (Fig 1).

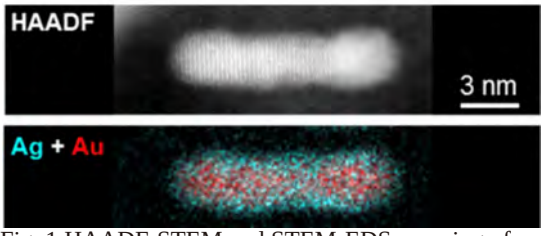


Fig. 1 HAADF-STEM and STEM-EDS mapping of an ultrathin gold nanorod with a silver shell.

[1] T. Ishikawa et al., ***J. Am. Chem. Soc.*, 145,** 12244–12254 (2023).
[2] S. Maity et al., ***Nano Lett.***, ASAP Article. DOI: 10.1021/acs.nanolett.4c03159

P4-06

Poster Award Nominee

Application of Nanometric Thermometry Based on Electron Spectroscopy of Phonons

Jun Kikkawa and Koji Kimoto
Center for Basic Research on Materials, National Institute for Materials Science (NIMS)

Recently, scanning transmission electron microscopy (STEM) and electron energy loss spectroscopy (EELS) have enabled the measurement of phonons with high spatial resolution. Through energy and momentum transfers between incident electrons and phonons, we measured phonon dispersion relations at the nanometer scale and detected vibrational modes localized at heterointerfaces [1]. Based on the principle of detailed balancing of phonon creation and annihilation, we also demonstrated the measurement of local temperature [2]. By using acoustic phonons, we found that temperature can be evaluated more precisely at low temperatures [2]. In this study, as an application of phonon spectroscopy based on the STEM–EELS method, we measured the local temperature of a diamond nanowire (DNW) during Joule heating [2]. Applying a voltage of 20 V to both ends of the DNW, we obtained EELS spectra along the DNW. EELS intensities located on both sides of the zero-loss peak were assigned to phonon modes, i.e., transverse acoustic (TA), longitudinal acoustic, transverse optical (TO), and longitudinal optical (LO) modes. Based on the intensity ratio of TA phonon creation and annihilation, we evaluated the temperature gradient along the DNW axis. The center of the DNW was determined to be 613 ± 5 K [2]. We also discuss the Joule heating mechanism in the DNW.

[1] J. Kikkawa, T. Taniguchi and K. Kimoto, ***Phys. Rev. B,* 104,** L201402 (2021).
[2] J. Kikkawa and K. Kimoto, ***Phys. Rev. B,* 106,** 95431 (2022).

P4-07

Poster Award Nominee

Direct Observation of Cu Sites in SCR Zeolite Catalysts Using Electron Ptychography

Masahiko Shimizu[1,2,3], Katsuaki Nakazawa[2], Kazutaka Mitsuishi[2], Hajime Matsumoto[1,2], Hisashi Shima[1], Takahiko Takewaki[1], and Ayako Hashimoto[2,3]
[1] Science & Innovation Center, Mitsubishi Chemical Corporation
[2] Research Center for Energy and Environmental Materials, National Institute for Materials Science (NIMS)
[3] Graduate School of Science and Technology, University of Tsukuba

Selective catalytic reduction (SCR) of NO_x is the mainstream method for cleaning diesel exhaust gas, and Cu-doped zeolites are widely used as SCR catalysts. It is thought that the local coordination of the active species Cu ions contributes to the catalyst's activity and degradation, but it has not yet been possible to analyze the structure at the atomic level. Therefore, in this study, we attempted direct observation using electron ptychography[1] to determine the Cu site and visualize the factors that cause hydrothermal degradation in SCR catalysts. Fig. 1 shows the phase image of Cu-CHA. In the poster, we will discuss the results of the observation of the structure of CHA zeolite after hydrothermal degradation, and the structural changes before and after hydrothermal test in AEI-type zeolite with hydrothermal durability.

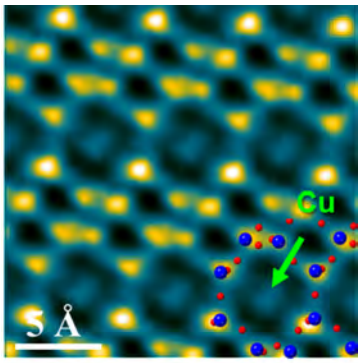


Fig. 1 Phase image of Cu-CHA zeolite observed from [100] direction. The scale bar is 5 Å. The arrow indicates Cu site with high possibility.

[1] K. Mitsuishi, et al., ***Sci. Rep.*, 13,** 316 (2023).

P4-08

Poster Award Nominee

Phase Mapping of Temperature Waves in Submicron-structured Ceramics Using PSTAM

Hieu Duy Nguyen[1], Isamu Yamada[2], Toshiyuki Nishimura[3], Hyunyong Cho[1], Takao Mori[4,5], Koji Kimoto[1], and Naoyuki Kawamoto[1]
[1] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)
[2] Yamada R&D Support Enterprise
[3] Research Center for Structural Materials, National Institute for Materials Science (NIMS)
[4] International Center for Materials Nanoarchitectonics (WPI-MANA), National Institute for Materials Science (NIMS)
[5] Graduate School of Pure and Applied Sciences, University of Tsukuba

Temperature waves were induced inside submicron-structured ceramics such as AlN and WB4-B composite, using a pulsed convergent electron beam of a scanning transmission electron microscopy (STEM) mode inside a transmission electron microscope (TEM). Strong contrast of phase delays between grains and grain boundaries, and different phases gives an idea to qualitatively characterize thermal properties and heat route inside submicron/nano-structured ceramics. This result provides a possibility to solve thermal-related issues in various applications such as thermal management of electronic devices, and development of heat sink and thermoelectric materials.

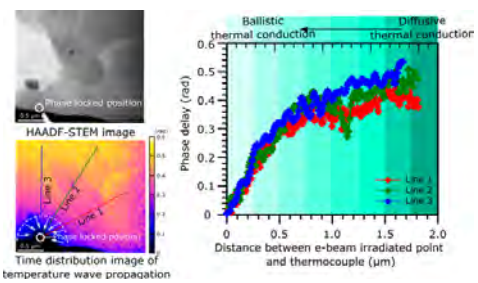


Fig. 1 Phase map of temperature wave propagation

Beside figure shows a HAADF-STEM image and a time distribution image of temperature wave propagation acquired by nano-sized thermocouple attached to the specimen.

[1] Hieu Duy Nguyen, Naoyuki Kawamoto et al., ***Sci. Adv,* 10,** eadj3825 (2024).

P4-09

Poster Award Nominee

Interpretable Structural Evaluation of Metal-Oxide Nanostructures in STEM Images via Persistent Homology

Ryuto Eguchi[1,2], Yu Wen[1,2], Hideki Abe[1,3], and Ayako Hashimoto[1,2]
[1] Research Center for Energy and Environmental Materials, National Institute for Materials Science (NIMS)
[2] Graduate School of Science and Technology, University of Tsukuba
[3] Graduate School of Science and Engineering, Saitama University

Persistent homology is a powerful tool for quantifying various structures, but it is equally crucial to maintain its interpretability for material design. In this study, we extracted interpretable geometric features from the persistent diagrams (PDs) of scanning transmission electron microscopy (STEM) images of self-assembled Pt-CeO_2 nanostructures synthesized under different annealing conditions. Analysis of the PD quadrants provided five interpretable features: average width and total length of striped CeO_2 phases, the number of CeO_2 phases from zeroth PDs, and the numbers of ring- and arc-like structures from first PDs. Principal component analysis (PCA) and its component mapping onto PDs clarified that the number of small arc-like structures is especially important for describing Pt-CeO_2 nano- structural changes. This descriptor enabled us to quantify the degree of disorder, namely the density of bends, in nanostructures formed under different conditions. By using this descriptor along with the width of the CeO_2 phase, we could classify 12 Pt-CeO_2 nanostructures in an interpretable way [1].

[1] R. Eguchi et. al., ***Nanomaterials*, 14,** 1413 (2024).

P4-10

Poster Award Nominee

Image Processing Techniques for Unveiling the Internal Structure of Crosslinked Rubber

Masato Suzuki[1,2] and Yasuhiko Igarashi[1,3]
[1] Institute of Systems and Information Engineering, University of Tsukuba
[2] The Yokohama Rubber Co., Ltd.
[3] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)

Rubber's unique elasticity and viscoelasticity among materials make it suitable for various applications, including tires and medical devices. These excellent properties are attributed to the crosslinking structure that connects the molecular chains [1]. However, significant noise makes it difficult to accurately understand the internal crosslinking structure of rubber, even with electron microscopy. This research focuses on improving the visualization of crosslinked network structures in rubber using image processing techniques. The study utilizes the Hessian matrix, a method commonly used in bio-medical imaging [2], to enhance the visibility of the network structure, even in noisy and hazy images. This allows for extracting parameters related to the network and its density, which correlates strongly with experimental results. This method successfully compared the internal structure of crosslinked rubbers of different formulations.

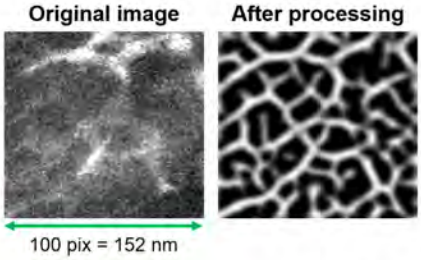


Fig. 1 Image processing using the Hessian matrix

[1] D. Y. Kim et al., ***Polymers*, vol. 12, no. 9,** 2020 (2020).
[2] B. P. Marsh et al., ***Sci Rep*, vol. 8, no. 1,** 978 (2018).

P4-11

Observation of Skyrmionic Vortex Using Electron Holography

Kodai Niitsu
Center for Basic Research on Materials, National Institute for Materials Science (NIMS)

The topological magnetic structure stabilized in a tetrahedral nanoparticle of B20-structure FeGe, a material hosting magnetic skyrmions, was determined. Using electron holography, magnetic-phase projections were obtained from multiple directions for one nanoparticle, and by integrating coupled analysis of micromagnetic simulation and finite element integration, the phase changes integrated across the same directions were calculated and imaged. As a result, it was found that the magnetic texture shapes a vortex structure with a spherical outline due to the chiral geometric frustration, which was named a skyrmionic vortex (see Figure).

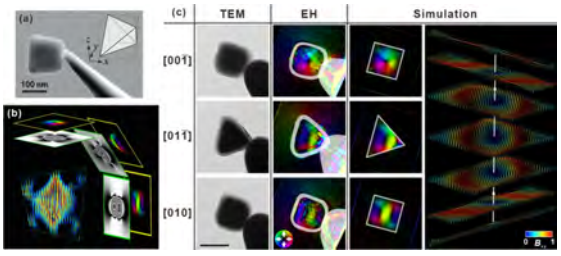


Figure. (a) FeGe tetrahedron on a tip, (b) Calculated phase map and its projections, (c) comparison of experimental and simulated magnetic-phase projections.

This study was conducted in collaboration with Y. Liu, X. Yu, D. Shindo, N. Nagaosa, Y. Tokura (from RIKEN), A. C. Booth, S. Jin (from U. New Hampshire), and N. Mathur, M. Stolt, J. Zang (from Univ. Wisconsin-Madison)

[1] K. Niitsu et al., ***Nature Materials,*** **21,** 305-310 (2022).

P4-12

Direct Imaging of Thermal Vibration Modes Using Frequency-Selective Electron Microscopy

Ovidiu Cretu, Han Zhang, and Koji Kimoto
Center for Basic Research on Materials, National Institute for Materials Science (NIMS)

In the absence of a driving force, objects experience thermal vibration, solely due to their non-zero temperature. Spatially resolved measurements of these vibrations are limited by their small amplitudes and by the overlap between different modes. We have developed a technique [1] which combines the extremely high spatial resolution of a STEM and fast signal acquisition electronics, which can display several thermal vibration modes simultaneously, with nanometer resolution.

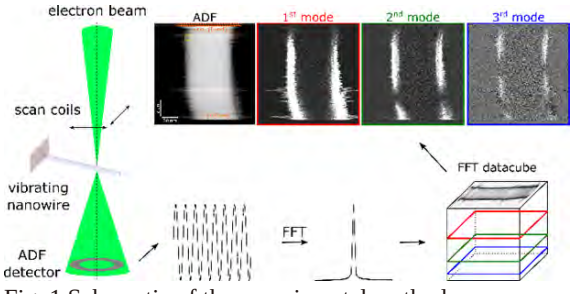


Fig. 1 Schematic of the experimental method.

This is showcased by mapping the first few thermal vibration modes of a nanowire, which agree well with classical vibration theory and FEM simulations. The influence of temperature on the vibration process as well as progress towards acquiring direct stroboscopic images of the vibration will also be discussed.

This work was supported by JSPS KAKENHI grants JP20H02624, JP22H05145, and JP24K08253.

[1] O. Cretu et al., ***Nano Lett.,*** **22,** 10034–10039 (2022).

P4-13

Deriving Sample Information from 4DSTEM Dataset by Electron Ptychography

Kazutaka Mitsuishi[1] and Katsuaki Nakazawa[2]
[1] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)
[2] International Center for Young Scientist (ICYS) ,National Institute for Materials Science (NIMS)

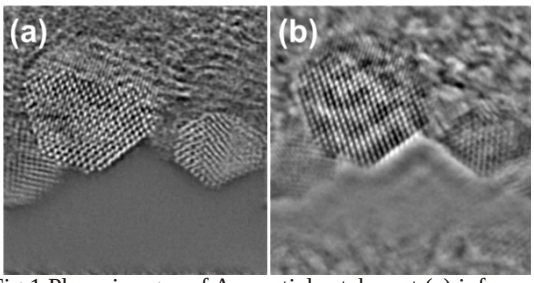


Fig 1 Phase images of Au particles taken at (a) infocus and (b) 100 nm defocused conditions reconstructed by ptychography.

The 4DSTEM measurement, which obtains diffraction patterns at each probe position during scanning transmission electron microscopy (STEM), has gained attention due to recent advancements in detectors. Ptychography [1] is a method to derive phase information from 4DSTEM data. This technique is noted for its high beam efficiency and its post correction capability, making it suitable for beam sensitive materials [2]. In this presentation, we will discuss the image features of ptychography. The figure shows the phase reconstructed from datasets of gold nanoparticles obtained under in-focus and 100 nm defocused conditions. Under the 100 nm defocused condition, it is usually challenging to visualize gold particles in conventional STEM images, but ptychography allows for the reconstruction of gold particles by estimating and correcting aberrations from the data.

[1] J.M. Rodenburg and R.H.T. Bates, ***Phil. Trans. R. Soc. Lond. A,*** **339,** 521(1992).
[2] K. Mitsuishi, et al., ***Sci. Rep.,*** **13,** 316 (2023).

P4-14

Characterization of Aberration-Corrected Lorentz TEM and STEM

Yu Jimbo[1], Yuto Tomita[2], Yuki Ninota[1], Kanako Kobayashi[1], Takeo Sasaki[1], Shigemasa Ohta[1], Takehiro Tamaoka[2], and Yasukazu Murakami[2]

[1] JEOL Ltd.
[2] Kyushu University

Lorentz microscopy is one of the powerful observation methods without the influence of magnetic field from the objective lens (OL) of a transmission electron microscope (TEM). Normally, the magnetic field around the TEM specimen is about 2 T. This field could adversely affect the observation of magnetic material. To avoid the influence, OL needs to be turned off and the lens under the OL is used as a focus lens, where it is called an objective mini-lens (OM) in JEOL instrument. We can use the OL to apply some amount of magnetic field to samples in Lorentz microscopy [1]. Recently, the spherical aberration correction was applied to Lorentz microscopy, the resolution was improved [2]. They showed the applied magnetic field with OL is possible with spherical aberration correction. However, the optimum setting for aberration-corrected Lorentz TEM has not been understood yet. In this research, we characterized the detailed capabilities of spherical aberration-corrected Lorentz TEM while applying magnetic field by the OL.

On the other hand, spherical aberration correction could be adapted to Lorentz STEM. In STEM case, condenser mini lens is used as focus lens. We confirm the resolution of corrected Lorentz STEM, and the resolution is 0.5nm. In presentation, the detail will be discussed.

[1] Xiuzhen Yu et al, ***JEOL NEWS,*** **50,** 2-10(2015).
[2] Takuro Nagai et al, ***PHYSICAL REVIEW B,*** **96,** 100405(2017)

P4-15

Poster Award Nominee

Observation Conditions for Grayscale HREM Image Interpretation via Persistent Homology

Ankit Singh[1], Ryuto Eguchi[1,2], Kazutaka Mitsuishi[3] and Ayako Hashimoto[1,2]
[1] Research Center for Energy and Environmental Materials, National Institute for Materials Science (NIMS)
[2] Graduate School of Science and Technology, University of Tsukuba
[3] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)

Persistent Homology (PH) is a mathematical tool that quantifies topological features like 'holes' by recording their 'birth' and 'death' in a persistent diagram (PD). PH is widely used in materials science for complex systems and recently applied to grayscale image analysis for structural patterns [1].

The accuracy of PH in interpreting structural patterns from grayscale images, particularly via High-Resolution Electron Microscopy (HREM), depends heavily on the imaging conditions. This study investigates the optimal observation conditions to minimize inaccuracy in structural pattern interpretation in HREM images. The images are based on a molecular-dynamics simulated model of amorphous carbon. Our findings reveal how observation parameters like defocus, sample thickness, and orientation affect PH's effectiveness in analyzing grayscale HREM images.

[1] Fumihiko Uesugi, and Masashi Ishii, ***Microscopy*, 71(3),** 161-168 (2022).

P4-16

Poster Award Nominee

Development of 5-dimensional STEM and Application to Glass Transition Phenomenon

Katsuaki Nakazawa[1], Kazutaka Mitsuishi[2] , Shinji Kohara[2], and Koichi Tsuchiya[1,3]
[1] International Center for Young Scientists, National Institute for Materials Science (NIMS)
[2] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)
[3] Research Center for Structural Materials, National Institute for Materials Science (NIMS)

In recent years, the development of high-speed pixelated scanning transmission electron microscope (STEM) detectors has made it easier to perform 4-dimensional STEM [1], which allows for the acquisition of spatial distributions of diffraction patterns.

We further advanced this technique to enable continuous observations using 4D-STEM, making it possible to acquire the spatiotemporal distribution of diffraction patterns. We call this method 5D-STEM since the time dimension is added to the conventional 4D-STEM [2]. In this study, we applied the developed 5D-STEM method to investigate the glass transition phenomenon in metallic glass. A correlation between local dynamics and atomic structures was revealed, which indicates that area with less-ordered structures tends to exhibit a shorter relaxation time.

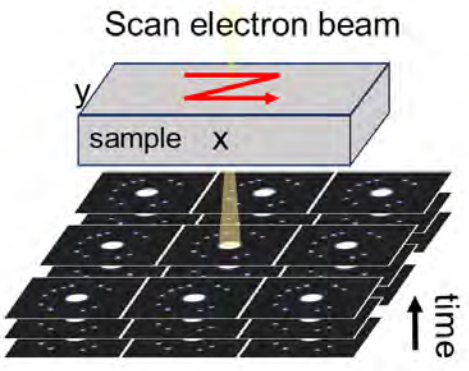


Fig. 1 Schematic of 5D-STEM

[1] C. Ophus, ***Microscopy and Microanalysis*, 25,** 563-582 (2019).
[2] K. Nakazawa and K. Mitsuishi, ***Microscopy*, 72,** 446-449 (2023).

P4-17

Poster Award Nominee

High Resolution and High Probe Current Electron Microscopy Application for LaB6 Nanostructured Emitter

Han Zhang
Center for Basic Research on Materials, National Institute for Materials Science (NIMS)

Electron microscopy applications, especially industrial use, demands both high resolution and high throughput (high probe current). It is vital to find an electron source with both brightness and monochromaticity as high as possible. Conventionally available electron sources, including thermionic electron source, Schottky electron source and W(310) cold field emission electron source, with their respective limitations, are insufficient to help overcome current technology barrier. We will introduce a new type of ultrahigh brightness cold field electron source made of low work function LaB6 single crystalline nanowire. We will first go over how nanostructured electron source surpasses conventional counterparts as a mechanistic discussion of basic emission properties. Then application examples in commercial S(TEM), SEM and semiconductor inspection instruments will be demonstrated.

[1] H. Zhang, Nature ***Nanotechnology*****, 11,** 273 (2016).
[2] H. Zhang, Nature ***Nanotechnology*****, 17,** 21 (2021).

P5-01

Poster Award Nominee

Simulation of Diffractive Electron Lenses Using Monte Carlo Method

Bo DA
Center for Basic Research on Materials, National Institute for Materials Science (NIMS)

Recently, Emanuel M. Avrahami et al. [1] reported that complex morphologies of biogenic crystals emerge from anisotropic growth of symmetry-related facets, demonstrating that the rotating crystal derives from asymmetric growth of symmetrically related crystallographic planes. Here, we present an even more interesting asymmetric crystal growth structure: the cylindrical symmetric rotating crystal (CSRC) [2]. The CSRC simultaneously exhibits island morphology in real space and Kikuchi diffraction patterns in momentum space in the raster scan mode of scanning electron microscopy. This new experimental observation suggests a potential mechanism beyond current diffraction theories.

For example, a CSRC could be designed to make the diffracted bright spots converge to the same point when the electron beam is incident on any position of the material. In this manner, it would be possible to produce a micron-scale electron lens, which is much smaller than current meter-scale electromagnetic lenses, and would facilitate development of portable electron microscopes. This will undoubtedly be of great significance to both materials characterization and industry. A CSRC thus provides broad opportunities for developing electronic components, and its application potential warrants further investigation.

[1] Emanuel M. Avrahami et al., ***Science,* 376,** 312–316 (2022).
[2] B. Da et al., ***Science and Technology of Advanced Materials: Methods*, 3:1** (2023).

P5-02

Poster Award Nominee

Computational Simulation of Material Behavior Using Image-based Finite Element Modeling

Ikumu Watanabe[1,2] and Tianwen Tan[1,2]
[1] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)
[2] Graduate School of Science and Technology, University of Tsukuba

Computational simulations are invaluable for studying the connection between material behavior and heterogeneous microstructure. The finite element (FE) method, with its ability to discretize domains into finite elements, is particularly adept at capturing complex heterogeneities. Nevertheless, constructing a computationally efficient FE model that accurately represents the actual microstructure remains a significant challenge. Furthermore, determining the local properties of individual constituents within the microstructure can be problematic. To address these limitations, various approaches have been proposed [1, 2]. In this paper, we present a case study demonstrating the application of these approaches to create an FE model based on an experimentally observed three-dimensional microstructure.

[1] I. Watanabe and A. Yamanaka, ***Int. Jour. Mech. Sci.,* 150,** 314 (2019).
[2] T. Chen and I. Watanabe, ***Sci. Tech. Adv. Mater. Meth.,* 2,** 416 (2022).

P5-03

Development of Fundamental Technologies for Data-Driven Battery Material Exploration

Yibin Xu, Yen-Ju Wu, Masao Arai, Huiping Li, Lei Fang, Shigenobu Hayashi, Ayako Oishi, Yuki Sakishita, and Natsuko Shimizu
Center for Basic Research on Materials, National Institute for Materials Science (NIMS)

We present a data-driven platform for exploring next-generation battery materials. At its core is the AtomWork Battery database, which compiles material data from over 1,000 selected papers on solid electrolytes and cathode materials. This data includes key properties such as chemical composition, crystal structure, ionic conductivity, and charge/discharge capacity. Additionally, we have developed a Python package, AtomWork Creator, designed for the exploration of superionic conductors. This package features tools for descriptor encoding/decoding, ionic conductivity prediction, and material design, leveraging the data from the AtomWork Battery database. This integrated approach accelerates the exploration of new superionic conductors and provides a continuously updated, comprehensive resource to advance battery material development through data-driven methods.

This work was supported by JST COI-NEXT “Center for Advanced Battery Collaboration” Grant Number JPMJPF2016.

[1] Y. Xu, Y. J. Wu, H. Li, L. Fang, S. Hayashi, A. Oishi, N. Shimizu, R. Caputo, P. Villars, ***Science and Technology of Advanced Materials,*** **25,** 2024. DOI: 10.1080/14686996.2024.2403328

P5-04

Exploration of Novel Eu^{2+}-Activated Phosphor Materials Using a Data-driven Approach

Yukinori Koyama[1], Takayuki Nakanishi[2], Naoto Hirosaki[2], and Takashi Takeda[2]
[1] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)
[2] Research Center for Electronic and Optical Materials, National Institute for Materials Science (NIMS)

Phosphor materials that use Eu^{2+} ions as the luminescent center utilize luminescence that accompanies electron transitions from 5d orbitals to 4f orbitals. As 5d orbitals are strongly affected by the host lattice, luminescence properties change greatly depending on the host. For example, the emission color changes from near-infrared to near-ultraviolet depending on the host. To rapidly develop phosphor materials for specific applications, it is necessary to design and search for host compounds that meet various requirements for phosphors. In this paper, we introduce the exploration of novel Eu^{2+}-activated phosphor materials using a data-driven approach.

[1] Y. Koyama, H. Ikeno, M. Harada, S. Funahashi, T. Takeda, N. Hirosaki, ***Mater. Adv.,*** **4,** 231-239 (2023).
[2] S. Takemura, Y. Koyama, T. Nakanishi, S. Funahashi, N. Hirosaki, H. Ikeno, T. Takeda, ***Scr. Mater.,*** **215,** 114686 (2022).
[3] S. Takemura, Y. Koyama, T. Nakanishi, S. Funahashi, N. Hirosaki, H. Ikeno, T. Takeda, ***J. Phys. Chem. Lett.,*** **13,** 11878-11882 (2022).

P5-05

A feature Mining Method Composed of Wavelet Filtering and PCA

Fumihiko Uesugi[1], Koji Harano[2], and Koji Kimoto[2]
[1] Electron microscopy unit, National Institute for Materials Science (NIMS)
[2] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)

The image processing method developed by Uesugi can perform feature extraction, image enhancement, and noise filtering by appropriately selecting and superimposing elements expanded by a concentric mother wavelet (CMW) [1]. In the feature extraction, size information of an object is extracted as wavelet coefficients using the CMW with the various radius, selecting, and reconstructed multiplying the coefficients and CMW.

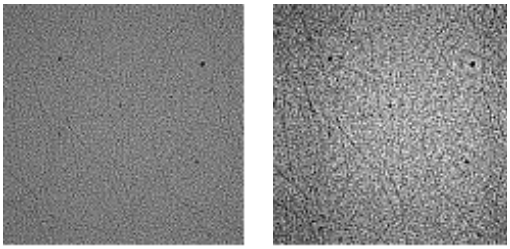


Fig.1 (Left) the original image, and (right) the optimizing result using PCA.

In this study, we tried to optimize the feature extraction by performing principal component analysis (PCA) on the wavelet coefficient data. Extracting the “feature” as loading vectors, the target object in the image can be reconstructed as score vectors. If feature extraction is possible, it is expected that the target object in another image will be selectively enhanced. The bottom right of the figure shows the result of feature extraction by PCA. The polymer image was reconstructed without losing the fine structure (Fig.1).

[1] Fumihiko Uesugi. Novel image processing method inspired by wavelet transform. ***Micron*, 168,** 103442 (2023)

P5-06

Poster Award Nominee

Information Extraction from Fermi Surfaces Using Unsupervised Machine Learning

Daichi Ishikawa[1], Kentaro Fuku[1],Yoshio Miura[2,3],Yasuhiko Igarashi[4], Yuma Iwasaki[5], Yuya Sakuraba[2], Koichiro Yaji[5], Alexandre Lira Foggiatto[1], Varadwaj Arpita[1], Naoka Nagamura[5], and Masato Kotsugi[1]
[1] Department of Material Science and Technology, Tokyo University of Science
[2] Research Center for Magnetic and Spintronics Materials, National Institute for Materials Science (NIMS)
[3] Electrical Engineering and Electronics, Kyoto Institute of Technology
[4] Institute of System and Information Engineering, University of Tsukuba
[5] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)

Fermi surface is crucial information for the designing various functions in spintronics devices. Particularly, electron states such as Weyl point and nodal line on Fermi surface contribute to spin polarization and anomalous Nernstian effects. In this study, we applied machine learning to the Fermi surface of Heusler alloy $Co_2MnGa_xGe_{1-x}$ (CMGG) and visualized the regions contributing to physical properties. We could confirm significant “jumps” in certain compositions in the reduced two-dimensional space. These jumps corresponded to compositions with varying spin polarization rates, and to compositions where the Weyl points appeared in the Fermi level. These results demonstrate the success of using unsupervised machine learning to reduce the dimensionality of the complex Fermi surface and visualize it in data space, allowing for the automatic extraction of noteworthy compositions and features.

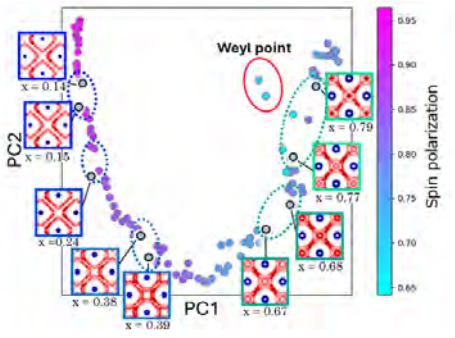


Fig. 1 Dimensional reductionof Fermi surface of CMGG

P5-07

Predictive Modeling of Two-Dimensional Electron Gas Formation at the β-$FeSi_2$/Si(001) Interface

Keisuke Sagisaka and Kazutaka Mitsuishi
Center for Basic Research on Materials, National Institute for Materials Science (NIMS)

As silicon-based electronic devices continue to shrink in scale, the exploration of novel two-dimensional materials compatible with silicon architectures becomes increasingly critical. In this study, we investigate the atomistic interface structure between β-iron silicide (β-$FeSi_2$) and a Si(001) substrate using cross-sectional scanning transmission electron microscopy and density functional theory (DFT) calculations [1]. Our results demonstrate that the β-$FeSi_2$(100) plane bonds to the Si(001) plane through two silicon dimers per unit cell. DFT band structure calculations further reveal the localization of metallic electronic states at the interface. This finding indicates the presence of two-dimensional electronic states at the β-$FeSi_2$/Si(001) interface, which could offer promising applications for silicon-based electronic devices.

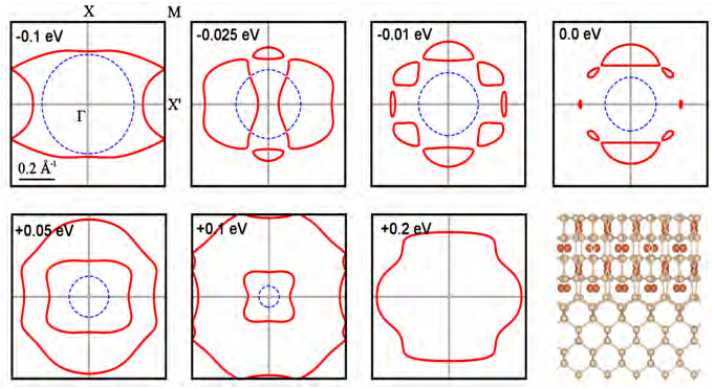


Fig. 1: Contour maps for the β-$FeSi_2$/Si(001) interface bands within the first Brillouin zone at the various energies around the calculated Fermi energy.

[1] K. Sagisaka, K. Mitsuishi, Submitted to Appl. Surf. Sci.

P5-08

Starrydata: an Open Database of Experimental Measurement Data from Published Plots

Yukari Katsura[1,2,3], Tomoya Mato[1], Yu Takada[1], Erina Fujita[1,4], Eiji Koyama[1], Atsumi Tanaka[1], Fumikazu Hosono[1], Dewi Yana[1], Naoto Saito[1], Yoshihiro Sakamoto[3], and Masaya Kumagai[3,5]
[1] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)
[2] Graduate School of Science and Technology, University of Tsukuba
[3] RIKEN Center for Advanced Intelligence Project, RIKEN
[4] The Institute of Statistical Mathematics
[5] SAKURA Internet, Inc.

We have developed Starrydata web system [1-2], an open database of experimental materials data collected by tracing plot images in literature. This web system allows users, including our data curators to share experimental data, with figure captions, sample information and other short explanatory text. The data on Starrydata are open to the public, and it can be used freely both for commercial and non-commercial purposes. We introduce our datasets for various functional materials extracted from plot images in published papers. Thermoelectric materials project is our largest data collection project on Starrydata, containing curves obtained from ~50,000 physical samples reported in ~10,000 papers, with compositions and fabrication methods. Data collection by the human curators were accelerated by improving the data digitizer and implementing an automatic retrieval system of sample information.

[1] Yukari Katsura, Masaya Kumagai et al., ***Sci. Technol. Adv. Mater.*, 20 (1)** 511-520 (2019).
[2] Starrydata2 web system: URL: https://www.starrydata2.org/

P5-09

Fermi Surface Analysis of Multi-component Co-based Heusler Alloys Using Machine Learning

Soichi Takase[1], Daichi Ishikawa[1], Kentaro Fuku1,Yoshio Miura[2,3],Yasuhiko Igarashi[4], Yuma Iwasaki[5], Yuya Sakuraba[2], Koichiro Yaji[5], Alexandre Lira Foggiatto[1], Varadwaj Arpita[1], Naoka Nagamura[5], and Masato Kotsugi[1]

[1] Department of Material Science and Technology, Tokyo University of Science
[2] Research Center for Magnetic and Spintronics Materials, National Institute for Materials Science (NIMS)
[3] Electrical Engineering and Electronics, Kyoto Institute of Technology
[4] Institute of System and Information Engineering, University of Tsukuba
[5] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)

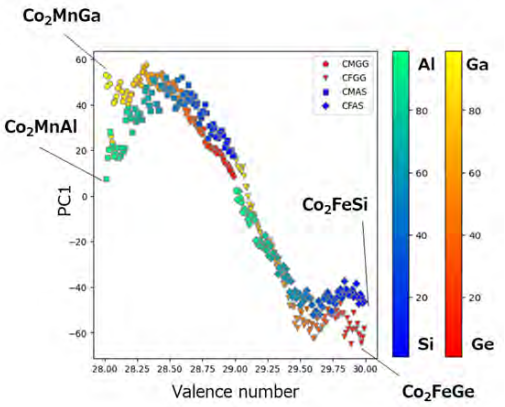


Fig. 1 Relationship between dimensional reduction results and valence electrons.

Cobalt-based Heusler alloys exhibit functional properties such as high spin polarization and ferromagnetism, rendering them promising candidates for spintronic applications. These properties are derived from the Fermi surface, yet extracting information from it remains a significant challenge. In this study, we utilized machine learning to analyze the Fermi surfaces in the k_x-k_y direction for four compositions: $Co_2MnGa_xGe_{1-x}$, $Co_2FeGa_xGe_{1-x}$, $Co_2MnAl_xSi_{1-x}$, and $Co_2FeAl_xSi_{1-x}$. Our findings reveal a correlation between the shape changes of the Fermi surface and the valence electron counts and magnetic moments in each composition. The results indicate that simple machine learning can extract parameters that correlate with physical quantities from the shape of Fermi surfaces.

P5-10

Poster Award Nominee

Real-time in-situ Machine Learning Analysis of RHEED Images for MBE Film-growth

Toshiro Osawa[1, 2], Asako Yoshinari[1, 2], Yasunobu Ando[3], Tarojiro Matsumura[4], Masato Kotsugi[1], and Naoka Nagamura[1,2]

[1] Tokyo University of Science, [2] National Institute for Materials Science (NIMS), [3] Institute of Science Tokyo, [4] National Institute of Advanced Industrial Science and Technology (AIST)

Molecular beam epitaxy (MBE) allows precise film-growth and reflection high-energy electron diffraction (RHEED) is used to evaluate structure and thickness. However, quantitative RHEED analysis requires expertise. We have developed machine learning approaches for automatic detection of surface superstructure changes and extraction of structural information[1]. In this study, we extend this method to a real-time structure evaluation during MBE film growth by integrating hardware and software. We applied this system to optimize the synthesis conditions for the target surface superstructures in MBE deposition of indium on a clean Si(111)”7×7” surface. During deposition, four steps were repeated every second: (1) RHEED image capture, (2) luminance histogram generation, (3) peak fitting using EMPeaks[2,3], and (4) plotting the maximum likelihood estimation results, including the standard deviation in each peak component. We succeeded in observing temporal changes in the standard deviation of a peak component in luminance histograms during deposition(Fig. 1). We found that the extreme values of the curve were the optimal conditions for the synthesis of $\sqrt{3}\times\sqrt{3}$-In, $\sqrt{31}\times\sqrt{31}$-In, and 4×1-In surface superstructures.

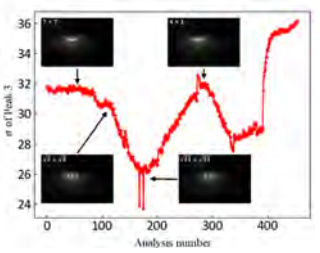


Fig. 1 Temporal changes in the standard deviation of a peak component.

[1] A. Yoshinari et.al., ***Sci. Technol. Adv. Mater.***: ***Methods 2***, 162 (2022). [2] T. Matsumura et al., ***Sci. Technol. Adv. Mater.*, 20,** 734 (2019). [3] EMPeaks (PyPI): https://pypi.org/project/EMPeaks/

P5-11

Exploration of New Alloy Compositions Using Prediction Model of Precipitation by Energetics

Yoshiaki Toda, Sae Dieb, Keitaro Sodeyama, and Masahiko Demura
Center for Basic Research on Materials, National Institute for Materials Science (NIMS)

Since the three-dimensional additive manufacturing is a new process, it is possible to manufacture with new compositional alloy systems that are not suitable for conventional forging or casting and may exhibit better properties than existing materials. However, it is very inefficient to search for new alloy systems only by experimental methods because of the huge cost in time and expense. In this study, we have proposed a model that can easily and quickly predict precipitation phenomena, which significantly affect high-temperature properties, by means of energetics. This model evaluates the total free energies of various microstructures that can appear in the process from supersaturated solid solution to equilibrium state and predicts the precipitation process of alloys based on the assumption of the steepest energy descent path. This model requires only a small number of input parameters for the calculation, and the prediction can be done with a relatively simple calculation of energy addition and subtraction only. Therefore, the composition, temperature, and time dependence of the precipitation process in new materials with unknown properties as well as practical structural materials in multiphase and multicomponent systems can be calculated in a short time using a personal computer. And, by combining an optimal solution search method based on information engineering, we attempted to search for heat-resistant nickel alloys with novel compositions suitable for additive manufacturing from a wide compositional space of multi-component systems [1].

[1] S. Dieb, Y. Toda, K. Sodeyama, M. Demura, ***Sci. Tech. Adv. Mater.: Method,*** **3 (1),** 2278321 (2023).

P5-12

Inverse Design Based on the Concept of Materials Integration

Masahiko Demura
Research Network and Facility Services Division, National Institute for Materials Science (NIMS)

The concept of Materials Integration aims to computationally link processing, structure, properties, and performance to accelerate materials research and development [1,2]. To realize this concept, we have developed a system called MInt [3]. In MInt, various prediction models based on computational simulations, theoretical or empirical formulas, and machine learning algorithms can be implemented as modules. These modules can be interconnected to design workflows that comprehensively predict material properties and performance from processing condition through microstructure evolution. Once forward predictions are established, inverse problems can be solved using AI optimizers.

We applied MInt to address the inverse problem of designing the aging process of a Ni-Al two-phase alloy, a model material for Ni-based superalloys. We constructed a computational workflow to predict high-temperature strength based on the aging process [3]. By incorporating Monte Carlo Tree Search (MCTS), one of the AI optimizers, into the workflow, we explored aging patterns that result in higher strength [4]. The AI algorithm identified 110 aging patterns superior to conventional isothermal aging. Based on these AI-discovered patterns, we proposed a novel two-stage aging concept.

[1] M. Demura & T. Koseki, ***Mater. Trans.,*** **61,** 2041 (2020).
[2] M. Demura, ***ISIJ International,*** **64,** 503 (2024).
[3] S. Minamoto et al., ***Mater. Trans.,*** **61,** 2067 (2020).
[4] T. Osada, et al., ***Mater. & Design,*** **226,** 111631 (2023).
[5] V. Nandal et al., ***Sci. Reports,*** **13,** 12660 (2023).

P5-13

A Tandem Bayesian Model for Probabilistic Search to Improve Weld Joint Creep Property

Hitoshi Izuno[1], M. Demura[1], M. Yamazaki[1], S. Minamoto[1], J. Sakurai[1], K. Nagata[1], Y. Mototake[2], D. Abe[3], and K. Torigata[3].
[1] Research Network and Facility Services Division, National Institute for Materials Science (NIMS)
[2] Hitotsubashi University
[3] IHI Corporation

The creep rupture of welded joints of heat-resistant steel initiated at the fine-grained heat-affected zone (HAZ) and its life is determined by the HAZ shape, which widely varies depending on the thermal history. This work aims at improving the creep rupture life of the weld joint through controlling the HAZ shape with optimizing the welding condition. We first constructed a forward workflow to predict the creep rupture life for arbitrary welding conditions by coupling the heat conduction analysis and subsequent creep damage analysis [1]. Then, using the workflow as a data source, we then developed a tandem Bayesian model that probabilistically connects two surrogate models: one is to predict the HAZ shape factors from the welding conditions; and the other is to predict the creep rupture life from the HAZ shape factors [2]. We finally proposed a framework where the model is sequentially updated by testing the candidates selected based on the probability of updating the longest rupture life obtained so far. The proposed framework has succeeded in improving the rupture life by 12% over the initial one just with the very small number of calculations (137 cases) compared with the huge design space of 78.

[1] D. Abe, K. Torigata, H. Izuno, M. Demura, ***Welding in the World,*** **68,** 1297–1311 (2024)
[2] H. Izuno, M. Demura, et al. ***Welding in the World,*** **68,** 1313-1332 (2024)

P5-14

First-principles Calculation of Electron-phonon Interaction

Atsushi Togo[1], Laurent Chaput[2], Henrique Miranda[3], Manuel Engel[3], Martijn Marsman[4], and Georg Kresse[4]
[1] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)
[2] LEMTA, University of Lorraine
[3] VASP Software GmbH
[4] Faculty of Physics and Center for Computational Materials Physics, University of Vienna

The electron-phonon interaction in condensed matter materials is related to properties such as the thermoelectric effect and conventional superconductivity. These properties can be predicted through first-principles calculations. There are several approaches to computing the electron-phonon interaction from first-principles calculations. We have developed a supercell approach within the projector augmented wave (PAW) method [1, 2]. This approach simplifies the computational procedure and expects to enhance robustness in systematic calculations against a variety of crystals. This method has been implemented in two software packages, the VASP and phelel codes. We overview the theory and methodology for computing the electron-phonon interaction and its related properties.

[1] L. Chaput, A. Togo, I. Tanaka., ***Phys. Rev. B,*** **100,** 174304 (2019).
[2] M. Engel, H. Miranda, L. Chaput, A. Togo, C. Verdi, M. Marsman, and G. Kresse, ***Phys. Rev. B,*** **106,** 094316 (2022)

P5-15

Physical Properties of Quantum Materials under Low Temperature and High Magnetic Field

Naoki Kikugawa
Center for Basic Research on Materials, National Institute for Materials Science (NIMS)

Quantum materials have attracted great attention as next-generation functional materials due to their rich physical properties, such as novel magnetism, multiferroicity, and unconventional superconductivity [1]. Recent advances in topological materials have also opened new windows to deepen our knowledge of the underlying materials science [2,3]. A key aspect of these materials is that their ground states can be controllable by relatively small perturbations: chemical substituting or doping of other elements, (uniaxial) pressure, gate tuning, and magnetic field. Understanding the intrinsic properties of bulk materials is essential because the magnetic, electronic, thermal, and topological properties are strongly linked. We present our recent achievements on the physical properties of quantum materials under low temperatures and high magnetic fields, where the bulk single-crystalline materials are grown by a floating-zone method [4]. We particularly focus on the magnetocaloric effect, a candidate magnetic Weyl semimetal, and unconventional superconductivity.

[1] N. Smith, ***Nature Materials*****, 16,** 1068 (2017).
[2] Y. Ando, ***J. Phys. Soc. Jpn.*****, 82,** 102001 (2013).
[3] B.A. Bernevig, C. Felser, and H. Beidenkopf, ***Nature*****, 603,** 41 (2022).
[4] N. Kikugawa, ***Crystals*****, 14,** 552 (2024).

P5-16

Poster Award Nominee

Observation of Nematicity in the Normal State in Sr-doped Bi_2Se_3

Yuhang Zu, Wenxi Wu, Tsuyoshi Tamegai and Yukio Hasegawa
School of Engineering, The University of Tokyo

Research on nematicity has been an important topic in the research field of unconventional superconductors. Nematicity means physics quantities show C_2 symmetry with high symmetry C_n in the crystal lattice. In previous work, such symmetry-broken electronic nematic phase widely found in high- T_c cuprates, iron-based superconductors and kagome superconductors. Recently, a similarly symmetry-broken behavior below T_c was found in topological superconductors $A_xBi_2Se_3$ (A=Cu, Sr, Nb), which is named nematic superconductivity. In theory and some experiments indicate that nematic superconductivity can be observed over T_c, but is limited to a small range above T_c. In this work, by carefully remove Planar Hall effect signal, we successfully got the numericity signal even in high temperature range (~200 K). Such result will have a huge influence on the understanding the mechanism of nematic superconductivity.

P5-17

Poster Award Nominee

Enhancing Corrosion Resistance by Electrodeposition of Mg-Al Layered Double Hydroxide (LDH) for AA6061 Alloy

Supicha Trakuldit[1,2] and Sachiko Hiromoto[2,1]
[1] Graduate School of Fundamental Science and Engineering, Waseda University
[2] Research Center for Structural Materials, National Institute for Materials Science (NIMS)

Aluminum alloys are utilized in contact with other metals, such as steel, in practical use. It promotes the corrosion of aluminum alloys by galvanic couple behavior. Electrodeposition of Mg-Al layered double hydroxide (Mg-Al LDH) was employed on AA6061 aluminum alloy to enhance the corrosion resistance. The influence of varied electrolyze concentrations was examined to optimize the coating condition. After electrodeposition, Mg-Al LDH islands preferentially formed on intermetallic precipitates. In a bath containing 1 M of $Mg(NO_3)_2$ and $Al(NO_3)_3$ solutions (1 M-bath), the Mg-Al LDH coated AA6061 showed a higher coverage of LDH islands on precipitates. Polarization and impedance tests in 0.1 M NaCl revealed that Mg-Al LDH coated AA6061 performed the corrosion protection ability, and AA6061 treated in the 1 M-bath has higher corrosion resistance due to more coverage of LDH on precipitates. In the wet-dry test, some localized corrosions were observed around the Fe-rich precipitates in the as-polished AA6061, while no corrosions occurred on the LDH coated AA6061, indicating that the presence of Mg-Al LDH on precipitates improved corrosion resistance of AA6061. This study provides the optimization of corrosion-protective Mg-Al LDH electrodeposition for AA6061 alloy.

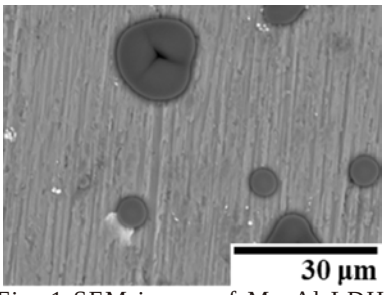


Fig. 1 SEM image of Mg-Al LDH electrodeposited AA6061.

[1] A. Ruiz-Garcia, V. Esquivel-Peña, J. Genesca, R. Montoya, ***Electrochimica Acta***, 449, (2023).

P5-18

Poster Award Nominee

Supercooled π-Gels Based on A Chiral Alkylated–Carbazole Liquid

Akito Tateyama[1,2] and Takashi Nakanishi[1,2,]
[1] Graduate School of Life Science, Hokkaido University
[2] Research Center for Materials Nanoarchitectonics, National Institute for Materials Science (NIMS)

In recent years, solvent-free functional molecular liquids composed of a π-conjugated unit and branched alkyl chains (alkyl–π liquids) have attracted attention.[1] To expand the usefulness of alkyl–π liquids, it is necessary to adjust their elastic modulus over a wide range. Therefore, we developed optoelectronically-active gel materials (alkyl–π gels) based on alkyl–π liquids using low-molecular-weight gelators.[2] This study focuses on the effect of chirality on the thermal and rheological properties of alkyl–π liquids and alkyl–π gels. Carbazole derivatives possessing a racemic (***rac*-CZL**) or an (R)-isomeric (***R*-CZL**) alkyl chain (Fig. 1a) were utilized. The as-obtained ***R*-CZL** was a supercooled liquid at room temperature; in contrast, ***rac*-CZL** was a practically stable liquid. Furthermore, adding 1 wt % low-molecular-weight gelator to ***R*-CZL** formed supercooled gel stable at room temperature (Fig. 1b). The gel exhibited unique temperature-dependent rheological properties due to its supercooling behavior.

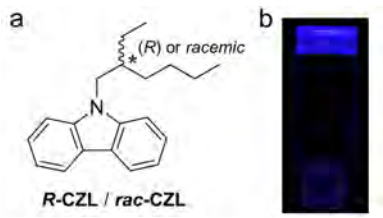


Fig. 1 (a) Molecular structures of ***R*-CZL** ((R)-isomer), ***rac*-CZL** (racemate). (b) Photo image of the gel based on ***R*-CZL** under 365 nm UV irradiation.

[1] A. Tateyama, T. Nakanishi, ***Responsive Mater.*, 1,** e20230001 (2023).
[2] A. Tateyama, T. Nakanishi, et al., ***Angew. Chem. Int. Ed.*, 63,** 202402874 (2024).

P5-19

Development of the Terahertz Magneto-spectroscopic System with Helium-3 Refrigerator

Kanji Takehana and Yasutaka Imanaka
Center for Basic Research on Materials, National Institute for Materials Science (NIMS)

The terahertz magneto-spectroscopy under high magnetic fields is a quit powerful tool to investigate the electron properties such as the effective mass and mobility [1, 2]. In general, the measurements at lower temperature are more advantageous to observe, for instance, the cyclotron resonance. It is, however, almost impossible to achieve the terahertz measurements at helium-3 temperatures, because the spectrum of blackbody radiation at the room temperature spread over the terahertz energy region.

We are developing the terahertz magneto-spectroscopy combined with the helium-3 refrigerator, using light pipe system which leads the prove light to the sample. The light pipe system has the advantage of reducing blackbody radiation from the room temperature. As the results, we succeeded to cool the sample down to less than 0.8 K. At the poster presentation, we will discuss the detailed optical system and further improvements.

[1] K. Takehana et al., ***Appl. Phys. Lett.*, 96,** 193110 (2010).
[2] K. Takehana et al., ***Current Applied Physics*, 14,** S119 (2014).

P5-20

Poster Award Nominee

Physical Modelling of Spatial Geometries at the Micro- and Macroscale Based on the Percolation Phenomenon

Robert Saraczyn
Faculty of Mechanical and Industrial Engineering, Warsaw University of Technology

The term percolation, most often, when used to describe materials refers to the process where a liquid or gas spreads through a network of interconnected pathways within porous or nonmetallic materials. Metal structures generally lack such networks, however, the geometry of objects can be shaped in such a way as to obtain it. Studies indicate that an appropriate use of the phenomenon in the design of mathematically defined spatial geometries allows the creation of components of low mass and high strength.

The term “phase percolation” refers to the process of percolation occurring between different phases or components within a composite material at the microscale level, where two or more distinct phases are combined to achieve specific properties. Phase percolation occurs when a continuous network forms between the phases, enabling the transfer of physical or chemical properties throughout the material.

Material properties are typically assessed based on the concentrations of specific phases or elements, but the identical chemical composition doesn’t ensure the same microscale structure. This leads to variability in properties due to the differences in spatial arrangement of phases. By determining the percolation threshold engineers can design composites with enhanced properties. Studies indicate that in the heat treatment processes the arrangement of phases can be modified to induce percolation, resulting in achieving desired mechanical properties.

P5-21

Poster Award Nominee

Anti-inflammatory Nanoparticles as Potential Treatment for Aortic Dissection

Maria Thea Rane Clarin[1,2,3], Eri Motoyama[3], Ahmed Nabil[2], Koichiro Uto[2], Sachiko Kanki[4], Kenichi Kimura[3], Hiromi Yanagisawa[3], and Mitsuhiro Ebara[2]
[1] Ph.D. Program in Humanics, University of Tsukuba,
[2] Research Center for Macromolecules and Biomaterials, National Institute for Materials Science (NIMS)
[3] Tsukuba Advanced Research Alliance (TARA) Center, University of Tsukuba,
[4] Osaka Medical and Pharmaceutical University, Osaka

Aortic dissection (AD) is characterized by the disruption of the aortic wall, which could be fatal as it might lead to rupture. More so, inflammation has been implicated in its development. Current treatments are still limited to surgery and anti-hypertensive agents. Thus, this research aims to develop nanoparticles that can be targeted in the aorta and suppress inflammation. Previously reported phosphatidyl serine-inspired polymeric particles (PSPs) known for modulating macrophages (MΦ) [1] were further validated using peritoneal MΦ. Lipopolysaccharide (LPS) was used to induce pro-inflammatory M1 MΦ. It has been observed that treatment with PSPs in LPS-induced MΦ reduces NF-kB signaling and significantly downregulates IL-6. This indicates its capacity to suppress inflammation. In our AD mouse model, we have observed the upregulation of vascular adhesion molecule-1, matrix metalloproteinases, and accumulation of M1 MΦ in the aortic lesions. These upregulated molecules will be further used in the design of targeting moiety for the modification of PSPs and its efficacy will be validated both in-vitro and in-vivo.

[1] Nakagawa et. al., ***ACS Macro Lett.*, Vol. 11, Issue 2,** 270–275 (2022).

P5-22

Rational Ligand Design for Enhanced Carrier Mobility in Self-powered SWIR Photodiodes Based on Colloidal InSb Quantum Dots

Cong Zhang[1,2], Subhashri Chatterjee[1,2], and Naoto Shirahata[1,2]
[1] Research Center for Materials Nanoarchitectonics, National Institute for Materials Science (NIMS)
[2] Graduate School of Chemical Sciences and Engineering, Hokkaido University

Solution-processed colloidal III–V semiconductor quantum dot photodiodes (QPDs) have potential applications in short-wavelength infrared (SWIR) imaging due to their tunable spectral response range, possible multiple-exciton generation, operation at 0-V bias voltage and low-cost fabrication and are also expected to replace lead- and mercury-based counterparts that are hampered by reliance on restricted elements (RoHS). Our previous work successfully synthesized InSb quantum dots (QDs) via a solution-based method and utilized these QDs to fabricate SWIR detection diodes. However, similar to other studies, our devices exhibited significant limitations such as excessive dark current and prolonged detection times, attributed to the high surface defect density of the QDs, which diminished their practical application potential.

In this study, we employed ligand exchange, utilizing sulfur ion oleylamine ligands to reduce the In_2O_3 oxide defects on the surface of the InSb QDs. This modification led to an enhanced photodetection response speed (rise time of 0.1s) and significantly reduced the dark current (as low as nA/cm²). Additionally, the reduced interdot spacing improved the carrier mobility within the QD layer of the device. As a result, the external quantum efficiency (EQE) of the ligand-modified device increased to 18.5%, thereby enhancing the potential of InSb QDs for infrared imaging sensor.

[1] S. Chatterjee, ***Nanoscale Horiz.*, 9,** 817-827 (2024).

P5-23

Poster Award Nominee

Does Uncertainty-based Active Learning Work in Materials Science?

Ai Koizumi[1], Guillaume Deffrennes[2], Kei Terayama[3,4,5], and Ryo Tamura[1,5,6]
[1] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)
[2] Univ. Grenoble Alpes, CNRS
[3] Graduate School of Medical Life Science, Yokohama City University
[4] MDX Research Center for Element Strategy, Tokyo Institute of Technology
[5] RIKEN Center for Advanced Intelligence Project
[6] Graduate School of Frontier Sciences, The University of Tokyo

Obtaining a fine approximation of a black box function (BBF) is important in the field of material design. Active learning aims to obtain a better BBF with less training data. In this study, we investigate whether Active learning based on uncertainty sampling (US, Fig. 1) can obtain a BBF in regression tasks using material databases. The liquidus surfaces of the ternary systems (the case of uniform and small dimensional inputs) are compared with the material databases of inorganic materials, small molecules and polymers (the case of non-uniform and large dimensional inputs). In the first case, US works. In the latter case, US is sometimes inefficient. And it works when the dimensions of the inputs are small. This study was supported by a project subsidized by the Core Research for Evolutional Science and Technology (CREST) (Grant number JPMJCR2234).

Fig. 1 Flow of uncertainty-based active learning (US)

[1] A. Koizumi et al., submitted.

P5-24

Poster Award Nominee

Kapok Microtubules Incorporated Carbon-Doped Graphitic Carbon Nitride for Photocatalytic H_2O_2 Production

Nur Shamimie Nadzwin Hasnan[1,2], Mohamad Azuwa Mohamed[1], and Lok Kumar Shrestha[2,3]
[1] Universiti Kebangsaan Malaysia
[2] Research Center for Materials Nanoarchitectonics, National Institute for Materials Science (NIMS)
[3] University of Tsukuba

Photocatalytic technology is appealing in producing H_2O_2 due to its environmentally friendly aspects of low energy consumption and no pollution. The photocatalytic H_2O_2 production as value-added chemicals and sustainable solar fuel has attracted enormous attention globally attributed to its sustainability process, where water and oxygen are abundant and ecologically natural resources, and solar light is applied to initiate the chemical reaction. In this study, kapok microtubules (t-KF) is utilized for the first time as an electron donor to boost the photocatalytic activity of carbon-doped g-C3N4 (CCN) through ligand-to-metal charge transfer (LMCT), significantly improving H_2O_2 production. Cellulose, a major component of kapok fiber, plays a promising role in photocatalysis due to its electron-rich hydroxyl groups, which can enhance photocatalytic activity. A simple hydrothermal grafting of CCN onto t-KF was accomplished by employing succinic acid (SA) as a cross-linker. The increase in the H_2O_2 production rate of CCN-SA/t-KF was 1.80-fold as compared to the pristine g-C_3N_4. This improvement is ascribed to the formation of the LMCT complex and the presence of carbon doping, which induced a charge transfer from the t-KF ligand to the metal CCN. This study highlights the potential of microtubular kapok fiber as a cost-effective, high-performance cellulose-based LMCT photocatalyst.

P5-25

Poster Award Nominee

Differences in Hydrogen Behavior Depending on Vanadium Grain Size

Souta Miyai[1], Tomoyasu Fujimaru[2], Tomoharu Hirayama[1], Eiji Tokumaru[1], Kouta Miyanouchi[1], Tomoko Kusawake[3], Yoshihisa Matsumoto[1], and Akiko N. Itakura[3]
[1] National Institute of Technology, Oita College
[2] Interdisciplinary Graduate School of Engineering Sciences, Kyushu University
[3] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)

We have been studying vanadium as a material for hydrogen separation membranes that can extract high-purity hydrogen gas from gas mixtures. It has been found that the amount of hydrogen permeation varies depending on the crystal grains [1]. In this study, we report the hydrogen diffusion in a rolled vanadium with a thickness of 0.5mm by hydrogen visualization using the silver decoration method [2]. First, a speckled pattern of permeated hydrogen was observed (Fig.1 left). It was found that the pattern corresponds to the shape of crystal grains, size of around 73μm, and the orientation. Next, we observed around the triple junction of large crystal grains, prepared by the unidirectional solidification method. Black dots were distributed throughout the surface (see Fig.1 right), and no orientation difference was found. These results suggest that not only the crystal orientation but also the crystal size affects the hydrogen diffusion behavior.

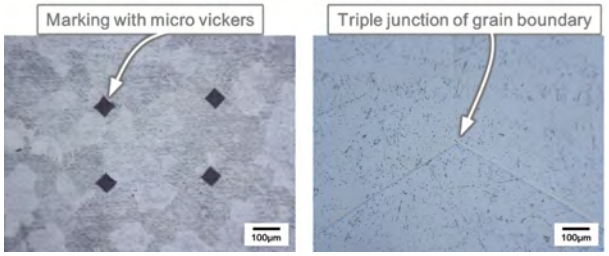


Fig.1 Silver decoration observation with an optical microscope. Left : rolled vanadium. Right : coarse grains of vanadium.

[1] T. Fujimaru et al., V***ac. Surf. Sci.*****, 66,** 608-612 (2023).
[2] A. N. Itakura et al., ***e-JSSNT*****, 22,** 174–178 (2024).

P5-26

Poster Award Nominee

Energy Performance Advancement by Tuning Nanospace of Hollow Carbon Spheres

Sabina Shahi[1,2] and Lok Kumar Shrestha[1,2]
[1] Department of Materials Science, Institute of Pure and Applied Sciences, University of Tsukuba
[2] Research Center for Materials Nanoarchitectonics, National Institute for Materials Science (NIMS)

Hollow carbon spheres, with their unique structural properties; hollow space at the center and carbon shells due to which they exhibit high surface area, have emerged as promising materials for energy storage/conversion and catalysts to drug delivery and sensing [1,2]. However, optimizing these materials still remains a challenge. We aim to enhance ion transport within these spheres, by manipulating the hollow spaces and nanopore engineering in the porous shell, improving their energy density performance to contribute to next generation energy storage technologies. In this contribution, we have used fullerene as a carbon source due to its ability to self-assemble and ethylenediamine as a structure-directing agent to synthesize the hollow carbon spheres with uniform particle size by simple dynamic liquid-liquid interfacial precipitation (DLLIP) method [2]. Systematic control over the nanoscale dimensions of the hollow spaces can improve ion mobility. Considering this, we successfully synthesize spheres with tunable cavity size. Furthermore, we chemically activated these hollow spheres using KOH and then carbonized at 900 °C. The morphology was intact even after carbonizing at high temperature. Spheres with high surface area (2189 m^2 g^{-1}) along with micro-mesopores on the shell and cavity at the center has been obtained. Electrochemical studies are going on to evaluate their performance as advanced electrode materials.

[1] Y. Sun, ***Carbon*****, 125,** 139-145(2017).
[2] L.K. Shrestha, ***Nanomaterials*****, 13,** 946(2023).

P5-27

Water-cooled Bitter Magnet for Measurement in High Magnetic Fields

Shinji Matsumoto and Yasutaka Imanaka
Center for Basic Research on Materials, National Institute for Materials Science (NIMS)

Semiconductors, magnetic materials, and superconductors exhibit interesting physical properties under conditions, such as low temperatures, high pressures, and high magnetic fields, as well as under combined conditions. Water-cooled magnets, superconducting magnets, and pulsed field magnets capable of generating high magnetic fields over 10 tesla are used for the measurements. NIMS has developed water-cooled Bitter coils to generate steady [1] and pulsed magnetic fields. The Bitter coil is shown in Fig. 1. The Bitter plate is a disk-shaped copper alloy plate with slits for coiling, holes for fastening stud bolts against electromagnetic force, and holes for cooling. Bitter plates are assembled into a solenoid shape with insulating sheets to form a Bitter coil. To achieve the desired magnetic field, an optimal design must be made, and the current density distribution, temperature distribution, magnetic field distribution, and stress distribution due to electromagnetic force in the coil must be evaluated, and an actual coil must be manufactured. By applying the Bitter coil to the pulsed field magnet, it is expected that repetitive magnetic fields can be generated by taking advantage of the water cooling.

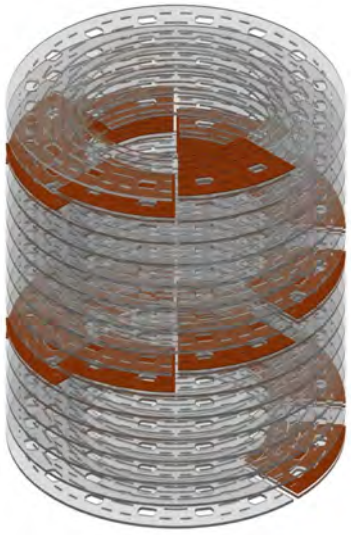


Fig. 1 Bitter coil

[1] T. Asano et al., ***IEEE Trans. Supercond.*, 16,** 965 (2006).

P5-28

Poster Award Nominee

Accelerating the Valid of Solid Electrolyte Candidates Through Machine Learning Force Fields: A Case Study on Li_8SeN_2 and $Li_{10}GeP_2S_{12}$

Meiqi ZHANG, Yen-Ju Wu, Yukinori KOYAMA, Masao ARAI, and Yibin XU
Center for Basic Research on Materials, National Institute for Materials Science (NIMS)

The discovery of high-performance solid-state electrolytes (SSEs) is critical for advancing all-solid-state batteries (ASSBs). However, traditional methods like ab initio molecular dynamics (AIMD), while accurate, are computationally expensive for large-scale screening.

This study demonstrates the use of Machine learning force fields (MLFFs)[1] to predict the ionic conductivity of Li_8SeN_2, a promising new SSE, and $Li_{10}GeP_2S_{12}$ (LGPS), a benchmark material. The MLFF, trained on first-principles data, accurately predicts ionic conductivity and ion migration pathways, showing excellent agreement with experimental results for LGPS. For Li_8SeN_2, MLFF simulations reveal their ionic mobility, providing critical insights into its structure and diffusion mechanisms. A major advantage of MLFFs is their ability to handle large systems and long timescales, making them ideal for material screening. In this work, MLFF enabled efficient simulation of Li_8SeN_2 across various conditions, yielding precise predictions at a fraction of the cost of AIMD. The flexibility to incorporate corrections for long-range interactions further enhances MLFF's accuracy in complex systems.

By significantly reducing computation time, MLFFs accelerate the valid of new SSE materials, allowing researchers to focus resources on the most promising candidates.

[1] R. Jinnouchi, F. Karsai, C. Verdi, R. Asahi, and G. Kresse, ***J. Chem. Phys.*, 152,** 234102 (2020).

P5-29

Poster Award Nominee

AI-Assisted Crystal Plasticity Analysis of Anisotropic Cold Rolling behavior in Ni_3Al

Jiyi Yang[1,2], Yoshinao Kobayashi[1], and Masahiko Demura[2]
[1] School of Materials and Chemical Technology, Tokyo Institute of Technology
[2] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)

The deformation behavior of Ni_3Al during cold rolling is highly anisotropic[1] and analysis based on the crystal plasticity is necessary to examine the mechanism behind it. The computational analysis requires not only the intrinsic understanding of the crystal plasticity but also the knowledge on a specific library or software for the simulation. This research presents an innovative approach that leverages a large language model such as ChatGPT to make codes necessary for the crystal plasticity analysis. Here we used the crystal plasticity simulation package, DAMASK[2]. As shown in Fig. 1, we fed proper prompting messages to ChatGPT together with the reference manual of DAMASK and could successfully obtain the codes such as input files for materials parameters and boundary conditions and python codes for executing, optimization, and post processing. Using the AI-generated codes, we conducted the crystal plasticity simulation and found that the anisotropic rolling deformation can be reproduced by assuming an exceptionally high value for the slip interaction of glissile junction pair.

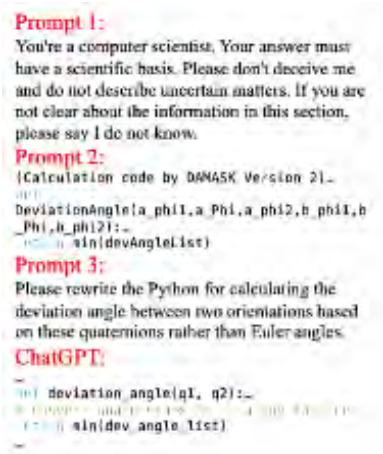


Fig.1. Part of the process of deviation angle calculation code generation.

[1] K. Kishida et al., ***Philos. Mag.*, 83,** 3029 (2003).
[2] https://damask-multiphysics.org

P5-30

Poster Award Nominee

Decoding Polymer Chain Using Nano Porous Material

Biplab Manna[1], Mizuki Asami[2], Nobuhiko Hosono[2], and Takashi Uemura[2]
[1] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)
[2] Department of Applied Chemistry, The University of Tokyo

Microstructures of polymer chains play a critical role in determining their properties. Therefore, researchers have devoted considerable efforts to developing techniques for synthesizing polymers with a controlled microstructure. However, there has been limited exploration into methods for identifying such microstructures of synthetic polymers. This study reports a new strategy for recognizing the monomer structures, compositions, and sequences of synthetic co polymers by introducing them into nano-sized pores of a metal organic framework (MOF) (Fig. 1). This technology is expected to create a new trend in separating and characterizing synthetic co polymers. Notably, this paradigm redefines the role of synthetic polymers from to serving as new information media, like how biosystems use nucleotide sequences of DNA as genetic information storage.[1]

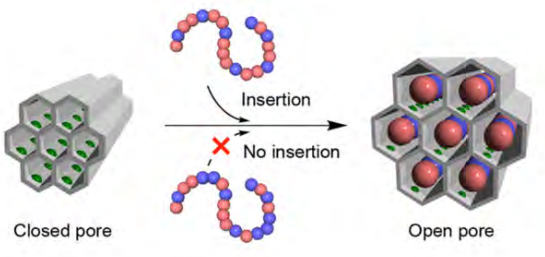


Fig.1: Schematic illustration of polymer Chain decoding using MOF material

[1] H. Ehara, T. Yokoyama,H. Shigematsu,S. Yokoyama,M. Shirouzu,1 S.-i. Sekine, ***Science*, 357,**921 (2017).

P5-31

Poster Award Nominee

Biomass-derived Carbon Nanostructures for Energy Storage Technology

Sarita Manandhar[1, 2] and L. K. Shrestha[1, 2]
[1] Research Center for Materials Nanoarchitectonics, National Institute for Materials Science (NIMS)
[2] Department of Materials Science, Institute of Pure and Applied Sciences, University of Tsukuba

Amidst the exploration of clean energy source and energy storage device, biomass carbon material has emerged to be one promising candidate [1] owing to their unique combination of high surface area, well-defined porosity, and intrinsic conductivity, hence particularly fitted to energy storage devices such as supercapacitors and batteries [2]. By using nanoarchitectonics, biomass carbon could be designed and applied precisely at the nanoscale for novel performance possibilities of sustainable energy storage technologies. This work presents the synthesis of high surface area, hierarchically porous carbon from Terminalia bellirica (Barro) seeds, using KOH activation and carbonization at 700-900°C in nitrogen atmosphere (1:1 weight ratio). The carbon materials were characterized by various techniques, and their electrochemical performance was tested in a three-electrode cell with 1 M H_2SO_4, using Ag/AgCl as the reference and Pt-wire as the counter electrode. The XRD and Raman spectrum confirms the amorphous nature of prepared carbon materials, having ultra-high surface area of 2321.2 m^2 g^{-1} that showed better electrochemical performance of 325.65 F g^{-1} at 1 A g^{-1} current density.

[1] J. Wang et. al., ***ACS Omega,* 7 (26),** 22689–22697 (2022).
[2] R. G. Shrestha et. al., ***Nanomaterials,* 10 (4),** 639 (2020). w

P5-32

Poster Award Nominee

Oxidation-Triggered Nanophase Separation: Numerical Simulation and Experimental Study.

Nasrat Hannah Shudin[1,2], Ryuto Eguchi[1,3], Ankit Singh[1], Ayako Hashimoto[1,3], and Hideki Abe[1,2]
[1] Research Center for Energy and Environment Materials, National Institute for Materials Science (NIMS)
[2] Graduate School of Science and Engineering, Saitama University
[3] Graduate School of Science and Engineering, University of Tsukuba

Nanophase separation of metal-oxide nanocomposites (MONs) triggered by internal oxidation were explored both through numerical simulation and experimental. Multiple pattern trends from lamellae-pattern to maze-pattern obtained from simulation were compared to *In-Situ* Transmission Electrons Microscope images (*In-situ* TEM) of phase-separated bulk Pt-CeO_2. [1, 2] In other experimental approach, Pt_5Ce precursor nanoalloy with particle sizes approximately ~10 nm supported on graphene nanoplatelets were observed to formed a heterostructure of Pt-CeO_2 with epitaxial interface upon internal oxidation of more oxyphilic species, Ce. Fast Fourier Transformation (FFT) patterns further confirmed Pt (110)//CeO_2 (110) epitaxial interface relationship.

[1] N.H. Shudin, R. Eguchi, T. Fujita, T. Tokunaga, A. Hashimoto and H. Abe, ***Phys. Chem. Chem. Phys.*, 26,** 14103-14107 (2024).
[2] Y. Wen, H. Abe, K. Mitsuishi and A. Hashimoto, ***Nanoscale,* 13,** 18987-18995 (2021).

Corporate Sponsors

株式会社菱光社　78th　(since 1947)

培った専門知識と、幅広い要素技術をソリューション営業に役立てませんか？

我が社の目指すソリューション営業・・・顧客の課題解決／目的達成／製品完成

専門知識だけでは目の前の課題は解決できても、製品を企画からプロデュースすることは難しいです。材料の分析・開発、材料を生かせる設備、検証する試験・測定、検査まで提案します。

これから求められる商社の知識は、広く浅くから、広くちょっと深くを求められています。

粉体に特化したソリューション資料

業界分野別、目的別に定期的に配信される菱光社のソリューション冊子

菱光社は幅広い業界の大手企業様とビジネス展開をしてます

半導体、パワーデバイス、電子部品、光学分野、精密加工、化学、材料、フィルム、パネル、電池、自動車、セラミック、磁性体、LD/LED、他

神奈川大学「海とみなと研究所（海中ソーラーパネル実験場）

令和2年に神奈川大学が中心となってサポインに採択をされました。
「高発電効率と汚れ防止機能を有する海中設置型 高機能ソーラパネルの研究開発」のテーマにおきまして
菱光社はアドバイザーとして任命を頂き貢献しました。

営業拠点

国内拠点

海外拠点

RYOKOSHA

AILIN VACUUM

Recommendation

オイルフリーポンプのベストセレクト

Kashiyama Vacuum Solutions

★ 非接触型ルーツポンプ★

NeoDry-Gシリーズ

600ℓ/min, 500ℓ/min, 250ℓ/min, 100ℓ/min

高性能、ﾒﾝﾃ周期：6年など従来の特徴を継承しつつ、更なる低騒音/低振動を実現！

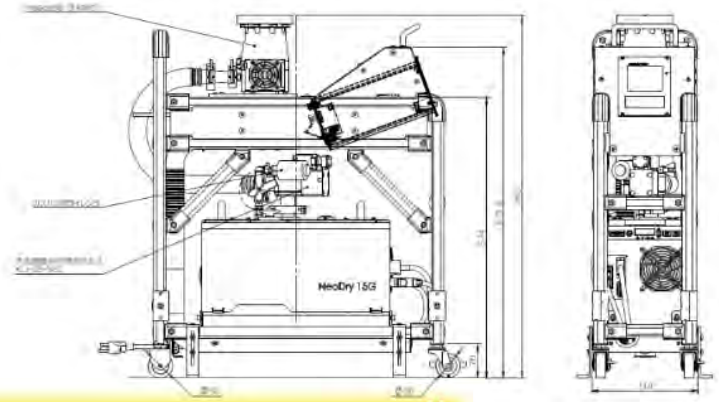
ｵﾌﾟｼｮﾝ装備を充実させ付加価値を高め、LED表示とﾓﾉﾄｰﾝのｽﾀｲﾘｯｼｭﾃﾞｻﾞｲﾝで装いも新たに!!

小型ターボ排気システム/ Neo TURBO Mini

AILIN VACUUM **Invention** **AV-EX80NEO**

NeoDry-Gｼﾘｰｽﾞより、15G型を基調とした真空排気ｼｽﾃﾑを考案！

コンパクト且つスリムな設計を重視しつつ、ターボポンプは70L/sクラスに加え、 300L/sクラスの搭載も可能。高速でクリーンな真空排気を行うことが可能な小型排気システム。NeoDryからターボポンプ、オプションの真空計まで一括制御可能なコントローラを採用。また停電など突然の有事より高真空側を保護/真空保持出来る様、大気開放弁付き緊急遮断電磁式バルブを装備し、安全面にも配慮。ターボポンプはハイブリット構造(上部：磁気軸受け式/下部：セラミックベアリング受け)で、約４年の長寿命サイクルの機体を採用し、メンテナンス性も追求。配管や真空計の増設など拡張性も有し、使用環境や用途に応じたフレキシブルな真空排気を提案致します!!



Neo TURBO Mini
AV-EX80NEO

- 吸気口： ICF114
- ターボ分子ポンプ排気速度： 67L/s（N2）
- 粗排気ポンプ排気速度： 250L/min
- 外形寸法： 210(W)x520(D)x730(H)
- 電源電圧： AC100V

お気軽にお問い合わせ下さい!!

株式会社アイリン真空

名古屋本社: TEL: 052-401-2061 FAX: 052-401-6960 E-mail: info@ailin-va.com
関東営業所: TEL: 048-769-7011 FAX: 048-769-7483 E-mail: hnakamura@ailin-va.com

Time-Resolved Scanning Tunneling Microscopy System

New

Developed in collaboration with Prof. Shigekawa group (Univ. of Tsukuba)

Financially supported by JST

Time-Resolved STM System UNISOKU-WEB

Feature 1 Compact Table-Top Optical System

- Temporal resolution ~ 80 ps
- Significantly improved operability
- Stable laser irradiation on the sample surface
- Possible integration into an existing STM system

※the optical system can be purchased separately

Feature 2 Nano-Scale Carrier Dynamics Measurements

- Spatial resolution ~ 1 nm
- Long-term time resolved measurements (~ 1 day)

New On-Site SPM Experimental Service

Service Description

We offer high-end low-temperature SPM systems that customers can use as a paid service. The measurement environments are available for on-site visits or online connections.

Available Systems

40 mK UHV STM

Now accepting

USM1600 publication list

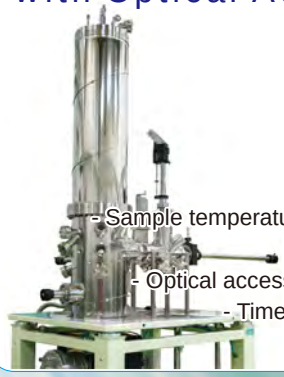
USM1300 publication list

Specifications

- 1.7-1.7-7 T vector magnet
- RF-STM
- Long-term dI/dV measurement

1.5 K UHV SPM with Optical Access

Now accepting



USM1200 series publication list

Specifications

- Sample temperature ≦ 1.5 K (when optical shutters closed)
- Compatible with AFM measurement
- Optical access capabilities by inertial-driven lens stages
- Time-resolved STM with high spatial resolution
- Shot noise measurement

Feel free to contact us about the details! **Contact: info@unisoku.co.jp**

UNISOKU Co., Ltd.

UNISOKU TII Group

E-mail: info@unisoku.co.jp Web site: https://www.unisoku.com/

2-4-3 Kasugano, Hirakata, Osaka 573-0131 Japan TEL +81-72(858)6456

SHIMADZU
Excellence in Science

ナノ領域を切り拓く島津表面構造解析装置

高分解能 走査型プローブ顕微鏡

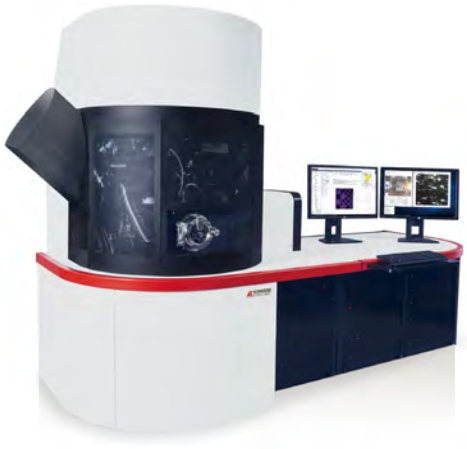
SPM-8100FM

HR-SPM 活きたナノ世界を観る

HR-SPMは周波数検出方式を採用した新世代の走査型プローブ顕微鏡です。従来のSPM（走査型プローブ顕微鏡）/AFM（原子間力顕微鏡）は、一般的にAM（振幅変調）方式ですが、FM（周波数変調）方式は、原理的に高感度測定法であり、より高い分解能での撮像が可能となります。大気中・液中における超高分解能観察だけでなく、固液界面の水和・溶媒和の測定が初めて可能となりました。

イメージングX線光電子分析装置

KRATOS ULTRA2



試料搬送から測定までを自動化した複合型表面分析装置 空間分解能はサブミクロンへ

装置構成の自由度の高さはそのままに、性能をアップしながら操作部分のすべてをコンピュータコントロール化した複合表面分析装置です。球面鏡アナライザーによる高速リアルタイムXPSイメージングの空間分解能は1 μmに達し、微細領域の化学状態分布を鮮明に視覚化することが可能です。豊富なオプション類により、in-situでの大気非暴露実験や高エネルギー XPS測定などの多彩な用途にお使いいただけます。

島津製作所　表面組成分析装置の情報はこちら

https://www.an.shimadzu.co.jp/surface/pindex.htm

トヤマの分析技術（モーメンタム分光器）

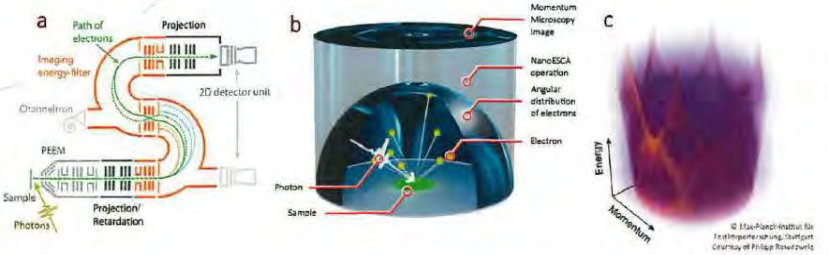
NanoESCA III　Next generation photoemission microscopy

Microscopy with Momentum and Imaging Spin-Filter (Au/Ir)

Matthias Escher[1], Nils B. Weber[1], Timna-Joshua Kühn[1], Marten Patt[1], Michael Merkel[1]

[1]FOCUS GmbH, 65510 Huenstetten, Germany - Corresponding author: m.patt@focus-gmbh.com

Momentum Microscopy

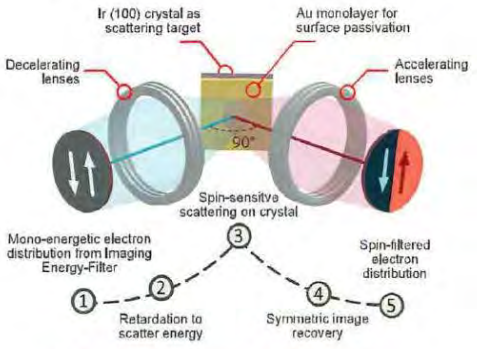


Momentum Microscopy is a new technique in surface science, in which the **momentum** (or the **real-space**) distribution of photoelectrons is projected onto an image plane (b) by using a **photoemission electron microscope** (PEEM) column. In case of momentum imaging the kx-ky plane can be energy-filtered by a double-hemispherical electrostatic analyzer (IDEA[1]) (a) to achieve a monochromatic momentum distribution. The ability of the method to map the complete angular distribution of photoelectrons is successfully used for **photoemission orbital tomography** (e.g. at the **NanoESCA in Trieste** [1]). Scanning the filter-energy of the NanoESCA allows to map the band structure of novel materials (c).

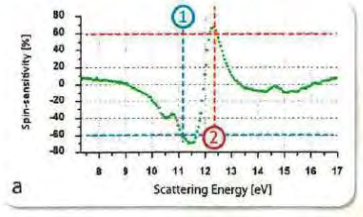
[1] M. Wießner et al., Nature Comm. 5 4156 (2014)

Spin-Filter working principal

The **monochromatic image** delivered by the **Imaging Energy-Filter**[2] of the **NanoESCA** is projected onto a **Au/Ir crystal**. For specific kinetic electron energies, **one spin polarization** is strongly preferred in the scattering process due to spin-orbit coupling. The reflected image is **spin-filtered**. The **Au passivated surface** of the Ir crystal keeps the scattering conditions **stable for weeks**.



The asymmetry of IV-curves of the Au/Ir (100) crystal and optimal scattering energies



Images at both scattering energies (FoV 66 µm)

Pre-characterizations of the **Au/Ir crystal** were done with **LEED** and a **Ferrum-Detector setup** [1] to find optimal **preparation conditions** and **scattering energies** for a high **single-point figure-of-merit** (with **Spin-sensitivity >60%** and **Reflectivity >1%**) [2]. The I-V-curve in (a) was measured with the Ferrum setup and shows, at which scattering energy the highest spin-sensitivity can be reached. Images (b,c) are then acquired at these **two energetically sharp working points** with the **NanoESCA** and are used to calculate the spin-polarization of the complete field-of-view.

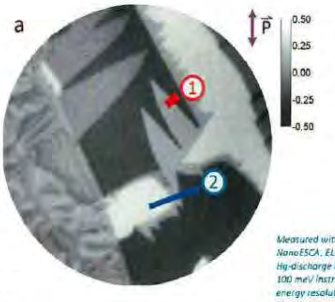
[1] Escher, et al., e-J. Surf. Sci. Nanotech. Vol. 9, 340-343 (2011)
[2] C.Tusche et al., Ultramicroscopy 159, 520–529 (2015)

Spin-polarization imaging of magnetic domains of poly-cristalline iron

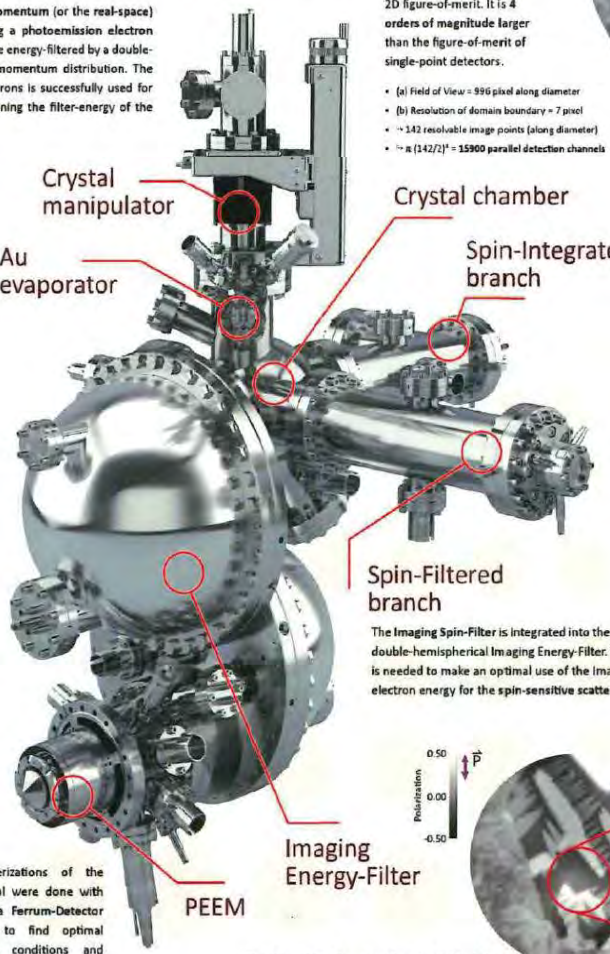
Parallel detection of spin-channels

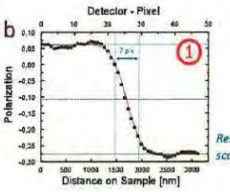
The **already high single-point figure-of-merit** (Sherman function > 60% and Reflectivity > 1%) is multiplied by the amount of **parallel detection channels** given in the imaging spin-filter to define an effective 2D figure-of-merit. It is **4 orders of magnitude larger** than the figure-of-merit of single-point detectors.

- (a) Field of View = 996 pixel along diameter
- (b) Resolution of domain boundary = 7 pixel
- → 142 resolvable image points (along diameter)
- → π (142/2)² = **15900 parallel detection channels**

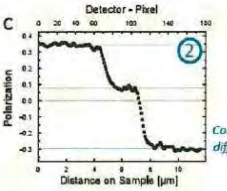


Measured with: NanoESCA, ELI-ALPS, Hg-discharge lamp, 100 meV instrumental energy resolution, Room temperature, 200 s exposure time, 66 µm lateral FoV



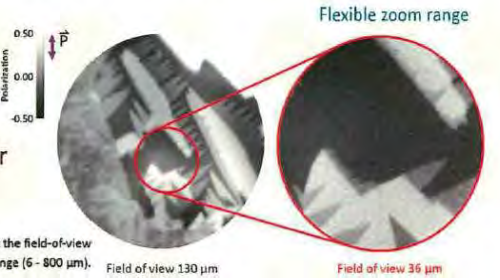


Resolution of scattered image



Contrast between different domains

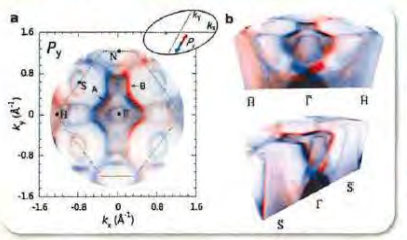
The **Imaging Spin-Filter** is integrated into the standard **NanoESCA III** analyzer, directly behind the **double-hemispherical Imaging Energy-Filter**. The **monochromatic image** behind the Energy-filter is needed to make an optimal use of the Imaging Spin-Filter, which needs a very defined kinetic electron energy for the **spin-sensitive scattering process**.



The NanoESCA allows to adjust the field-of-view over a wide range (6 - 800 µm).

Spin-Filtered band structure mapping

Adapted from: Ying-Jiun Chen, Christian Tusche et al., Comm. Phys. (2021) 4:179 (CC-by 4.0 License)



The **Imaging Spin-Filter** works in the momentum microscopy mode in the same way as in the real-space microscopy mode. The graphic shows the **spin-resolved Fermi surface of W(110)** (a) as well as full 3D spin-resolved momentum maps (momentum vs. binding energy) (b). Note, that a W (100) crystal was used as scattering target in this experiment.

Measured with: NanoESCA, Elettra (Trieste, Italy), Synchrotron radiation, hν = 50 eV, p-polarized, T = 130 K

TOYAMA
Pioneering New Horizons in Science

本　　社：〒258-0112　神奈川県足柄上郡山北町岸3816-1
TEL 0465-79-1411　E-mail salesdept@toyama-jp.com
関西営業所：〒670-0935　兵庫県姫路市北条口1-35 藤和シティコア姫路駅前101号
TEL 079-226-8373
東北営業所：〒984-0051　宮城県仙台市若林区新寺3-5-31 パークフロント1F
TEL 022-297-6880

Dry Pump Unit

DRYFORCE SLIM

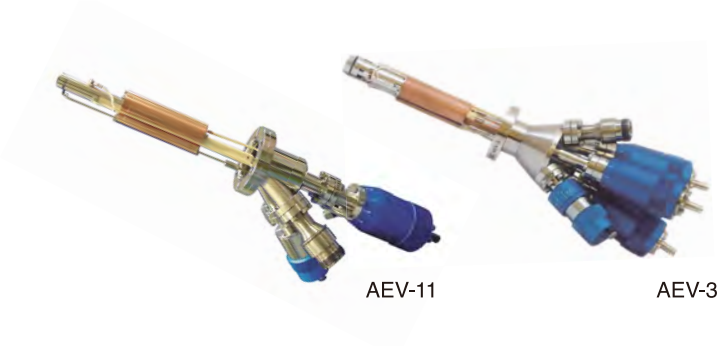
Dry & Turbo Pumping System

AUTO DRIVE MODE

MANUAL DRIVE MODE

- Clean vacuum pumping system with turbo molecular pump and dry roots pump
- Single-touch start/stop operation
- Compact and space-saving; W300 x D600 mm

UHV Evaporator



AEV-11 AEV-3

Mouting flange:	ICF70-FH
In-vacuum length:	195 mm (AEV-11)
	190 mm (AEV-3)
Equipped with:	Manual shutter
	Water-cooling shroud
	Flux monitor

Dedicated controller is available.
Filament current: 0-5 A
HV output: 0-1000 V at 300 mA

AEV-1P-300

UHV 3kV Ion Gun

ACIG-3

Mounting flange:	ICF70-FH
Ion source:	Electron impact
Acceleration voltage:	Max. 3 kV
Emission current:	0-30 mA
Ion current:	3 μA (at Acc. 3 kV)
Beam spot size:	ϕ1 mm (at Acc. 3 kV)
XY deflection:	+/-20 mm

Dedicated power supplies are available.

Power Supply
ACIG-3P-2

Scanning Controller
ACIG-3P-S

R-DEC Co., Ltd.

1-16-10 Ninomiya, Tsukuba, Ibaraki 305-0051 Japan
Phone : +81-29-858-0211 Fax : +81-29-855-9877
mail: info@rdec.co.jp https://www.rdec.co.jp/

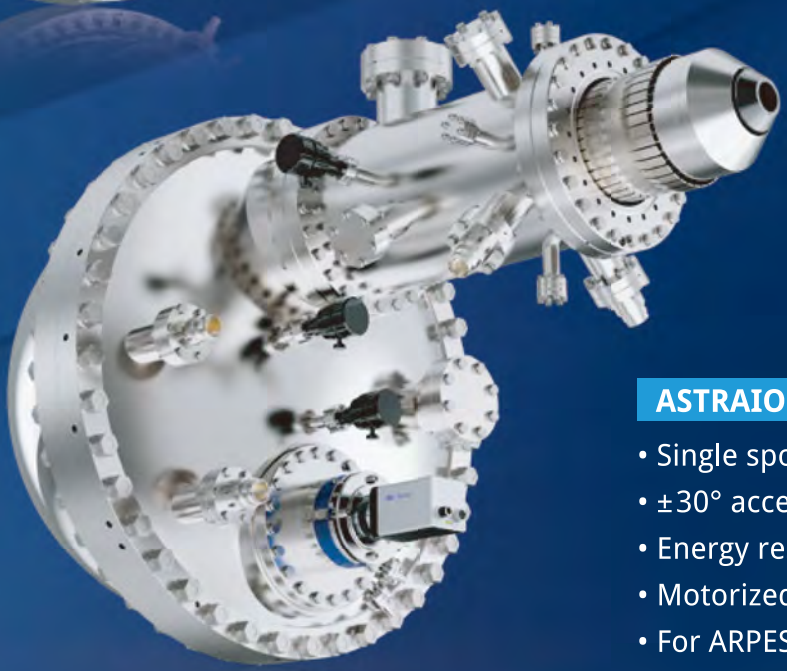
KREIOS 150 & ASTRAIOS 190

HIGH PERFORMANCE MOMENTUM MICROSCOPY
AND HIGH RESOLUTION 2D MAPPING ARPES

SPECS™

KREIOS 150

- Ultimate Acceptance Angle ±90°
- μARPES (<2 μm field of view)
- Extractor zoom lens design
- Kinetic energy range 0–1500 eV
- Energy resolution <5 meV
- k-resolution <0.01 $Å^{-1}$



ASTRAIOS 190

- Single spot parallel shifting lens
- ±30° acceptance angle
- Energy resolution <1.5 meV
- Motorized entrance slit
- For ARPES and Spin-ARPES

東京インスツルメンツ
TOKYO INSTRUMENTS
グローバルにネットワークを広げ、最先端の科学をお客様に提供

本　社：〒134-0088 東京都江戸川区西葛西6-18-14 T.I.ビル　Tel. 03-3686-4711
営業所：〒532-0003 大阪府大阪市淀川区宮原4-1-46 新大阪北ビル　Tel. 06-6393-7411
URL：https://www.tokyoinst.co.jp　Mail：sales@tokyoinst.co.jp

TII Group Company

UNISOKU TII Group　超高真空・極低温走査型プローブ顕微鏡 高速分光測定装置、クライオスタット

LOTIS TII　Nd:YAGレーザー、Ti:Sレーザー OPOレーザー

総合カタログ2024-2026をお求めのかたはコチラ！

＊価格帯は、WEBカタログには付属しません。
配送分のみの取扱いになります。

TOKYO 23 FOOTBALL CLUB　東京インスツルメンツは、東京23FCを応援しています。

世界の科学技術を支えて75年

日本電子は戦後間もない1949年5月に、創業者の風戸健二が科学技術による国の復興を願い、
電子顕微鏡の開発会社として発足し、おかげさまで創立75周年を迎えることができました。
これも長きにわたる皆様の温かいご支援とご指導の賜物と深く感謝申し上げます。
創業以来弊社は、「世界の科学技術を支える」という強い想いを持ちながら、
最先端の理科学・計測機器、産業機器そして医用機器の開発に邁進してまいりました。
そしてこれから進んでいく方向性を、「世界の科学技術を支えるニッチトップ企業へ」と明確に定め、
世界中のJEOLグループ社員とともに新しい挑戦を続けてまいります。
これからも皆様からの変わらぬご支援ご協力をどうぞよろしくお願い申し上げます。

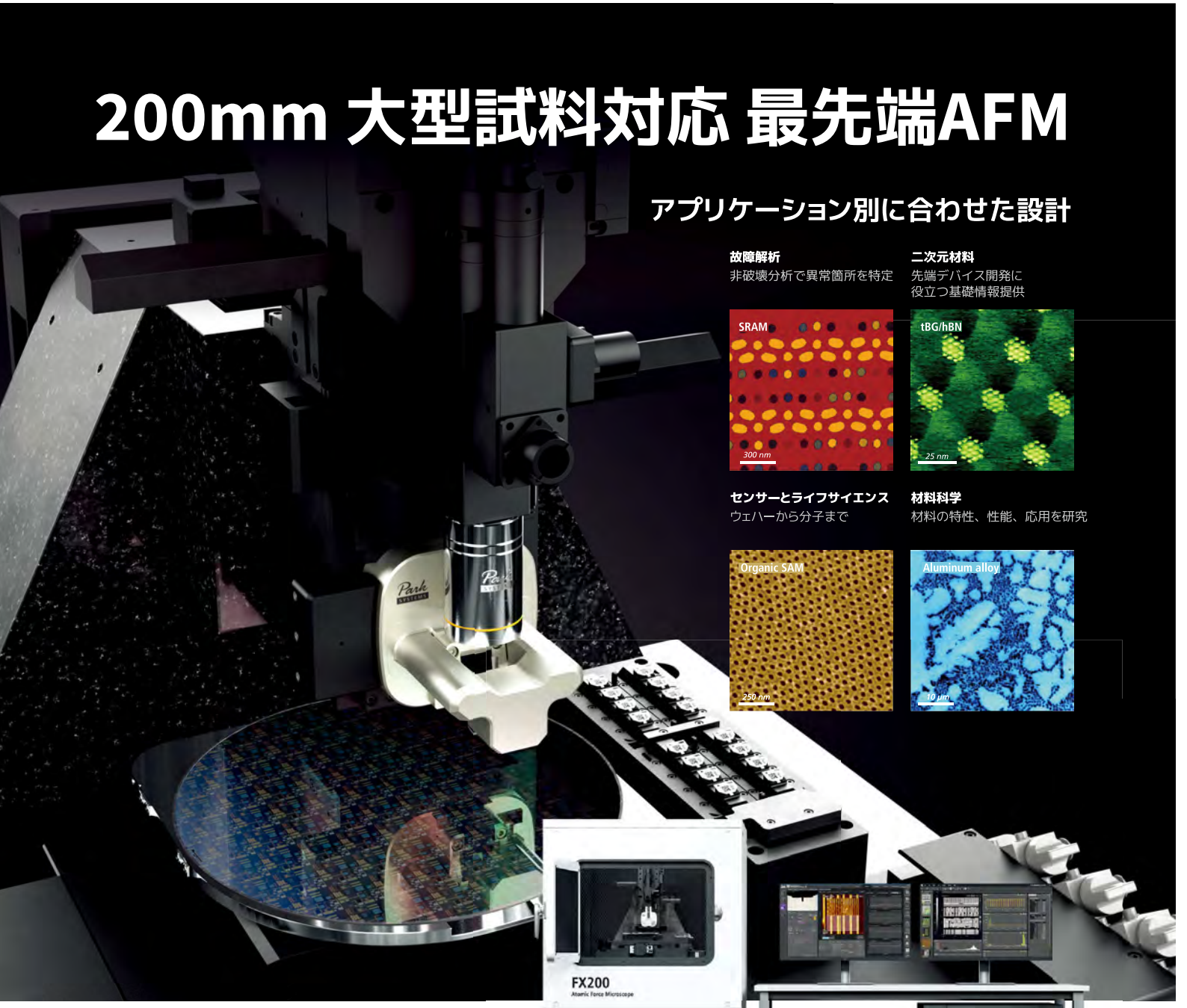
日本電子最初の製品であるDA-1型電子顕微鏡。
現存する唯一のDA-1が日本電子本社に所蔵されています。

JEOL 日本電子株式会社

本社・昭島製作所　〒196-8558　東京都昭島市武蔵野3-1-2　ISO 9001・ISO 14001 認証取得

JEOLグループは、「理科学・計測機器」「産業機器」「医用機器」の3つの事業ドメインにより事業を行っております。
「理科学・計測機器事業」電子光学機器・分析機器・計測検査機器　「産業機器事業」半導体関連機器・金属3Dプリンター・成膜関連機器/材料生成機器　「医用機器事業」医用機器

200mm 大型試料対応 最先端AFM



アプリケーション別に合わせた設計

故障解析
非破壊分析で異常箇所を特定

二次元材料
先端デバイス開発に
役立つ基礎情報提供

センサーとライフサイエンス
ウェハーから分子まで

材料科学
材料の特性、性能、応用を研究

新発売

Park FX200

Park FX200は、パーク・システムズの最新の原子間力顕微鏡技術を搭載した200mmの大型試料に対応した最先端原子間力顕微鏡です。このモデルは、ノイズフロアを劇的に低減し、熱ドリフトを最小限に抑える先進的な機械構造を備え、卓越した安定性を提供します。高速なZサーボ性能と改善されたハイパワーサンプルビューにより、作業効率とイメージング能力が向上し、自動プローブ認識、プローブ交換、レーザービームアライメント、フルサンプルビュー用のマクロ光学系などの機能により、ユーザーエクスペリエンスが簡素化され、生産性が最大限に向上します。光学式オートフォーカス、ナビゲーション、複数の座標での連続測定、自動AFMスキャンパラメーター設定、自動データ解析などと複雑な操作を簡素化させる機能を多数搭載しており、研究と産業アプリケーションの両方に理想的な選択肢です。優れた性能と使いやすさを兼ね備えたFX200は、科学者やエンジニアがナノスケールのイメージングと分析において、新たな洞察と進歩を達成できるようサポートします。

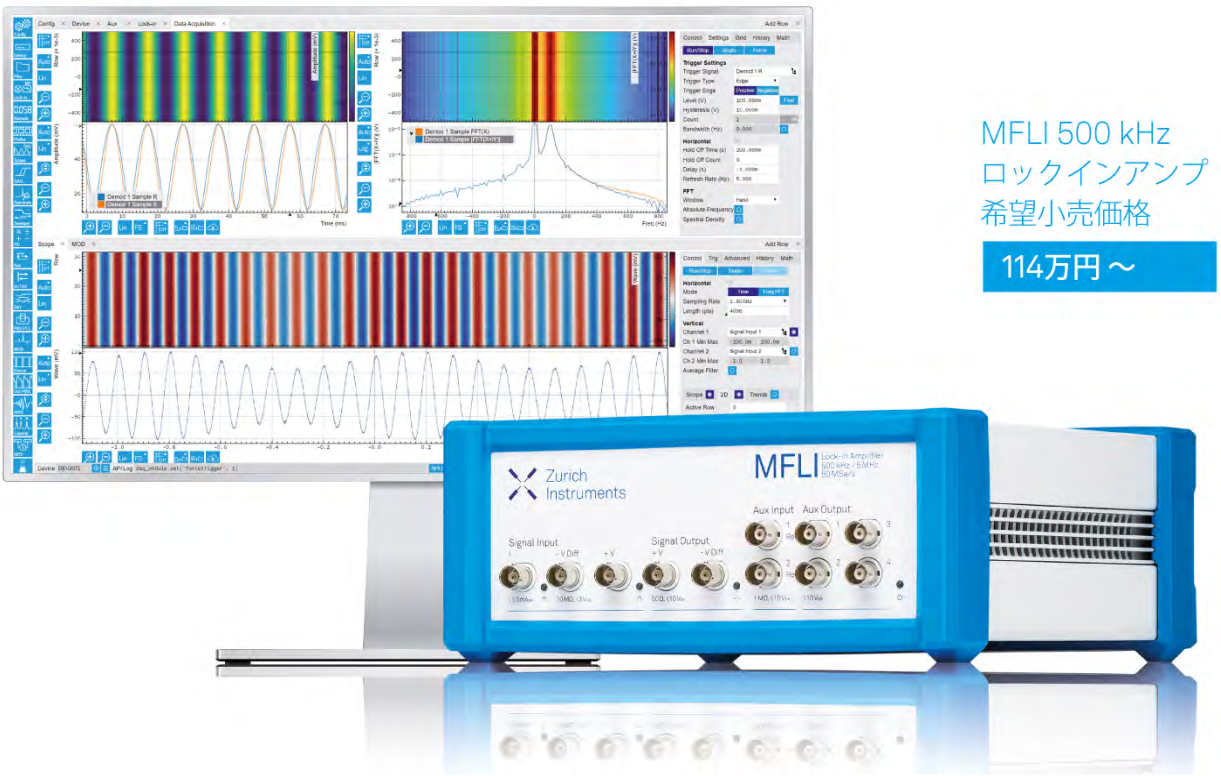
Park Systems Japan
詳しくは、ウェブサイトparksystems.com/jp/fx200または、
inquiry@parksystems.comまでお問い合わせください。

Park SYSTEMS

気になったら

難題お待ちしてます

周期波形の検出でお困りではありませんか?
より少ない時間と労力で最高の結果を得られるよう
装置、ソフトウェア、サポートを提供しています



MFLI 500 kHz
ロックインアンプ
希望小売価格

114万円 ～

Zurich
Instruments

Provide consistent support of research and development with extensive experience

Kitano Seiki's high flexible and high-quality finished vacuum equipments for research and developments. High quality products, experimental environments of good quality research and development are supported by our technical strength and know-how fostered with our extensive experience and actual performance. We pursue the goal of "We don't compete, but we create through competition." First, based on the communication with our clients, we set our rule of conduct of "We deal with it because of difficult task." This is our basic stance we definitely reflect a desire up to even the single part. It is our pleasure to have the achievements and success by customers' research and developments.

- Design
- Machine processing
- Welding processing
- Leak test
- Surface processing
- Cleaning
- Assembling
- Vacuum start up

Line of business

- Instruments and equipments for research and development
- Instruments and equipments for ultrahigh vacuum
- Thin film production equipments (MBE, CVD, EB, Spattering, etc.)
- Surface analysis equipments (FIM, STM, TEM, CMA, etc.)
- Cryogenic-cooling equipments, instruments, parts
- Multi-spindle manipulators
- Various linear and rotation introduction machines (single axle, biaxial)
- Transfer rod
- Ultrahigh vacuum chamber
- Various repairs, maintenances, retrofit, relocation operations

KITANO SEIKI CO.,LTD.
7-17-3 Chuo Ohtaku, Tokyo Zip Code143-0024 Tel: 03-3773-3956 Fax:03-3778-0379
E-mail: info@kitano-seiki.co.jp http://www.kitano-seiki.co.jp

All for Researchers.
KITANO

ThermoFisher SCIENTIFIC

Aberration-corrected STEM

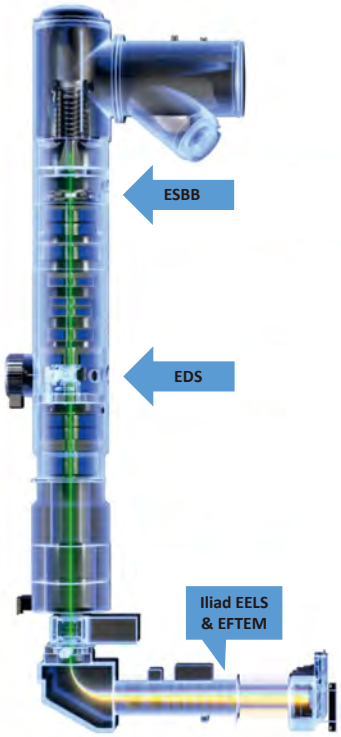
Iliad (S)TEM

完全に統合されたEELSで常識を変える

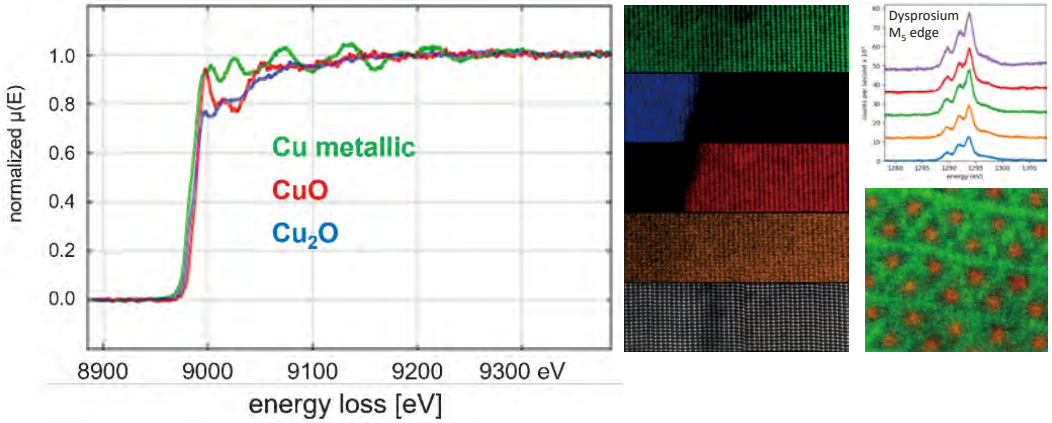
イリアドは2024年夏発表の新型収差補正STEMです。
高品質EELSデータ取得が容易になった、新しいスタンダード。

Iliad EELSの主な特長

- TEMカラムとEELSシステムが初めて完全統合
- 10個の多極レンズによる自動高次収差補正
- MultiEELSで最大５つのエネルギー範囲を同時取得
- 常にフォーカスのあったスペクトル取得により、超高エネルギーロス領域でのスペクトルも明瞭に（下図）
- 優れた自動調整により、生産性を向上
- ナノパルサー 超高速静電ビームブランカー（ESBB）による電子線照射量の制御および試料ダメージの低下
- 観察結果とEELSおよびEDS分析結果、すべての情報をVeloxソフトウェア上で一元化。新しい知見を見逃しません。



詳細はこちら: **thermofisher.com/iliad**



2024.12.16
Webinar開催！
登録はこちら

https://forms.office.com/r/YZWrYC2C1g

thermo scientific

未来の製品開発目標を実現する最適な微細構造検査ソリューション

Struersは、いかなるお客様の製品目標にも対応し微細構造検査工程の最適化に必要な専門知識と将来性のあるソリューションを提供します。

ENSURING CERTAINTY

Struers

株式会社ストルアス
141-0022　東京都品川区東五反田
3-14-13 高輪ミューズビル1F
電話番号：03-5488-6207
Email : info@struers.co.jp

NIMS Award Symposium 2024

Organizer: National Institute for Materials Science (NIMS)

Sponsor: Ministry of Education, Culture, Sports, Science and Technology (MEXT)

NIMS Award Committee

Chair: Takashi Taniguchi (NIMS)

Nobutaka Hanagata (NIMS)

Koichi Hayashi (Nagoya Institute of Technology)

Shingo Ichimura (The National Institute of Advanced Industrial Science and Technology, AIST / Waseda University)

Toshihiko Kamada (NIMS)

Koji Kimoto (NIMS)

Yasuo Koide (NIMS)

Takuya Masuda (NIMS)

Masanori Mitome (NIMS)

Tadakatsu Ohkubo (NIMS)

Takahito Ohmura (NIMS)

Yuji Otsuka (Toray Research Center, Inc.)

Kaoru Sato (JFE Techno-Research Corporation)

Hidemi Shigekawa (University of Tsukuba)

NIMS Award Symposium 2024 Action Committee (NIMS)

Chair: Koji Kimoto

Ayako Hashimoto

Shigeki Kawai

Shinji Kohara

Masanori Mitome

Kazutaka Mitsuishi

Chihiro Uchibori

Koichiro Yaji




November 6th (Wed) - 7th(Thu), 2024
TSUKUBA International Congress Center

State-of-the-art Characterization to Accelarate Materials Innovation

マテリアル革新力強化をもたらす最先端計測