

National Institute of Advanced Industrial Science and Technology (AIST) Department of Materials and Chemistry

# AIST-UTokyo Advanced Operando-Measurement Technology Open Innovation Laboratory





# Greeting

Human beings have started to gather knowledge on nature by observation, that is, by accurate inspection.

Nanotechnology has developed similarly: it began with nano-observation. In other words, you cannot make a thing you cannot see.

Buddhism has eight basic practices that constitute the Noble Eightfold Path: Right View, Right Resolve, Right Speech, Right Action, Right Livelihood, Right Effort, Right Mindfulness, and Right Concentration. This pro-

cess holds true in scientific procedures in basic science, as well, including processes in basic science employed in applied research and those leading to product development for the welfare and happiness of human beings in the end.

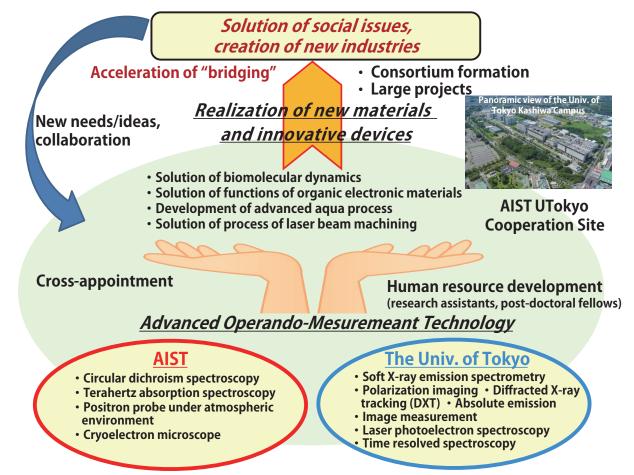
This is exactly the aim of "AIST-UTokyo Advanced Operando-Measurement Technology Open Innovation Laboratory (OPERANDO-OIL)." We utilize **techniques to measure materials/devices in actual working conditions (operando measurement)** to deepen our understanding of basic science, and simultaneously make efforts to proceed to product development.

We expect interested researchers and companies to actively participate in OPERANDO-OIL.

Yoshiyuki AMEMIYA Director, Laboratory

# Aim of OPERANDO-OIL

OPERANDO-OIL combines fundamental technologies for advanced measurement and materials with new physical properties developed by the University of Tokyo (UTokyo) and research potentials for precise measurement and material/device technology put forth by the National Institute of Advanced Industrial Science and Technology (AIST), to establish the Advanced Operando-Measurement Technology and develop it further for application to a broad range of innovative materials, devices, and manufacturing technologies, and to act as a "bridge" between companies.





# Organization



Director, Laboratory:

Prof. Y. AMEMIYA (Project Prof. UTokyo)



PhD T. SASAKI



PhD J. ISHII



Principal Researc Manager: PhD S. HARA

Laboratory Team			
	Tough Composite Ma PhD Y. HAKUTA* (AIST)	aterials Process Team (p.4) Prof. K. TERASHIMA <sup>+</sup> (UTokyo)	
	Organic Device and PhD M. MUKAIDA (AIST)	d Spectroscopy Team (p.5) Prof. H. OKAMOTO*,† (UTokyo)	
	Advanced Coherent PhD R. KURODA* (AIST)	Photon Process Team (p.6) Prof. Y. KOBAYASHI (UTokyo)	
EC/Eoscibility Stud	PhD K. MIO* (AIST) * : Laboratory	Dynamics Team (p.7) Prof. Y. SASAKI † (UTokyo) Team Leader † : AIST cro	oss-appointment fellow
FS(Feasibility Study) themes* Innovative operando microscopic technique realizing the evaluation of			
next-generation nanodevices under operation           PhD. H. AKINAGA (AIST), Prof. S. SHIN (UTokyo)         (p.8)			
Operando measurement-based exploration of health functions of underused materials originating from bioresources PhD. K. TOMINAGA (AIST), Prof. Y. OHYA (UTokyo) (p.9)			
Evaluation of structural vacancy in an icosahedral cluster solid by positron probe and creation of semiconducting quasicrystals and high-performance thermoelectric materials PhD N. OSHIMA (AIST), Prof. K. KIMURA (UTokyo)(p.10)			
Research on the sophistication of secondary batteries by ultrahigh resolution soft X-ray spectroscopic analysis PhD H. MATSUDA (AIST), Prof. Y. HARADA (UTokyo) (p.11)			
			(4.1.1)

\* : Themes conducted in FY2017

# Tough Composite Materials Process Team

Leaders: Y. HAKUTA (AIST), K. TERASHIMA (UTokyo)

# Purpose

Our team aims at creating tough composite materials that have both high functional property and mechanical strength. We have focused on inorganic particles with high functional property and slide-ring polymers exhibiting flexible and tough mechanical properties. In order to create a composite material of both materials in which inorganic particles serve as cross-linking junction points, we will develop an innovative process (advanced aqua process) for promoting a reaction to create a composite by introducing a solvent, notably water, to be used in the reaction fields of synthesis to a supercritical or plasma state. Furthermore, we will understand the properties of composite materials in an actual environment and the generation efficiencies and reaction mechanisms of reaction species in reaction fields by using operando measurement techniques and we will aim for the speedy development of the advanced aqua process and the realization of tough composite materials.

# Our research

1) Development of an advanced aqua process and tough Inorganic nanoparticle composites

We will develop an advanced aqua process, which integrates solution processes, including the production of tough composites, along with a supercritical fluid process and a plasma process 1) to improve the compatibility between polymers and inorganic particles or between these particles and solvents, which is key to synthesizing tough composite materials, and 2) to realize particle surface modification/functionalization, which is effective for preventing aggregation of the same type of particles, and thus inhibits homogeneous mixing. We will also synthesize polyrotaxane, which is a necklace-like supermolecule suitable for the realization of tough composite materials, and on the basis of a strategy of materials design, we will obtain a composite of polyrotaxane with inorganic particles, and perform structure analysis, mechanical characterization including fracture behavior, and evaluation of physical properties such as thermal conduction property and electric conduction property.

2) Development of techniques for process and material evaluation via operando measurement

For the production of tough composites, it is important to understand the reaction chemical species and reaction mechanisms in a reaction field, the dispersion state of inorganic particles in a composite, and their interfacial state with the polymer. We will measure the hydration structure of the aqua process and various chemical species using soft X-ray spectroscopy and ultraviolet-visible spectroscopy, utilize an operando measurement technique that analyzes the void structure of the composite material via positron measurement, understand the process reaction field and the basic principle of expression of materials function, and feed the understanding back to polymer design, aqua process, and kneading process development to accelerate the synthesis of the composite material.



rganic nanoparticle Slide-ring polymer

Figure 1 Conceptual diagram of tough composite materials

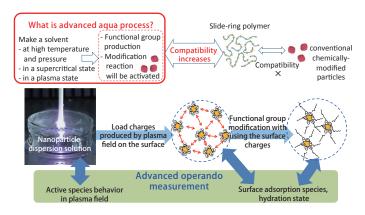


Figure 2 Surface modification of nanoparticles by plasma (advanced aqua process)

The results obtained will not only be presented at academic conferences and exhibitions but also be disseminated promptly in periodic workshops. We call for the early participation of not only material manufacturers but also large manufacturers in the fields of electronics and automobiles to combine our results with industrialization through joint research and technology transfer.

# Organic Device and Spectroscopy Team

Leaders: M. MUKAIDA (AIST), T. ISHIDA (AIST), H. OKAMOTO (UTokyo), J. TAKEYA (UTokyo)

# Purpose

For the development of all-in-one wearable devices, the improvement of performance of the main electronic materials—organic semiconductors for field-effect transistors (FETs), thermoelectric conversion materials for power generation, and organic ferroelectrics for memory—is an essential issue.

By applying advanced spectroscopy including femtosecond laser spectroscopy, terahertz spectroscopy, Raman microspectroscopy, and synchrotron radiation X-ray spectroscopy, to these materials and devices, we will clarify the factors limiting the performance from the standpoint of electron theory and reveal necessary conditions for the performance improvement. On the basis of this result, we will attempt to enhance the performance of these materials and devices and eventually develop all-in-one wearable devices.

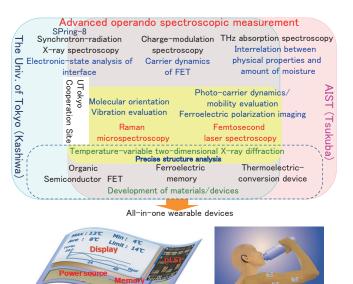


Figure 1 Research system

Femtosecond pump

Photon energy (meV) 10 20 30

# Our research

## 1) Development of materials and devices

- On the basis of the synthesis techniques of organic semiconductors for FETs, thermoelectric conversion materials for power generation, and organic ferroelectrics for memory and the techniques for converting them into devices, high-performance materials/devices will be developed.

### 2) Advanced operando measurement

- Mobility and scattering probability of carriers will be evaluated by applying charge-modulation spectroscopy to organic semiconductor FETs to analyze the optical spectrum and the limiting factors of conduction mechanism, and the mobility will also be clarified.
- Carrier mobility will be evaluated by applying wide-band femtosecond transient spectroscopy to organic semiconductors and thermoelectric conversion materials, and the con-

 $t_{\rm d} = 4 \, {\rm ps}$ (S/cm) 0.02 Re 0.0 0.05 High-mobility organic semiconductor (left) and circuit technology (right) Frequency (THz) PEDOT:PSS Measurement of carrier dynamics of organic semiconductor by femtosecond transient spectroscopy Mid-infrared ed light Photon energy (eV) 2 0.4 0.6 0 High-efficiency thermoelectric material (left) and thermoelectric-conversion module (right) 100 20 Frequency (THz) Detection of carriers in FET by Polarization domain imaging of a ferroelectric charge-modulation spectroscopy

Figure 2 Representative material/device manufacturing techniques and operando measurement techniques employed by the Organic Device and Spectroscopy Team

duction mechanism will also be clarified. Moreover, in conjunction with the result of Raman spectroscopy, the origin of lattice vibration and defects affecting carrier mobility will also be clarified.

- The performance of ferroelectric crystals, thin films, and devices will be evaluated by applying terahertz radiation spectroscopy, which uses a femtosecond laser, to measure the spatial distribution of polarization and dynamics.
- Space-resolved electronic state analysis of organic materials and devices will be performed using synchrotron radiation X-ray spectroscopy.

On the basis of the aforementioned results, we will clarify the requirements for the improvement of performance of materials and the problems arising in devices, and we will remarkably improve their performance by feeding them back to the development stage of the materials and devices.

# **Efforts toward industrialization**

We will improve the performance of integrated circuits with an organic semiconductor transistor, organic thermoelectric modules, and organic ferroelectric memory, which are the main elements, and we will transfer the possibilities of practical use thus arising to companies.

# Advanced Coherent Photon Process Team

Leaders: R. KURODA (AIST), Y. KOBAYASHI (UTokyo), H. AKIYAMA (UTokyo)

# Purpose

Our team has been developing processing techniques using light and operando measurement technologies to apply them to practical use as microfabrication techniques and quality assessment techniques. For light processing techniques, we will develop advanced laser microfabrication techniques using deep UV laser and femtosecond laser to perform nonthermal processing and microfabrication of various materials, and we will promote medical and biotechnological applications. Furthermore, we will clarify the deterioration mechanisms of laser processing and solar cells in the course of development of advanced laser technologies and advanced operando measurement technologies and we will perform the optimization of processing conditions etc. Moreover, we will demonstrate the usefulness of a technique for absolute light intensity measurement of photoluminescence (PL) as a quality assessment technique, and we will transfer it to the society as a technique supporting the development and efficiency improvement of solar cells, bio- and chemiluminescence probes, and other light-energy conversion materials.

# Our research

For the development of a laser processing technique, we have equipped our laboratory with a deep UV pulse laser processing machine (wavelength: 266 nm, power: 0.2 W, pulse width: nanosecond) and a femtosecond laser processing machine (fundamental wavelength: 800 nm; frequency-doubled 400 nm is available; power at the repetition frequency of 10 kHz: 4 W), and we will perform nonthermal processing and microfabrication of materials including hard-to-process indwelling materials such as stents, biocompatible materials such as zirconia, heat-sensitive biodegradable polymers, and materials for solar cells (Figure 1).

As the techniques of advanced operando measurement during laser processing and device operation, we will also promote the development of techniques for ultra-fast time-resolved measurement of scattering and reflection measurements during processing, absolute light intensity measurement of PL (Figure 2), and photoelectron spectroscopy. For example, laser-processed sites of solar cells will be assessed using the absolute light intensity measurement of PL. Furthermore, based on the experimental analysis of processed materials using a laser microscope and theoretical analysis using a theoretical calculation technique, we will elucidate the physical mechanisms of laser processing and solar cell deterioration and optimize the processing conditions.

The usefulness of the absolute light intensity measurement of PL as a quality quantitative evaluation method for solar cells and bio-and chemiluminescence probes will be demonstrated. In the field of bio- and chemiluminescence probes, we aim toward developing the absolute light intensity measurement of PL as a method to obtain absolute values of calibration curves of the amount of luminescence and luminous efficiency of a fluorescent reagent itself and as a method to evaluate the sensitivity and detection limits of luminescence analyzers with absolute values.

# Efforts toward industrialization

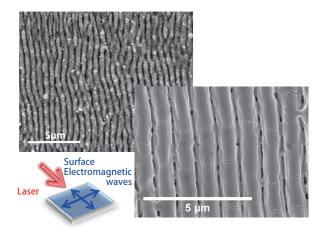


Figure 1 Example of microfabrication of ceramics using femtosecond laser

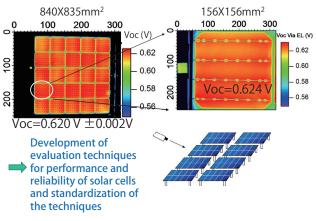


Figure 2 Operando image measurement of single-crystal silicon solar cell panel

We aim at establishing laser microfabrication techniques for indwelling materials, biocompatible ceramic materials, and biodegradable polymers, which are highly required in industries. We also aim at commercializing operando measurement techniques, including a technique for the absolute light intensity measurement of PL, as measurement instruments and providing them to the society for utilization in the industrial work place. We will construct a laser processing platform and database in the medical and biotechnological fields, form a laser processing consortium in cooperation with a manufacturing-oriented NEDO project "Technology Association of Cool laser Machining with Intelligence (TACMi)", promote open innovation of our techniques, and conduct the search and survey of materials necessary to efficiently satisfy the requirements of companies. Through creation and dissemination of our techniques and provision of our findings, we hope to contribute to the industrialization of laser processing techniques, laser-processed products, and high-efficiency solar cells and bio- and chemiluminescence probes and eventually lead to the reduction of CO<sub>2</sub> emissions, dissemination of clean energy sources, and sophistication of medical services.

# **Biomolecular Dynamics Team**

Leaders: K. MIO (AIST), Y. SASAKI (UTokyo)

# Purpose

To usher a revolution in health and food sciences, we will reveal the unknown functions of macromolecules and biomimetic materials by using advanced measurement techniques for single molecule dynamics (combination of diffracted X-ray tracking (DXT) and electron microscopy).

# **Our research**

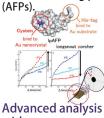
By combining the single-molecule analysis technique of UTokyo and the membrane protein analysis technique of AIST, we are developing next-generation sensors based on mechanisms of biomolecules for, e.g., taste, smell, and temperature sensing. We also aim at developing technologies for extending expiration dates of food stock, preservation of organs for transplant, and solving issues such as food allergies.

- Using advanced single-molecule analysis techniques including DXT and cryo-electron microscopy (cryo-EM), we analyze the internal motion of target molecules at high speeds with a high precision. We will also search for useful molecules that can be applicable for high-performance sensors.
- In order to resolve worldwide concerns regarding health, food, and energy, we aim at technological innovations by focusing on nanoscale molecular motion.
- We will elucidate the potential of anti-freezing proteins (AFPs), which inhibit the formation of ice crystals and protect hibernant animals and Antarctic fish from freezing. We analyze the molecu-

lar dynamics of AFPs and attempt to use these as food and tissue/organ preservatives with novel mechanisms.

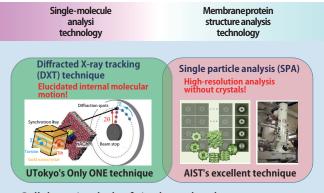
- With combination of the DXT method and the positron probe method, we will elucidate the interaction mechanisms between nanobubbles and proteins. We will also attempt to clarify the supersaturation phenomenon, in which clusterization holds the key, and also attempt its development into a solution for energy issues. <u>1. Sophistication of</u> analysis

For applications in drug discovery and industries, we elucidate the sophisticated molecular motion of TRP channels and anti-freezing proteins



with a new camera

# First-ever visualization of tRP channels capsacion receptor) Output of the provided of the provided



Collaboration hub of single-molecule measurement

Figure 1 World's first innovative analysis of single biomolecule dynamics realized by AIST-UTokyo

### 2. Dissemination of diffracted X-ray tracking (DXT) method

We develop a novel DXT method for "multipurpose screening" in collaboration with device manufacturers. This uses a laboratory X-ray source instead of synchrotron X-ray. e develop a novel DXT



Efforts for technology dissemination

Figure 2 Aspects of this research

# 3. Motion analysis in living cells and individuals

For realizing "advanced OPEANDO-measurement," we develop technologies not only for protein molecules but also for living cells and Caenorhabditis elegans.



From molecules to live cells and to individual level

# Efforts toward industrialization

We aim at (i) sample analysis, molecular search, and novel material development based on molecular dynamics and (ii) development of novel multipurpose screening devices.

# Innovative operando microscopic technique realizing the evaluation of next-generation nanodevices under operation

Leaders: H. AKINAGA (AIST), S. SHIN (UTokyo)

# Purpose

It is believed in the semiconductor device area that micro-/nanofabrication techniques have recently approached their limits and that it is difficult to continue following Moore' s law. Accordingly, research and development of next-generation nonvolatile memory, based on new principles and structures that are not the extension of, but are completely different from, conventional techniques, are proposed and promoted energetically. Above all, resistive random access memory (ReRAM), magnetic random access memory (MRAM), and phase change memory (PCM) have been receiving attention as promising candidates. However, these devices show increased variation in the recording state as they become finer and the decrease in reliability becomes more critical. This is a bottleneck in the application of high-density memory. In order to solve these problems and accelerate research and development, a "nanoscale operando measurement technique" that visualizes the recording state of fine memory elements under operation one-by-one in real time is indispensable. In order to be the first to realize this technique in the world, this study will develop the laser photoelectron microscopy (laser PEEM) technique, which features high resolution, deep detection depth, and visualization of the recording state. By applying it to the actual operation of ReRAM devices, we also aim to realize a microscopic method of nondestructive observation of nanostructures of a device under operation (operando) in real time.

# Our research

Our group has proposed the laser PEEM, a new microscopic technique combining the advantages of the "light" and "electron" microscopic methods, and achieved the world's highest spatial resolution of 2.6 nm by introducing a continuous-wave ultraviolet laser light source and electron optics for aberration correction (Figure 1). Considering the characteristics of the photoelectrons emitted, the laser PEEM is considered to have the capability to detect a nanostructure embedded at a depth of 10 to 100 nm and therefore paves the way for the realization of nondestructive observation under operation, i.e., operando observation. This study will perform the demonstration experiments and arrempt the first-ever observation of memory under operation. Furthermore, after the development of the aforementioned laser PEEM, we will actually measure devices using the laser PEEM. In other words, we will work on operational ReRAM devices, observe them as they stand, and attempt to determine the cause of variation of the devices and decrease in reliability (Figure 2). If the developed operando laser PEEM is successfully applied to practical use, it will be the first-ever technique for nondestructively and comprehensively evaluating the operation validation and reliability of major next-generation recording devices including not only ReRAM but also MRAM and PCM, and it will produce an extremely large ripple effect.

# **Efforts toward industrialization**

From the beginning of development, we have designed the laser PEEM assuming that its price will fall within a suitable price range such that users can use it in fundamental research in universities and the development process of device manufacturers. We will transfer our technology from Shin Laboratory to analytical instrument manufacturers when the laser PEEM will be applied to practical use.

Moreover, we are collaborating with a company developing memory in the research on ReRAM using the operando laser PEEM in order to quickly feed our findings back to the front line of the development. Furthermore, we have been promoting the development of non-von Neumann type information processing (artificial intelligence) devices, which are indispensable to the advance of industries.

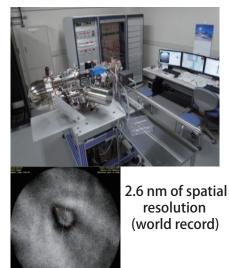


Figure 1 Ultrahigh-resolution laser photoelectron microscope (laser PEEM)

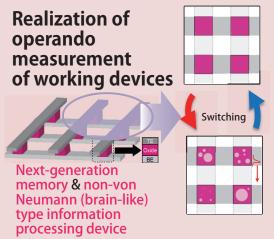


Figure 2 Operando measurement of a working device using laser PEEM

# Operando measurement-based exploration of health functions of underused materials originating from bioresources

Leaders: K. TOMINAGA (AIST), Y. OHYA (UTokyo)

# Purpose

A stressed society and an aging society are characteristic problems in the modern society, which have a great influence on the physical and mental health, cognitive functions, emotions, and actions of people; securing and improving the quality of life has thus been an ongoing issue, particularly in developed countries. Because of this, various pharmaceuticals have been sought active materials derived from natural products as safer candidates holding promise for immediate efficiency and tolerability.

By clarifying the cell activity function of underused materials originating from bioresources, including products from microalgae, using am advanced operando cell observation technology such as the morphological profiling method, we aim to identify functional ingredients that are safer and have immediate efficiency and tolerability and establish a principle to search for new candidate compounds on the basis of the clarified mechanism of action of the ingredients and, in the end, put them to practical use in the medical and food industries.

# **Our research**

The morphological profiling method developed by the Ohya Laboratory at UTokyo is a method of chemical genomics that predicts gene products with which a compound interacts in cells based on the similarity of morphological information of the cells. Ohya Laboratory has succeeded in the identification of intracellular targets of three breakdown products of woody biomass and interactions of compounds, observed under the working conditions of the gene.

In this study, we use budding yeast as a model of eukaryotic cells. Various materials originating from bioresources are reacted with budding yeast and the consequent morphological changes in the cells are informatically analyzed to observe the action of the materials in the cell under the working conditions of the gene.

For bioresource-originated materials showing the desired activity, we will search for and synthesize a group of compounds with analogous structures, evaluate the structure-activity relationship by the morphological profiling method and other methods, and use it as a principle to search for and synthesize compounds with further desired activities.

# **Efforts toward industrialization**

To share the outcome with industrial circles, AIST has established a consortium— "Food, Medicine and Material Innovation Based on Bio-resource and Catalyst Technology"—and UTokyo has established the "Functional Bio-Research Support Forum." We will strongly promote research toward practical use under an industry–academic–government cooperation system based on good cooperation between the two organizations.

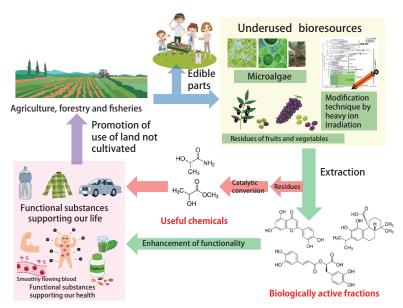
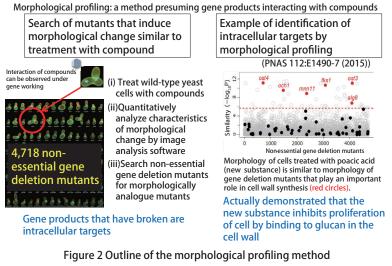


Figure 1 Full use of underused bioresources

# Identification of intracellular targets by morphological profiling



# Evaluation of structural vacancy in an icosahedral cluster solid by positron probe and creation of semiconducting quasicrystals and high-performance thermoelectric materials

Leaders: N. OSHIMA (AIST), K. KIMURA (UTokyo)

# Purpose

A quasicrystal is a solid showing high regularity of arrangement but not having a periodic arrangement like that of a crystal. Quasicrystals having the nature of semiconductor (semiconducting quasicrystals) have not yet been discovered and their existence has been a basic topic of debate in solid state physics. Because semiconducting quasicrystals have many carrier pockets due to the symmetry of the icosahedron being greater than that of the cubic crystal cluster solid and have low thermal conductivity due to their complicated structures, they are strongly expected to be high-performance thermoelectric materials and have thus attracted interest in development-oriented research.

Generally speaking, conversion of metallic properties to semiconducting properties can be achieved by increasing the ratio of covalent or ionic bonds to metallic bonds. Because Al- or B-based icosahedral cluster solids have covalent bonds, their evaluation and control are important for the development of semiconducting quasicrystals. Moreover, because these covalent bonds are considered to be correlated to structural vacancies being at the center of icosahedral clusters consisting of Al or B, evaluation of the structural vacancies is thought to be important in promoting studies in this field.

Positrons annihilate in a short time of less than one nanosecond after incidence in a material. Lifetime of positrons varies according to the presence or absence of vacancies in the material; thus, vacancies can be evaluated by positron probes with high sensitivity.

The aim of this study is to establish an evaluation method for covalent bonds in icosahedral cluster solids (quasicrystals and approximant crystals) using positron probes, to create semiconducting quasicrystals using the evaluation method, and to accelerate the development of high-performance thermoelectric materials.

# Our research

In Al-based icosahedral clusters in Al-based quasicrystals or approximant crystals, metallic-covalent bonding conversion occurs according to the presence or absence of an atom at the center (Figure 1). Such a vacant center of icosahedral clusters is called a structural vacancy and positron probes are useful for evaluation of the vacancy.

First, using Al-based approximant crystals and B-based crystals, structures of which can be analyzed by using electron or X-ray diffraction analyses, correlation of the increase and decrease in covalency with results of the vacancy analysis by positron probes will be investigated. On the basis of the results, positron probes will be applied to quasicrystal structures that are difficult to analyze by electron or X-ray diffraction analyses.

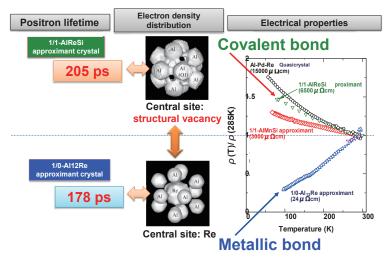


Figure 1 Metallic -covalent bonding conversion in Al-based icosahedral cluster and positron lifetime [1]

At the same time, the semimetal and semiconductor band structure found in AI- or B-based approximant crystal models based on an experimentally obtained structure will be analyzed by maximally-localized Wannier functions to elucidate a bandgap formation mechanism.

# Efforts toward industrialization

To attain a scenario where the obtained outcome is used efficiently, we are investigating the needs of companies. We also intend to develop an analytical method for other materials through the framework of OIL.

[1] Y. Takagiwa, K. Kimura, Science and Technology of Advanced Materials 15, 044802 (2014).

# Research on sophistication of secondary batteries by ultrahighresolution soft X-ray spectroscopic analysis

Leaders: H. MATSUDA (AIST), Y. HARADA (UTokyo)

# Purpose

To realize a sustainable low-carbon society, a breakthrough that leads to truly innovative materials for energy storage to contribute to achievement of the carbon dioxide emissions reduction target is desired. For effective and efficient promotion of the development of innovative materials, it is important to understand the characteristics of the material at a fundamental level using advanced measurement techniques and establish a principle of design based on the findings.

Our aim is to clarify the electronic state of the electrodes of the secondary battery i.e. a representative device using materials for energy storage, in element-, valence-, and orbital-selective manners by ultrahigh-resolution soft X-ray spectroscopic analysis under the operating potential, to elucidate the charge/discharge mechanisms at the electronic orbital level, to propose a guiding principle for the design of new materials, and to significantly contribute to the development of an innovative secondary battery that exerts an influence on the expansion of cruising range and improvement of acceleration performance of electric vehicles.

# **Our research**

On the University-of-Tokyo Synchrotron Radiation Outstation Beamline at the SPring-8 synchrotron radiation facility, an angle-resolved high-resolution soft X-ray photoelectron spectroscopy system and/or a soft X-ray emission spectrometer are combined with electrode chips with coatings e.g. epitaxial films developed by AIST, we will perform angle-resolved operando measurement of materials for secondary batteries with operating the potential of epitaxial films to obtain information about each electronic orbital. We will analyze data making optimal use of the facilities offered by AIST and UTokyo, such as first-principles calculations and multiplet calculation of a cluster model, and will consider charge/discharge mechanisms at the electronic orbital level. On the basis of the findings, we will attempt to propose a guiding principle for the design of new materials with high energy density, long-term stability, and durability against repeated charge/discharge cycles with intercalation of charge carriers.

# **Efforts toward industrialization**

- We hope that domestic automobile manufacturers and battery manufacturers participating in national projects understand advanced soft X-ray spectroscopy techniques and their superiority and perform a feasibility study of practical materials.
- We hope to develop this study into a large-scale joint research venture, to offer the measurement system on a larger scale, and to accumulate and diversify knowledge. We also intend to propose a guiding principle for the design of materials for innovative batteries in cooperation with companies and accelerate "bridging" research.
- We also aim to cooperate with overseas companies that have a subsidiary company in Japan and intend to work as a bridge between domestic companies.



Figure 1 Angle-resolved high-resolution soft X-ray photoelectron spectroscopy system and soft X-ray emission spectrometer

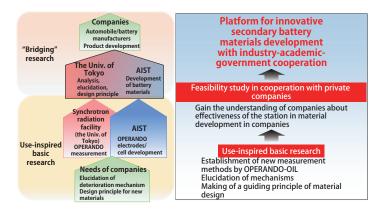
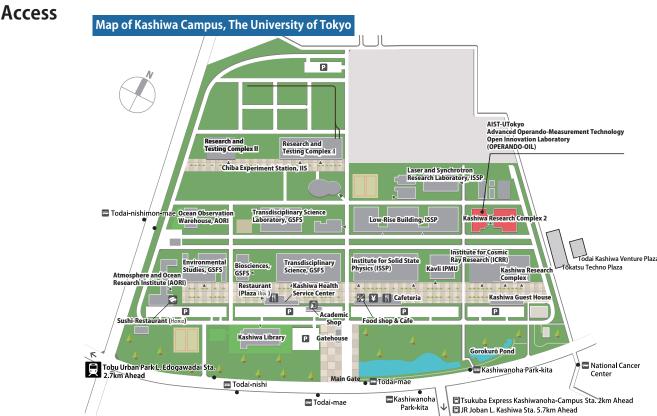
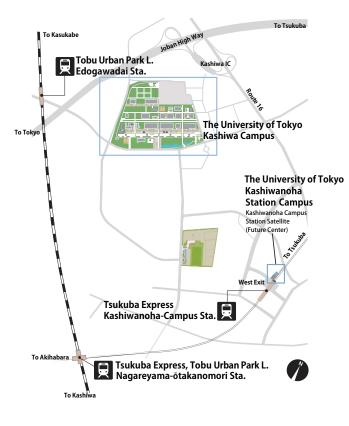


Figure 2 System to provide a guiding principle for development and design of materials for innovative secondary batteries





# **By Train**

- From Kashiwanoha-campus station (west entrance) of TSUKUBA EXPRESS (TX) Line

- Tobu Bus "Nishikashiwa03 (西柏03)" for east entrance of Nagareyama-otakanomori Station → get off at "National Cancer Center" stop.
- Tobu Bus "Nishikashiwa04 (西柏04)" for east entrance of Edogawadai Station → get off at "National Cancer Center" stop.
- Tobu Bus "Nishikashiwa10 (西柏10)" for east entrance of Edogawadai Station → get off at "Todai-mae" stop.
- About 25 minutes' walk from Kashiwanoha-campus station to the campus
- From Kashiwa station (west entrance) of JR Joban Line
  - Tobu Bus "Nishikashiwa01 (西柏01)" or "Kashiwa44(柏44)" for National Cancer Center → get off at "National Cancer Center" stop.
- From Edogawadai Station (east entrance) of Tobu Urban Park Line
   Tobu Bus "Nishikashiwa04 (西柏04)" or "Nishikashiwa10 (西柏10)" for Kashiwanoha-campus station west entrance → get off at "National Cancer Center" stop.
  - Tobu Bus "Nishikashiwa10 (西柏10)" for Kashiwanoha-campus station west entrance → get off at "Todai-mae" stop.

# **By Car**

Take the Joban Expressway and get off the Kashiwa Interchange (in the direction of Chiba). Drive into the National Rout 16 and follow it for 500 m. Turn right at the "Toyofuta Industrial Estate Entrance" crossroads.

# Contact

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