

ANNUAL REPORT

2018

**Institute of Advanced Energy
Kyoto University**

Gokasho, Uji, Kyoto 611-0011
Japan

CONTENTS

Foreword	1
1. Staff List	2
2. Organization Chart	10
3. Research Activities	11
3-1. Research Activities in 2018	13
Advanced Energy Generation Division	
Quantum Radiation Energy Research Section	15
Advanced Atomic Energy Research Section	23
Advanced Particle Beam Energy Research Section	29
Advanced Plasma Energy Research Section	37
Advanced Energy Research Section	45
Advanced Energy Conversion Division	
Advanced Energy Materials Research Section	47
Advanced Laser Science Research Section	55
Advanced Energy Structural Materials Research Section	59
Complex Plasma Systems Research Section	67
Clean Energy Conversion Research Section	75
Advanced Energy Utilization Division	
Chemical Reaction Complex Processes Research Section	79
Molecular Nanotechnology Research Section	85
Biofunctional Chemistry Research Section	89
Structural Energy Bioscience Research Section	95
Advanced Energy Utilization Division	103
Laboratory for Complex Energy Processes	107
Self - Assembly Science Research Section	107
High-Temperature Plasma Equipment Engineering Research Section	111
Environmental Microbiology Research Section	117
3-2. Award	121
4. Joint Usage/Research Program	129
5. Collaboration Works in the Laboratory for Complex Energy Processes	137
6. Projects with Other Universities and Organizations	145
7. How to get to the IAE	150

FOREWORD



Institute of Advanced Energy (IAE) was established in 1996 for pursuing research aimed at the development of energy science and the creation of advanced technology that drives it. This work, which is outstanding both in terms of environmental harmony and social acceptance, is conducted by 3 divisions with 14 research sections (including two with guest researchers) that engage in research on energy generation, conversion, and advancement, as well as the Laboratory for Complex Energy Processes with 3 research section, which specializes in highly project-oriented cross-disciplinary R&D.

IAE has leveraged the strengths as a research institute to focus on “plasma and quantum energy” and “soft energy” as fields of vital importance. It is devoted to R&D on nuclear fusion and advanced atomic energy, regulated by the science under extreme conditions, on distributed energy sources, typified by sunlight and biological systems, and on the advanced materials and effective energy utilization systems that support these technologies. IAE also has emphasized international collaborative research on advanced energy to lead the field of energy science and technology as an international pioneer.

Since AY2011, IAE has emphasized operating as a “Joint Usage / Research Center (JURC)” under the title of “Zero-Emission Energy (ZE) System”, which minimizes load/dissipation of energy, and generation/emission of harmful substance. Under this initiative, the institute employs its broad variety of resources to promote collaboration/ cooperation across different academic research areas. Encouraged by this assessment, we have continued our efforts in leading the zero-emission energy research and community formation. We have successfully finished the first term of the activity at 2016 and started the second term from 2017. These are ascribed to the continued strong support from all of you in related communities, which we deeply appreciate.

This annual report summarizes the IAE’s research findings for FY2017 (April 2017-March 2018). Due to the space limitation, only key results including publication and presentation performed in the year in each division and research section, and also in Laboratory for Complex Energy Processes are edited. Please contact to each researchers for more detail information.

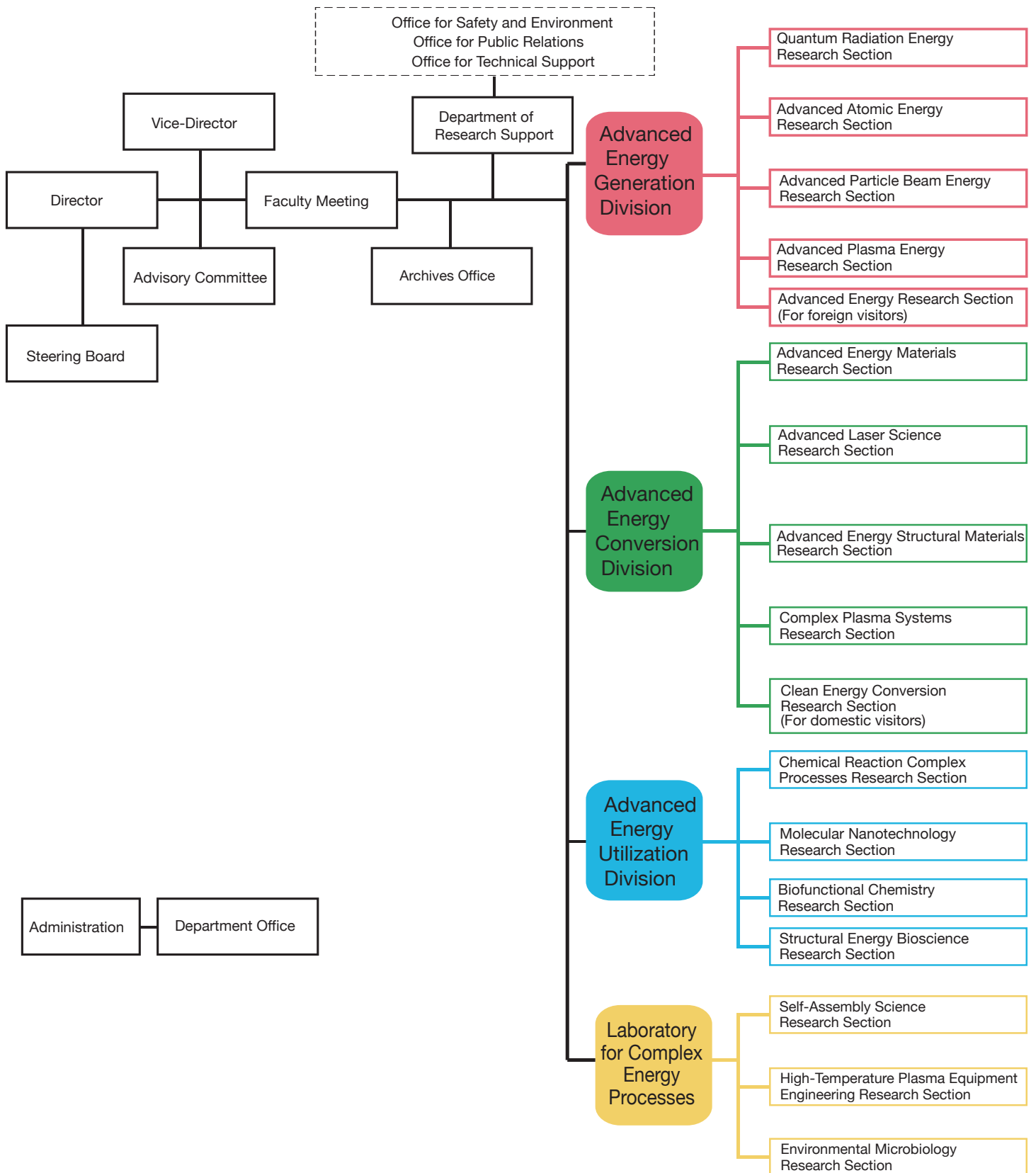
We would appreciate it if we could have your continuous support and encouragement for our institute.

A handwritten signature in black ink that reads "Yasuaki Kishimoto". The signature is written in a cursive, flowing style.

March 2019

Yasuaki KISHIMOTO
Director
Institute of Advanced Energy
Kyoto University

2. ORGANIZATION CHART



3. RESEARCH ACTIVITIES

3-1. RESEARCH ACTIVITIES IN 2018

Quantum Radiation Energy Research Section

H. Ohgaki, Professor
 T. Kii, Associate Professor
 H. Zen, Assistant Professor
 K. Sakaue, Part-time Lecturer
 K. Poolsawat, ogram-Specific Assistant Professor
 K. Miura, Specially Appointed Professor

1. Introduction

Coherent-radiation energy with wide wavelength tunability, high power and high efficiency is quite promising in the 21st century that is sometimes called the "era of light". The research in this section aims at developing the technology to generate new quantum-radiation energy and apply the radiation in various fields; atomic energy including plasma heating, energy transportation in the universe, material science, material synthesis, electronic device, medical and biological science, etc. Free-electron laser (FEL) is one of candidates for the new quantum radiation, and it is sometimes called the light source of next generation.

2. Free-electron Laser

FEL is regarded as a light source of the next generation because of its wide wavelength tunability where the conventional lasers cannot reach, potential high efficiency, and high power. However, the system is usually much larger and the cost is higher than conventional lasers. We are going to overcome these difficulties by exploiting an RF (radio-frequency) gun, an undulator, etc.

2.1 KU-FEL

The target wavelength of KU-FEL is MIR (Mid infra-red) regime, from 5 to 20 μm . The high power tunable IR laser will be used for basic researches on energy materials and systems. Figure 1 shows a schematic drawing of the KU-FEL system. The KU-FEL consists of a 4.5-cell thermionic RF gun, a 3-m travelling wave accelerator tube, a beam transport system, and a 1.8-m undulator and a 5-m optical resonator. The FEL device now can cover the wavelength range from 3.4 to 28 μm . The maximum macro-pulse energy which can provide is around 40 mJ in a 2- μs macro-pulse at the wavelength of 4.9 μm . The FEL is routinely operated and opened for internal and external users.

Another topic of KU-FEL development is introduction of photo-cathode RF gun, which enables us to generate higher peak power and wider tunable range MIR-FEL. Development of a UV-laser system for illuminating photo-cathode has been completed under collaboration with Dr. R. Kuroda, Researcher of AIST. In

FY2014, we have achieved FEL lasing with photo-electron beam generated from LaB₆ cathode. Further study is undergoing to use this operation mode for user experiments.

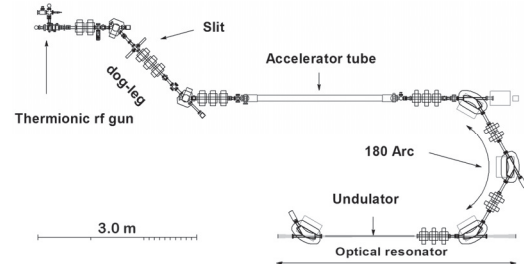


Fig. 1 Schematic drawing of the KU-FEL

2.2 MIR-FEL Application in the Energy Science

Mode-selective phonon excitation (MSPE) is important issue for the bulk solid material to develop the energy saving devices. An MIR-FEL pump, visible pico-second laser probe system has been constructed for measuring the dynamics of phonon vibration which is induced by MIR-FEL irradiation.

High-resolution photoacoustic spectroscopy (PAS) system for solid samples using an MIR-FEL has been also developed and demonstrated.

2.3 THz Coherent Undulator Radiation Source

A new compact terahertz coherent undulator radiation source has been constructed. It consists of a 1.6-cell RF-gun, a solenoid magnet, a magnetic chicane bunch compressor, a triplet quadrupole magnet, a planar undulator, and a laser system for photocathode. Schematic view of the proposed system is shown in Fig 2. In this device, short electron bunches are generated by the photocathode RF gun and the bunch compressor. The electron bunches are injected to the undulator and intense coherent undulator radiation can be generated.

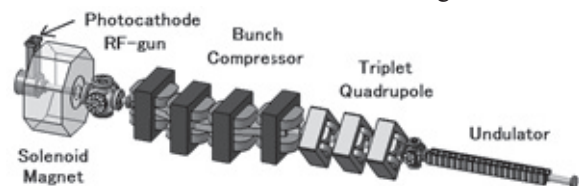


Fig. 2 3D image of THz coherent undulator radiation source.

In order to know the basic performance of the device, detailed experiments have been conducted. As the results, it was confirmed that the device can provide quasi-monochromatic THz radiation from 160 to 650 GHz. Intensity saturation due to space charge effect has been observed. This saturation should be avoided to generate THz radiation with higher peak power. Several methods to mitigate the space charge effect has been investigated. We found that the manipulation of laser pulse shape is a candidate to mitigate the space charge effect and to increase the peak power of the THz-CUR source.

3. Bulk HTSC Staggered Array Undulator

An undulator with strong magnetic field will play an important role in future synchrotron light sources and free electron lasers. We have developing a new undulator which consists of stacked bulk high critical temperature superconductors array and a solenoid magnet. As a next prototype of the new undulator, we installed a new solenoid magnet with GM cryocooler whose maximum field was 6 T.

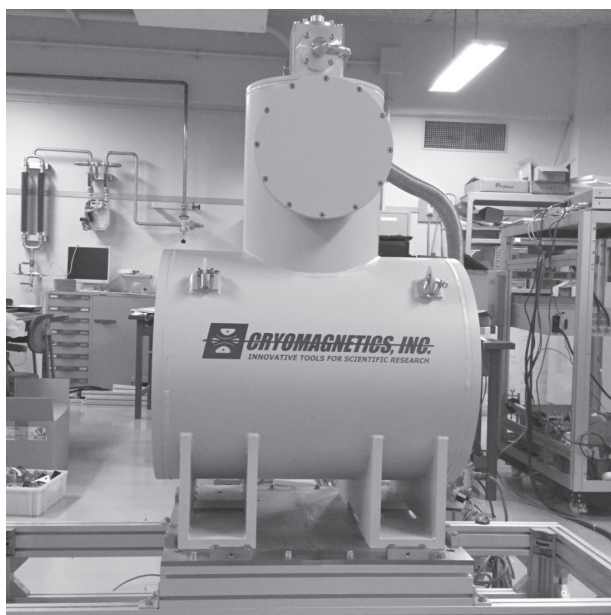


Fig. 3 A 6T solenoid magnet with GM cryocooler.

4. Isotope Imaging for Nuclear Security

A Nuclear Resonance Fluorescence (NRF) method is a powerful tool for investigation not only of the nuclear physics, but also of isotope imaging inside the nuclear waste canisters. We have been developing an isotope imaging technique by using NRF. The absorption can be measured by sample material and “witness target”.

A demonstration experiment of the NRF-CT imaging by using LCS gamma-ray beam has been carried out at the LCS gamma-ray beamline, BL-1U, at UVSOR-III where 5.4 MeV LCS gamma-rays with a flux of 1×10^7 photons/s can be available.

By using NRF absorption method a NRF-CT image

has been taken for a sample target consists of aluminium, stainless steel, and lead rods (shown in Fig. 4 (a)). The NRF signals from the witness target (natural lead) were measured by a Ge detector. At the same time, transmission gamma-rays have been measured by a $\text{LaBr}_3(\text{Ce})$ detector which gives a density distribution of the sample target. The segmented CT reconstruction method has been developed and we obtained clear ^{208}Pb distribution as shown in Fig. 4 (b). The LCS gamma-ray in UVSOR-III has been upgraded to generate 5.5 MeV LCS gamma-rays with a flux of more than 1×10^7 photons/s in 2018.

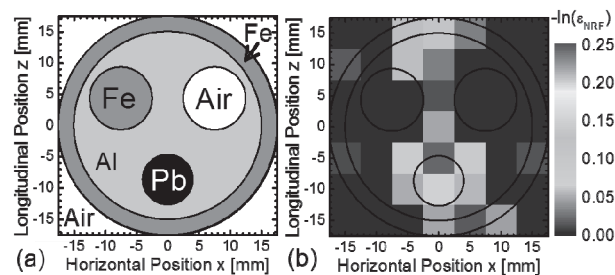


Fig. 4 (a) Result of NRF-CT measurement. (b) Arrangement of the sample target.

6. Japan-Thailand Project for Effective Use of Biomass Wastes as well as Low-rank Coals

Our section has organized a Japan-Thailand joint research project entitled “*Development of clean and efficient utilization of low rank coals and biomass by solvent treatment*” as one of the projects that are supported by the Japan Science and Technology Agency (JST) and the Japan International Cooperation Agency (JICA) through the program called Science and Technology Research Partnership for Sustainable Development (SATREPS). More than 15 Japanese researchers from Kyoto University, Akita University, Central Research Institute for Electric Power Industry (CRIEPI), and Kobe Steel Co. Ltd and 12 Thai researchers from the Joint Graduate School of Energy and Environment at King Mongkut’s University of Technology Thonburi and PTT Public Company Limited are involved in the project.

Through 6 years of cooperation starting from 2013 we are to develop several technologies to convert biomass wastes as well as low rank coals into valuable products such as carbon fiber, biofuel, high quality solid fuel, etc. based on a novel degradative solvent extraction technology developed at Kyoto University.

Acknowledgment

These works were partially supported by the Grant-in-Aid for Scientific Research and challenging Exploratory Research, by the Ministry of Education, Culture, Sports, Science and Technology of Japan, and The Collaboration Program of the Laboratory for Complex Energy Processes, Institute of Advanced Energy, Kyoto University.

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大垣英明, NSTDA (タイ), JASTIP、WP2

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大垣英明, University of Malaya (マレーシア), Study on Energy Usage and Quality of Life for Rural Community Through Rural Electrification using Renewable Energy

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大垣英明, Institute of Technology of Cambodia (カンボジア), A study on economic and technical impacts of mass integration of solar home system on power distribution system

三浦孝一, エネルギー・環境連合大学院/キングモンクット大学トンプリ校 (タイ), タイ石油公社 Research & Technology Institute (タイ), 低品位炭とバイオマスのタイ国におけるクリーンで効率的な利用法を目指した溶剤改質法の開発

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Advanced Atomic Energy Research Section

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1. Introduction

Main objective of our research section is to realize advanced energy systems for the sustainable development under global environmental constraints. We propose a Zero-emission energy scenario based on fusion energy with biomass-based recycling system where biomass waste is converted into liquid fuel or hydrogen, and further isolate CO₂ in the atmosphere by a carbonization process. Our research section focuses on development of impurity control system including hydrogen isotopes for liquid breeding blankets, fusion material R&D, feasibility study for fusion-biomass hybrid power system, conversion of biomass waste, and fusion neutron generation/measurement. Followings are main research achievements in the fiscal year of 2018.

- Generation of fusion neutron by the cylindrical discharge fusion device and a two-dimensional neutron measurement by imaging plate.
- Development of liquid lithium lead droplet system for efficient recovery of hydrogen isotope and heat.
- Electrochemical approach for impurity monitoring and reduction in liquid tritium breeding material
- Fundamental research on the additive manufacturing of ODS steel
- Economic feasibility analysis of fusion-biomass hybrid system, including an experimental approach to produce char as carbon sequestration.

2. 2D neutron measurement by imaging plate

Neutron distribution monitoring in fusion blanket is a key issue to ensure the self-sufficiency of the tritium fuel. Development of 2D (quasi-3D) neutron measurement is required, so that activation analysis quantified by

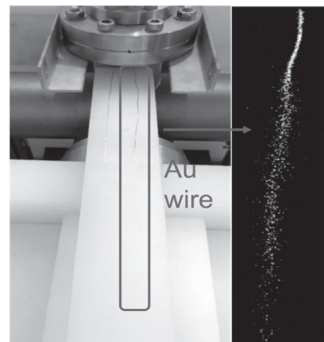


Fig. 1 Gold wire placed by the neutron source (left) and its radiation trace on the imaging plate (right).

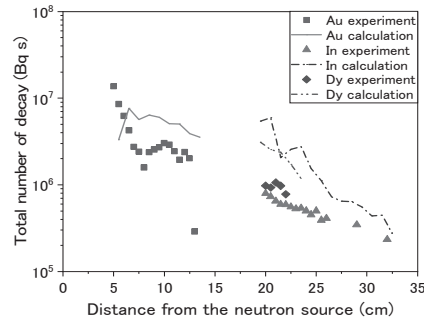


Fig. 2 Radioactivation dependence on the distance from neutron source.

imaging plate is investigated, using a cylindrical discharge (D-D) fusion device. Several kinds of metal wires and foils (Au, In, and Dy) are placed around a neutron source as shown in Fig.1, where polyethylene blocks are assembled to moderate and shield neutron. The activated sample was placed on an imaging plate and the activity was quantified by scanner to be compared with the estimation by calculation (code: MCNP5) as shown in the Fig.2 where rough agreement was observed.

3. Development of liquid lithium lead droplet system

Lead lithium eutectic alloy (Pb-17at%Li, Pb-Li) is a candidate liquid breeding material with low chemical reactivity and good tritium breeding ratio. Effective tritium recovery method from the liquid must be developed for the blanket system with minimal tritium loss. The vacuum sieve tray (VST) method, tritium recovery from the liquid droplet surface falling in vacuum, is a candidate developed in this section. This fiscal year, a collaboration work with National Institute for Fusion Science (NIFS) is started, to demonstrate VST device continuously in a Pb-Li loop in NIFS. A test device (4 nozzles system) shown in Fig. 3 was constructed and its stand-alone test was successfully completed followed by the transportation to NIFS. Connection to the loop and operation will be performed in the next fiscal year.

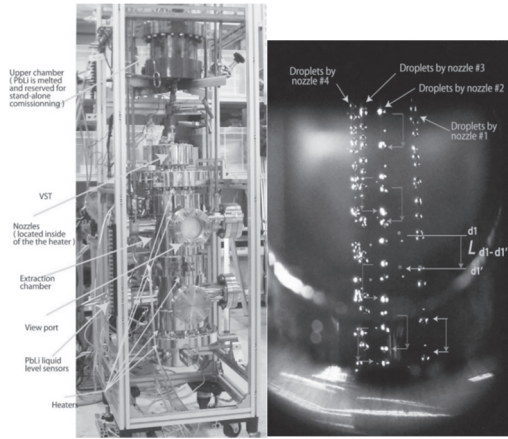


Fig. 3 The VST device during a stand-alone test (left) and Pb-Li droplets in the chamber (right).

4. Electrochemical impurity monitoring and recovery from liquid breeding material

Impurities in liquid breeding material (O, H in Pb-Li; H, N, O in Li; HF, H₂O in molten salt, etc.) play significant role on the corrosion of materials. Also controlling hydrogen isotopes are important from the view point of tritium fuel cycle. In this fiscal year, nitrogen impurity in liquid lithium is studied to develop the concentration monitoring method based on electrochemistry with compatible chloride molten salt. On LiCl-KCl (59:41 atomic ratio, 100~120g) bath, liquid lithium (2~4g) in stainless steel tube guide is placed. Unlike fluoride molten salt (FLiBe, FLiNaK, etc.), LiCl-KCl does not react with metallic lithium. Pure Ni wire (0.3 mm ϕ) is dipped in the salt bath to be used as a working electrode (WE). Li₃N powder is fed to the lithium, which is also used as a counter electrode (CE). The experimental setup is shown in Fig.4. Peak height corresponding to the reduction of nitride ion in cyclic voltammetry is acquired and its dependence on

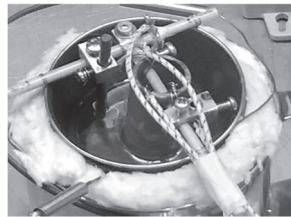


Fig. 4 Electrochemical cell (salt bath, Li CE, Ni WE).

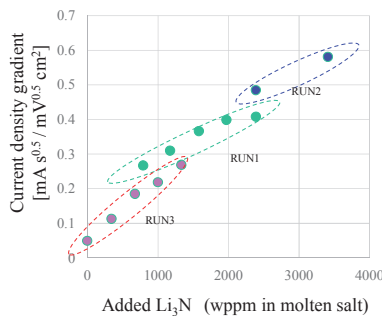


Fig. 5 Electrochemical cell and the change in CV depending on the Li₃N addition.

the potential scanning rate is calculated and shown in Fig.5. There is a linear relationship, which suggests the possibility of nitrogen concentration measurement and electrochemical reduction for liquid lithium.

5. Fundamental research on the additive manufacturing of ODS steel

ODS (Oxide dispersion strengthened) steel is a major structure material candidate for fusion reactors. However the fabrication method of complex structure from this material has not been established, because simple melting method, such as welding or casting, results in the aggregation of the dispersed oxide particles to invalidate the strengthening effect. The additive manufacturing (3D printing) can be the solution due to the very limited period of melting. As a first step, Fe powder with 1wt%Y₂O₃ nano-powder was melted with a single-pulse laser. The sample powder was prepared in a ball-mill from pure Fe powder and Y₂O₃ powder. As shown in Fig. 6, some part of the Y powder seems to remain in the Fe matrix suggesting possible ODS effect.

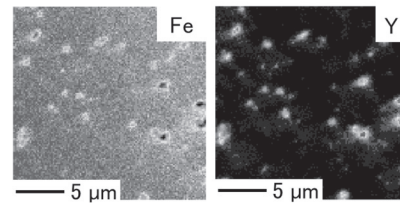


Fig. 6 surface element mapping of sintered Fe-1%Y₂O₃ pebble, 400W-5ms.

6. Economic feasibility of fusion-biomass hybrid

Fusion biomass hybrid system, in which the heat from fusion reactor is supplied to a biomass plant to produce combustible gas (H₂, CO) or liquid fuel (e.g. diesel through FT reaction) is a key concept to enhance the possibility of fusion energy. In this fiscal year, new type of fusion-biomass hybrid is proposed and investigated: producing char as a carbon sequestration medium. One of the representative result is shown in Fig.7. Depending on the heat cost of the fusion reactor (2~6000 USD/kW) and the annual cost of operation and maintenance (1~13% of initial cost), economically feasible emission credit (USD/ton-CO₂) is calculated, giving 10 % IRR (Internal rate of return).

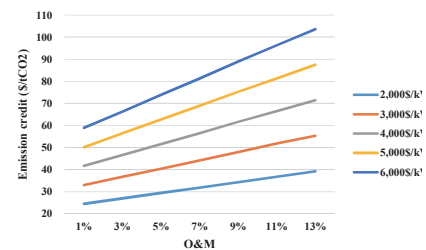


Fig. 7 Relationship between fusion heat cost, O&M cost and emission credit.

Collaboration Works

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Advanced Particle Beam Energy Research Section

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1. Introduction

Advanced and innovative control methods for the collective behavior of charged particles are being developed in this research section to bring about enormous contributions to human beings. Studies of nonlinear interactions between charged particles and electromagnetic fields are particularly emphasized. We focus on the following subjects; improvement and understanding of confinement and transport in fusion plasmas, development of heating and current drive systems using high power millimeter waves, development of advanced diagnostics in high temperature plasmas, development and application of compact and portable neutron/proton sources driven by fusion reaction, and production/diagnostics of highly brilliant relativistic electron beams for advanced light sources such as free electron laser.

2. Measurement of temperature distribution on electron gun cathode

Beam emittance reduction caused by the space charge effect can improve the quality of a high-intensity electron gun. Such a phenomenon called self-linearization has been discovered through numerical simulations but has not yet been experimentally observed. The emittance evolution is known to be affected by the temperature distribution on the surface

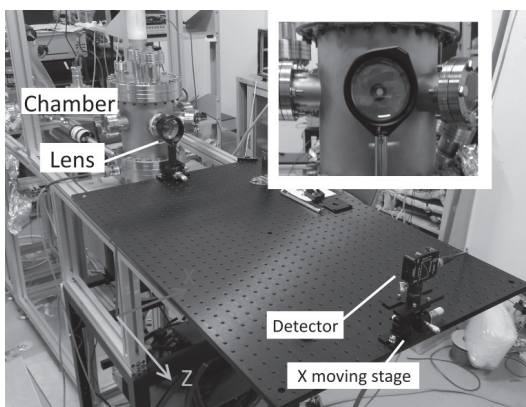


Fig. 1 Experimental setup

of the thermionic cathode. Thus, the development of a diagnostic system to monitor temperature profile on a cathode is needed to prove the self-linearization phenomenon in an experiment. In this study, a temperature distribution of a LaB₆ test cathode was measured with the developed system shown in Figure 1. A cathode image with 1.72mm diameter magnifies by 5.8 times through a lens, and an InGaAs photodiode detector is scanned to measure temperature profile on the cathode, resulting in a spatial resolution of 0.172 mm on the cathode. Figure 2 shows an example of temperature distribution on the cathode. The temperature resolution of the system was estimated to be 0.062K at 1500 °C, suggesting that the present system is capable of contributing to experimental studies of the self-linearization phenomenon.

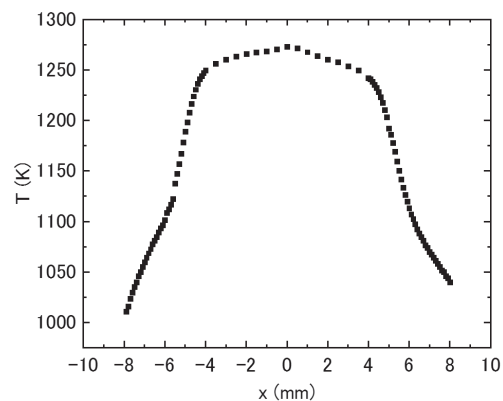


Fig. 2, Temperature distribution of test cathode measured with the developed system

3. Application of 3D peripheral plasma transport code to the Heliotron J

Design of divertor structure is an essentially important issue to control extremely high heat and particle fluxes to the divertor of fusion reactors.

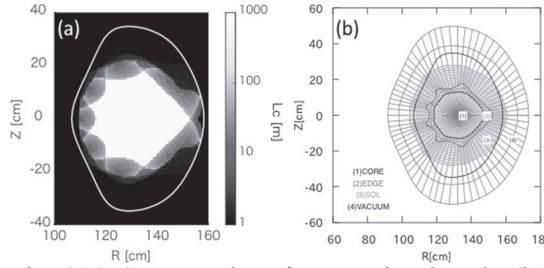


Fig. 3(a) Contour plot of connection length, (b) The computational grid The white line in (a) and black line in (b) represent chamber wall respectively.

Helical devices have 3D geometries intrinsically, hence the analysis and modeling of peripheral plasma transport should be done with considering the 3D effects. We applied 3D peripheral transport code, EMC3-EIRENE to the Heliotron J for the 3D modeling of peripheral plasma and reveal how magnetic field topology affects peripheral transport of plasma and neutrals.

The EMC3-EIRENE code requires a 3D grid with high resolution in the peripheral plasma region to reproduce the fine plasma structure. Figure 3 (a) shows connection length L_c distribution of a poloidal cross section in the standard configuration of Heliotron J. The grid has four domains, CORE, EDGE, SOL and VACUUM, as shown in Figure 3 (b) and labeled as (1) - (4), respectively. The confined region of the plasma is covered by CORE and EDGE domains. The boundary between CORE and EDGE domains is set at $r/a \approx 0.8$ and the outer boundary of EDGE domain is at the last closed flux surface (LCFS). Outside of the LCFS is covered by SOL and VACUUM domains. The outer boundary of SOL domain is defined to cover the region with connection length $L_c > 10$ m. The VACUUM domain is defined to cover the chamber wall. Transport equation of neutral particles is solved in the entire domains, and of plasma is solved only in EDGE and SOL domains. The grid in

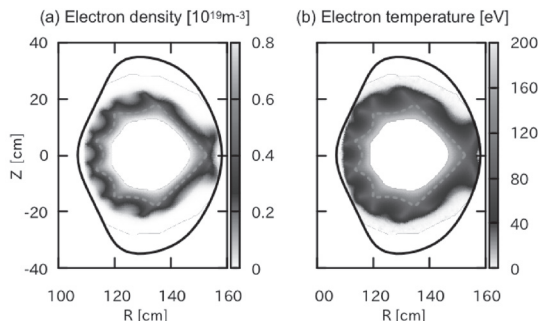


Figure 4 (a) Contour plot of electron density, (b) electron temperature obtained with EMC3-EIRENE

EDGE and SOL domains have a field-aligned structure in the toroidal direction to reduce aliasing error arising from finite resolution of the grids.

After the preparation of the 3D grid, we carried out EMC3-EIRENE calculation. Figures 4(a) and (b) show examples of calculation results for electron density and electron temperature, respectively. The distributions well reflect the structure of the connection length shown in Figure 3 (a).

We are preparing 3D grids for other magnetic configurations and discuss the effect of magnetic field structure for peripheral plasma transport in a three-dimensional magnetic confinement device.

4. Investigation of ^{10}B Quantitative Analysis by Tension Metastable Fluid Detector for BNCT Pharmacokinetic Evaluation

Establishment of a cancer treatment method that can be applied to elderly patients with an extremely low burden is an urgent issue in realizing a society of health and longevity. Boron Neutron Capture Therapy (BNCT) is one of the promising methods aiming at high tumor selectivity and accumulation for cancer treatment. The BNCT requires a neutron source, and however nuclear reactors cannot be easily utilized and so alternative neutron sources are necessary to accelerate the BNCT research. This work aims to develop a novel quantitative analysis method of ^{10}B for BNCT.

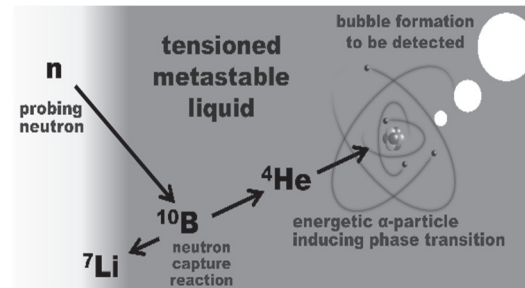


Fig.5 The principle of α particles detection by TMFD Q

Our proposed technique shown in Fig.5 is based on detecting α -particles generated from the $^{10}\text{B}(n,\alpha)^7\text{Li}$ nuclear reaction using Tensioned Metastable Fluid Detector (TMFD). We have utilized Kyoto University Reactor (KUR), which can provide pure thermal neutrons as a neutron source. We tried to verify the principle by investigating the correlation between alpha particle detection rate and the amount of boron in simulant liquid. We successfully demonstrated the possibility of quantitative analysis of target ^{10}B concentration ($10 \mu\text{g} / \text{mL}$) by using pure thermal neutrons from KUR and TMFD.

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Advanced Plasma Energy Research Section

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1. Introduction

The current subjects of this research section are to study the properties of high temperature plasmas in order to control and improve the plasma energy confinement from the physical viewpoint of nuclear fusion research. The experimental and theoretical investigations for the optimization of the helical-axis heliotron configuration are in progress under the collaboration with other groups of the international/national institutes and also groups of other universities under the auspices of the Collaboration Program of the Lab. Complex Energy Processes, IAE and the Collaborative Research Program of NIFS (National Institute for Fusion Science).

In this report, a remarkable result obtained in the Heliotron J experimental study in FY2017 is reported focusing on radial electric shear formation in high density NBI plasmas based on poloidal flow velocity measurement.

2. Study of seed plasma generation for NBI plasma startup using non-resonant microwave launch [1].

To extend the operation region of the Heliotron J experiment, development in initiation scheme independent to the requirement of the resonance condition is required. We have tested the seed-plasma generation for NBI plasma startup using non-resonant microwave launch [1]. This section describes the detailed characteristics of the seed plasmas produced by the non-resonant microwave launch [2].

Figure 1(a) shows a visible-image of seed plasmas produced by the non-resonant 2.45-GHz microwave obtained using the fast framing camera. The magnetic field strength was 0.83T and power of 2.45-GHz microwave was 5 kW. The visible light of the seed plasmas appears around the magnetic axis, which implies that the seed plasmas that had significant electron temperature to ionize the background neutral gas existed only around the magnetic axis. The radial profile of the visible light intensity along with the horizontal line crossing the magnetic axis is shown in Fig. 1(b). The visible light intensity has a peaked profile with a maximum value around the magnetic axis position. Since the density and temperature are lower than the detection limits of the YAG laser Thomson scattering diagnostic in Helio-

tron J, information of the density profile for the seed plasmas was not obtained yet. Nevertheless, the density profile is expected to be peaked. If the seed plasma is distributed to the 1/3 of the last closed flux surface, the electron density is expected to be more than $1 \times 10^{18} \text{ m}^{-3}$, which is more than 10 times higher than that of the O-mode cutoff density ($7.6 \times 10^{16} \text{ m}^{-3}$) for 2.45-GHz microwaves. In this report, the line-averaged electron density (\bar{n}_e) normalized by the path length of the interferometer crossing the last closed flux surface is used as an indicator.

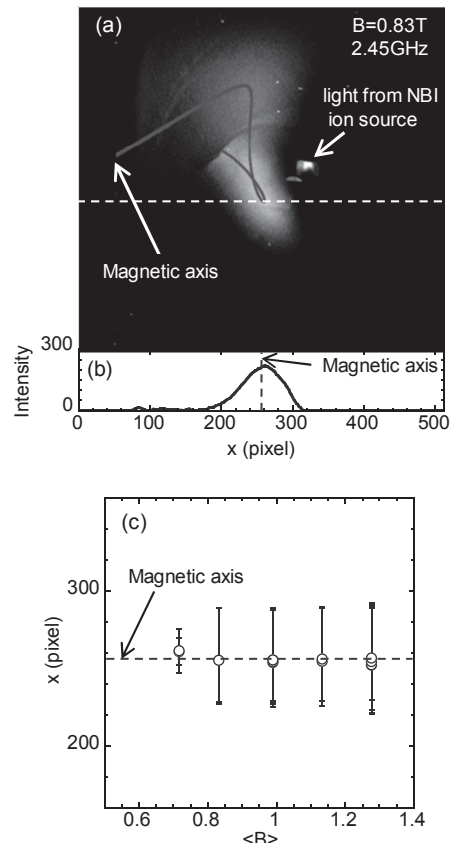


Fig. 1. (a) Tangential camera image of seed plasmas produced by 2.45-GHz microwaves, (b) visible-light intensity profile as a function of horizontal pixel position crossing magnetic axis, and (c) center of gravity calculated from intensity profile as a function of magnetic field strength. The error bar is the full-width at half maximum of the intensity profile.

The center of gravity (COG) calculated from the intensity profile of the visible-light emission is plotted as a function of field strength in Fig. 1(c). The error bar is the full width at half maximum, which corresponds to the width of the electron density of the seed plasmas. The COG position is almost at the magnetic axis and does not change when the magnetic field strength is varied. The width of the intensity profile is almost the same until the field strength is down to 0.8 T. For a magnetic field strength of 0.7 T, the width of the intensity profile becomes about half that for higher magnetic field strength, and the seed plasma density profile is expected to be narrow. This affects the plasma initiation after NBI. In fact, the NBI plasma start-up did not succeed in this case. The dependence of COG on the magnetic field strength implies that the mechanism of the plasma production is quite different from that with plasma initiation achieved using the second harmonic 70GHz ECH of Heliotron J. From an experimental study of plasma breakdown by the 70GHz ECH, the plasma initiated around the crossing point between the injected electron cyclotron beam and the resonance layer. The initial plasma moved as the crossing point was shifted when the magnetic field strength or the launch position of the electron cyclotron beam was changed.

The effect of seed plasma conditions on plasma breakdown by NBI was investigated by scanning the magnetic field strength and the microwave power. Figure 2(a) shows the operational range of the successful NBI plasma start-up as a function of \bar{n}_e and the magnetic field strength. The 2.45-GHz microwave power ($P_{2.45\text{GHz}}$) was varied from 1 to 5kW. The electron density was taken at the time just before NBI was turned-on. The plasma could be produced by NBI when the initial seed plasma density was above $0.4 \times 10^{18} \text{ m}^{-3}$, which indicates the existence of a density threshold for successful plasma start-up with NBI under the present experimental conditions, (injection power: $\sim 1\text{MW}$; acceleration voltage: 25-27 kV; pulse width: 100ms). At a field strength of $B = 0.8 \text{ T}$, the plasma could be produced at $P_{2.45\text{GHz}} = 5 \text{ kW}$, while the minimum required microwave power was 2-3 kW for $B = 1.3 \text{ T}$. These results show that the required microwave power for rapid start-up increases with decreasing the field strength. The obtained seed plasma density increases with the field strength for a given microwave power.

Figure 2(b) shows the relation between the electron density and neutral gas pressure at the pumping port at the time NBI was turned-on. Successful plasma start-up could be achieved under low neutral gas pressure and high electron density conditions. For $B = 1.3 \text{ T}$ and $P_{2.45\text{GHz}} = 3\text{-}4 \text{ kW}$, the plasma start-up did not succeed even though the electron density was close to the threshold. In this case, the neutral gas pressure was higher than that in the successful plas-

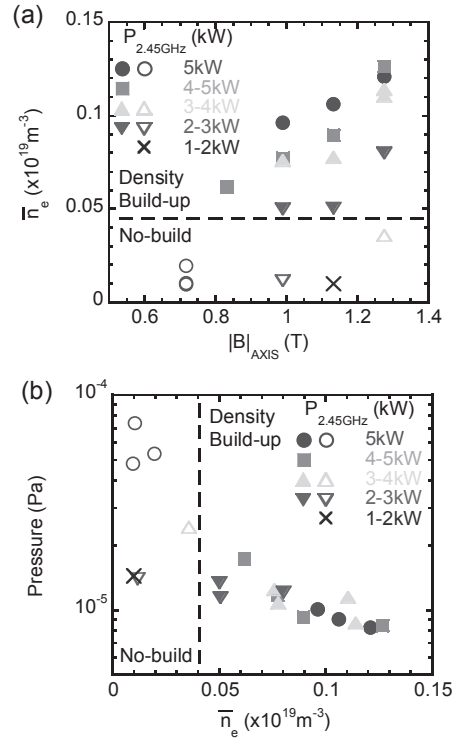


Fig.2 (a) Line-averaged electron density as a function of magnetic field strength. The data were obtained by varying the microwave power from 1 to 5kW. (b) Neutral gas pressure at pumping port as a function of line-averaged electron density.

ma start-up, which suggests that higher neutral gas pressure deteriorates the seed plasma condition for successful NBI plasma start-up. Therefore, careful adjustment of gas fueling is required for the present experimental conditions.

Additional gas puffing during the microwave launch was tried in an attempt to increase the seed plasma density and to generate target plasma that is preferable for NBI start-up. In the case that the additional gas fueling was applied during the phase at which significant radiation and carbon impurity line emission intensities were observed, the electron density increased more than $3 \times 10^{18} \text{ m}^{-3}$ in 60 ms after gas puffing, which was more than 4 times higher than that obtained without additional fueling. In such the case, even in the low NBI power (0.3MW) condition, rapid NBI plasma start-up ($< 10 \text{ ms}$) could be achieved. In fact, the density growth rate ($\delta\bar{n}_e/\delta t$) is about $4 \times 10^{20} \text{ m}^{-3} \text{ s}^{-1}$, which is almost 5 times faster than that obtained without additional fueling discharge. In summary, we have successfully developed the generation scheme for the plasma startup independent to the resonance condition.

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Advanced Energy Research Section

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1. Summary

The author spent three months (Jan 4, 2019-Mar 31, 2019) as a visiting professor at Institute of Advanced Energy (IAE), Kyoto University (Uji Campus) hosted by Prof. Hideaki Ohgaki under a supervision of Prof. Koichi Miura.

Here the author reports about the study on propensity to spontaneous heating of torrefied biomass under dry air and water vapor at over 100 °C using TG-DSC.

2. Introduction

Torrefaction is a low-temperature thermal treatment method to improve fuel properties such as heating values of raw biomass prior to be used in pyrolysis/gasification system. The chemical structure of biomass is complex and consists of three major components; cellulose, hemicellulose, and lignin. This affects to its fuel properties after torrefaction. Moreover, like coal, the torrefied biomass could be possibly self-ignited at low temperature after exposed to humid air during storage [1]. This study aims to investigate propensity to spontaneous heating of torrefied biomass under dry air and water vapor (steam) at over 100 °C using TG-DSC.

3. Experimental observations

Biomass model compounds; cellulose, xylan as a representative of hemicellulose, and lignin, and agricultural residues; rice husk (RH), cassava roots (CR), and palm kernel shell (KS) were used as raw materials in this study. The chemical compositions of each selected biomass sample are shown in Table 1.

Table 1. Chemical composition of biomass samples

Samples	wt% (dry-ash-free, d.a.f.)			
	Extractives	Cellulose	Hemicellulose	Lignin
RH	2.06	53.91	6.85	37.18
CR	10.98	29.94	32.82	26.25
KS	3.60	21.29	18.64	56.47

Approximately 10–20 mg of biomass samples were dried at 107 °C and then torrefied at 260–320 °C for 60 min, then in-situ cooling to 107 °C in TG-DSC. After stabilization under nitrogen, fresh torrefied samples were exposed to dry air or water vapor at 107 °C for 30 min to examine heat generation. Typical data expressing changes of temperature, relative weight, and heat generation along with time obtained by TG-DSC experiments can be interpreted as Fig. 1.

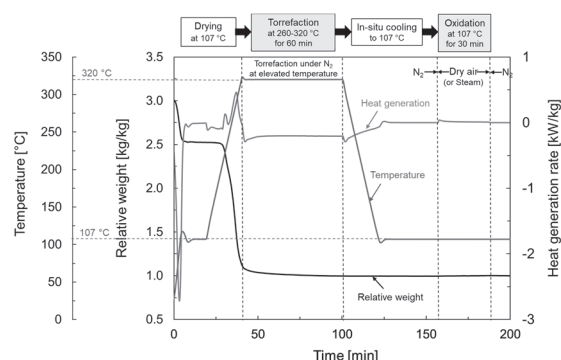


Fig. 1. Typical data obtained by TG-DSC experiment to study oxidation of torrefied biomass at low temperature. (Example; xylan was torrefied at 320 °C for 60 min, then in-situ oxidized under dry air at 107 °C for 30 min)

(1) Weight loss during torrefaction of biomass

Fig.2 shows weight loss during torrefaction of biomass samples at 260–320 °C for 60 min in TG-DSC. Cellulose (Fig. 2 (a)) was hardly decomposed at 260°C, but immediately degraded and reduce the yield to lower than 20 wt% when torrefied at 320 °C. Xylan (Fig. 2(b)) was mostly decomposed at 260 °C and almost stabilized at the yield of about 40 wt%

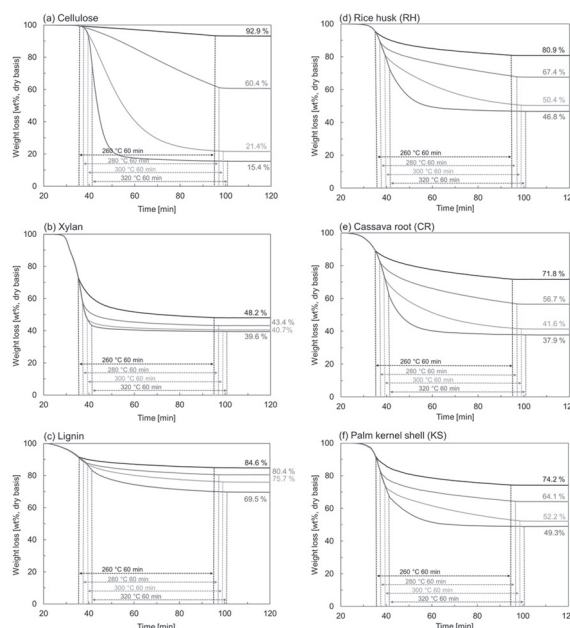


Fig. 2. Weight loss during torrefaction of (a) cellulose, (b) xylan, (c) lignin, (d) RH, (e) CR, and (f) KS at 260, 280, 300, and 320 °C for 60 min using TG-DSC.

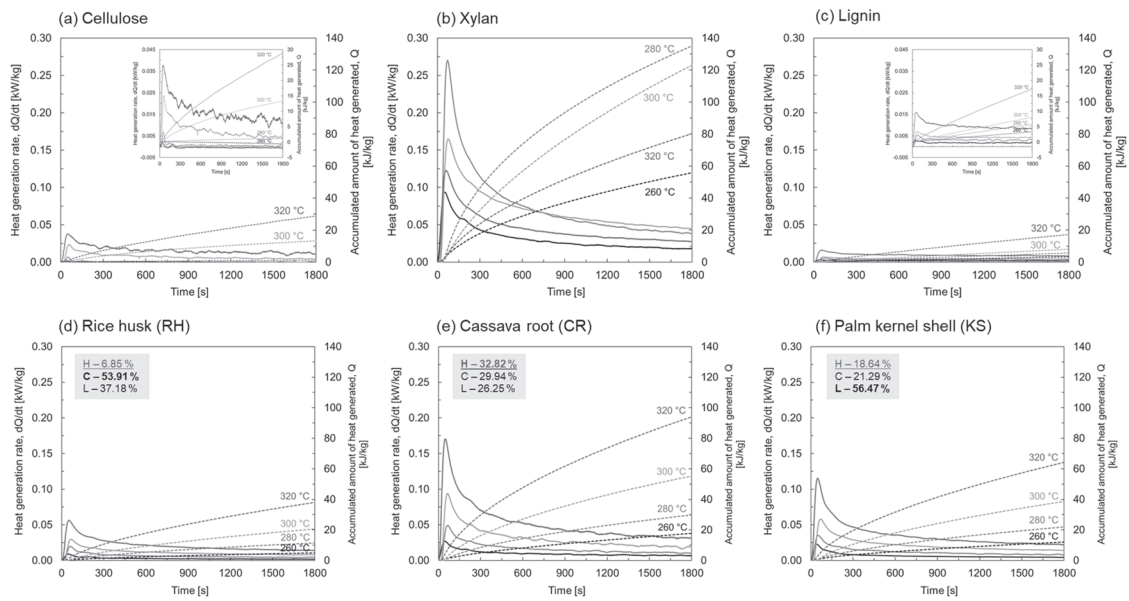


Fig. 3. Changes of heat generation rate, dQ/dt , (solid lines) and accumulated amount of heat generated, Q , (dashed lines) during in-situ oxidation in dry air at 107 °C o (a) cellulose, (b) xylan, (c) lignin, (d) RH, (e) CR, and (d) KS torrefied at 260–320 °C for 60 min.

when being torrefied above 300 °C for 60 min. Lignin (Fig.2 (c)) was slightly decomposed during the torrefaction, while other biomass residues (Fig.2 (e–f)) showed the weight loss during the torrefaction dependent on the composition ratio of major components in their structure.

(2) Heat generation during dry air oxidation

For an investigation of heat generation during dry air oxidation, Fig. 3 shows that the accumulated heat tended to increase when increasing the torrefaction temperature from 260 to 320 °C for almost all samples. However, xylan torrefied at 280 °C expressed the highest amount of heat generated (approximately 135 kJ/kg) during the air oxidation. They released relatively lower amount of heat when the samples were torrefied at above 300 °C. This could be explained from the weight loss curves in Fig. 2(b) that xylan was almost completely decomposed and then stabilized at high torrefaction temperatures. This agree with the previous results that stabilized char generated less amount of heat during the oxidation at 107 °C compared to fresh char [2]. Since the heat generated during dry air oxidation of torrefied cellulose and lignin were rather low at less than 35 kJ/kg (Fig. 3 (a) and (c)), the torrefied biomasses showed the trend of heat generated during air oxidation mainly depending on the amount ratio of hemicellulose (xylan).

(3) Heat generation during water vapor oxidation

Since torrefied xylan indicated the highest amount of heat generated during dry air oxidation, the experiments using water vapor were conducted for comparison. Fig. 4 (a) shows that the weight during steam oxidation rapidly increased in less than 5 min due to water adsorption on the torrefied biomass especially at higher temperature at 320 °C. Moreover,

heat generation during steam oxidation at 107 °C of torrefied xylan significantly increased due to heat of evaporation of adsorbed water on torrefied biomass.

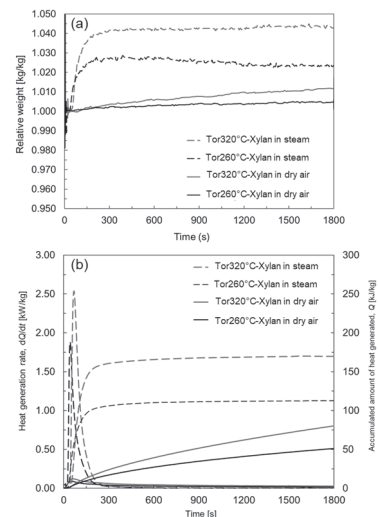


Fig. 4. Changes of (a) relative weight and (b) heat generation rate, dQ/dt , and accumulated amount of heat generated, Q , under dry air and water vapor oxidation for 30 min of xylan torrefied at 260 and 320 °C for 60 min.

(4) Conclusions and future work

Significant amount of heat generated during dry air and water vapor oxidation at 107 °C of torrefied biomass samples were observed. This related to propensity of the spontaneous heating of torrefied biomass. The kinetics and interaction behaviors during low-temperature oxidation of torrefied biomass should be further investigated.

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Advanced Energy Materials Research Section

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1. Introduction

We are working on basic and applied research of nano-materials from a viewpoint of optics and material science. Our research aims at exploring new physical and chemical phenomena leading to applications of novel nano-materials including carbon nanotubes, layered transition metal dichalcogenides, perovskite for efficient utilization of light energy and development of future optoelectronic devices with ultra-low energy consumption. The Multi-Scale Testing and Evaluation Research Facility are also used for development of new composite materials. Followings are main research achievements in the year of 2017.

1. Physics of Excitonic Valley Relaxation in Atomically Thin 2D Semiconductors

A “valley” is an electronic degree of freedom in momentum space, and its potential applications as information carriers in future electronics or optoelectronics devices are called valleytronics. Monolayers of transition metal dichalcogenides (1L-TMDCs) MX_2 ($M = \text{Mo}, \text{W}; X = \text{S}, \text{Se}, \text{Te}$) have recently emerged as promising two-dimensional (2D) materials for developing valleytronics because they have hexagonal lattice structures similar to that of graphene but are semiconductors with finite direct band gaps in two inequivalent $+K$ and $-K$ valleys related by a time-reversal operation in the 2D hexagonal Brillouin zone. Because of the reduced screening resulting from the atomically thin 2D structures of 1L-TMDCs, their excitons, which are mutually attracting electron-hole pairs that interact through Coulomb interactions, have extremely large binding energies and dominate their optical responses even at room temperature. In addition, the strong spin-orbit interactions in these materials give rise to large spin splitting in the valence band. This large valence spin splitting and a lack of inversion symmetry in these materials lead to spin-valley coupling that enables exclusive access to the excitonic valley pseudospins ($+K$ or $-K$) with right- or left-circularly polarized photons. These unique characteristics of 1L-TMDCs have provided unprecedented platforms for the study of valley-exciton physics in 2D systems, as well as

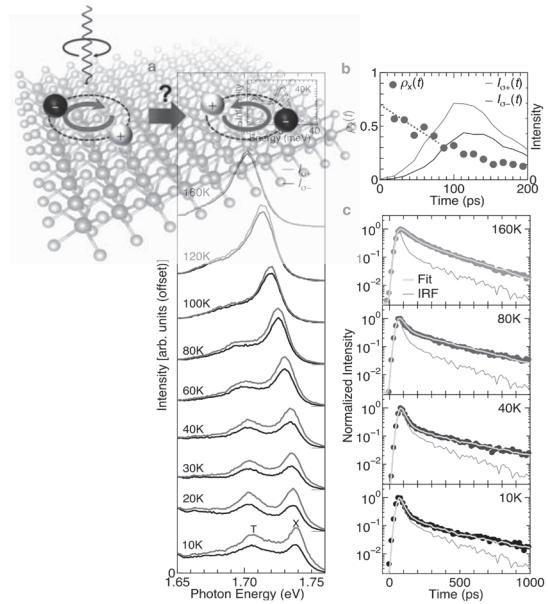


Fig. 1 (a) Schematic of excitonic valley polarization. Temperature dependence of valley polarization. (b) Polarization resolved photoluminescence (PL) decay. (c) Temperature dependence of PL decay profiles.

offering opportunities for developing future optoelectronic devices using the excitonic valley degrees of freedom.

Here, we provided experimental evidence that the excitonic valley relaxation times and their temperature dependence in naturally carrier-doped 1L-TMDCs are dominated by momentum-dependent $e-h$ exchange interactions screened by a 2D electron gas. We measured the valley polarization, linewidth, and time-dependent photoluminescence (PL) decay profile of excitons in 1L-WSe₂ to examine the valley relaxation times of an exciton in the linear response regime. We show that the low-temperature exciton valley relaxation times in 1L-WSe₂ can be excellently reproduced using a framework of an intervalley exciton scattering mechanism via momentum-dependent long-range $e-h$ exchange interactions screened by naturally doped 2D carriers. The temperature dependence of the Coulomb screening function deduced from the experimental data clearly demonstrates the 2D nature of the doped carriers; this

is a unique manifestation of the true 2D structure of 1L-TMDCs. Moreover, we demonstrate that the developed framework can be used to predict the valley relaxation times and polarizations under various experimental conditions with various exciton linewidths, exciton lifetimes, carrier densities, and exciton densities. We also demonstrate that the valley polarization in 1L-WSe₂ can be actually engineered via artificially modifying these parameters according to the theoretical prediction. Our findings therefore provide a unified framework through which the temperature-dependent exciton valley relaxation times and valley polarization in 1L-TMDCs can be understood and predicted; this framework may facilitate the development of TMDC-based opto-valleytronic devices.

2. Realization of Type I Heterostructures in Monolayer MoTe₂/WSe₂

Artificial van der Waals heterostructures of two-dimensional layered materials are attractive from the viewpoint of the possible discovery of new physics together with improved functionalities. Stacking various combinations of atomically thin semiconducting transition metal dichalcogenides, MX₂ with a hexagonal crystal structure, typically leads to the formation of a staggered Type II band alignment in the heterostructure, where electrons and holes are confined in different layers. Here, we performed comprehensive studies on heterostructures prepared from monolayers of WSe₂ and MoTe₂ using various spectroscopic methods. The MoTe₂/WSe₂ heterostructure shows strong PL from the MoTe₂ layer at 1.1 eV, which is different from the quenched PL from the WSe₂ layer. Moreover, enhancement of PL intensity from the MoTe₂ layer was observed because of the near-unity highly efficient photocarrier transfer from WSe₂ to MoTe₂. These experimental results

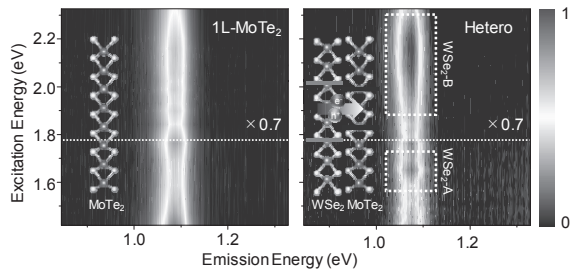


Fig. 2 (a) Schematic of monolayer MoTe₂. 2D map of PL excitation spectra in 1L-MoTe₂. (b) Schematic of monolayer MoTe₂/WSe₂. 2D map of PL excitation spectra in WSe₂/MoTe₂.

suggest that the MoTe₂/WSe₂ heterostructure has a Type I band alignment where electrons and holes are confined in the MoTe₂ layer. Our findings extend the diversity and usefulness of ultrathin layered heterostructures based on transition metal dichalcogenides, leading to possibilities toward future optoelectronic

applications.

3. Particle Dispersion Silicon Carbide Composites by Liquid Phase Sintering

Silicon carbide (SiC) is one of very attractive engineering ceramics in particular for severe environment. Silicon carbide composites basically require weak fiber/matrix interphase like carbon (C) or boron nitride (BN). The interphase material and its thickness are keys to determine mechanical properties. However precise control of the interphase is the critical issue in particular for large scale production and affects material cost significantly. The objective of this work is to develop oxidation resistant SiC composites without fiber/matrix interphase by applying particle dispersion in SiC matrix.

Silicon carbide composites were fabricated by liquid phase sintering (LPS) method. Silicon carbide with BN matrix was formed by mixture of SiC powder and BN powder in LPS composites. Prepreg technique was developed for industrial application. Mechanical properties were characterized by various methods including tensile test and fatigue test in air up to 1200C. Microstructures and fracture surfaces were characterized by FE-SEM.

The BN particle dispersion composites showed excellent high temperature oxidation resistance. Oxidation was limited to near surface. The BN particle dispersion composites don't require fiber/matrix interphase. It decreases material cost significantly. Productivity is also excellent compared to conventional SiC composites. The BN particle dispersion composites didn't break applying 175MPa following 1 million cycles at 1200 C of fatigue test in air without any coating. Machinability of BN particle dispersion composites is good. Stress-strain curves of the material fabricated by LPS seems brittle. However it has reliable matrix cracking stress and lower notch sensitivity like pseudo-ductile composites. figure 1 shows silicon carbide fibers, prepreg and BN particle dispersion SiC composites.

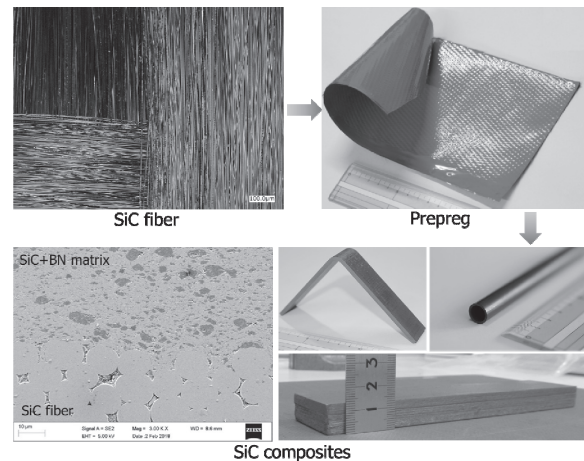


Fig. 3 silicon carbide fibers, prepreg and BN particle dispersion SiC composites.

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檜木達也, Oak Ridge National Laboratory (アメリカ), 原型炉プラズマ対向機器開発のための要素技術の工学的評価 (Phenix)

檜木達也, OECD NEA, Generation IV International Forum, GFR system

檜木達也, OECD NEA, The Expert Group on Accident Tolerant Fuels for Light Water Reactors (EGATFL)

檜木達也, SCK-CEN (ベルギー), Innovative Cladding Materials for Advanced Accident-Tolerant Energy Systems

檜木達也, 東北大学金属材料研究所, SiC/SiC 複合材料の中性子照射効果

檜木達也, 核融合科学研究所, 高延性タングステン複合材料システムの開発

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宮内雄平, 挑戦的萌芽研究, 遷移金属ダイカルコゲナイド超薄膜におけるバレー分極緩和メカニズムの解明

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染谷隆史, 特別研究員奨励費, 遷移金属ダイカルコゲナイドにおけるバレースピノ分極ダイナミクスの解明

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Advanced Laser Science Research Section

T. Nakajima, Associate Professor

1. Introduction

We utilize various kinds of lasers in one way or the other to investigate the various laser-induced phenomena towards the efficient use of laser-based devices in energy science. In this year we focus on the two subjects, i.e., size-controlled synthesis of polymer-metal nanocomposite films using a CO₂ laser and tuning the surface plasmon resonance of laser-induced nanostructures in Ag films.

2. Size-controlled synthesis of polymer-metal nanocomposite films using a CO₂ laser

Nanocomposites typically consist of nanometer-size materials (filler) in another material (matrix), and they are used for a variety of applications such as reinforced materials, sensors, optics, electronics, catalysis, etc. Among the various methods to synthesize nanocomposites, in-situ fabrication of polymer-metal nanocomposites have some advantages over the ex-situ one to realize the uniform dispersion of synthesized nanoparticles in the polymer matrix. The well-known techniques for the in-situ fabrication are the chemical reduction, photo reduction, microwave reduction, and thermal reduction. Recently we have developed a simple and efficient alternative. Our method utilizes a CO₂ laser, and its role is to promote the reduction of the precursor (typically metal salt) of metal nanoparticles in the polymer matrix. The main finding is that several to a few tens of seconds are sufficient to synthesize the polymer-metal nanocomposite films with the CO₂ laser at a very modest laser power (0.4~1 W).

The fabrication procedure is as follows: The mixture of the polymer solution (polyvinyl alcohol (PVA)) and the solution of silver nitrate (AgNO₃) is cast on a cover glass and then spin-coated to prepare the AgNO₃-PVA film. After drying the AgNO₃-PVA film in air the film is irradiated by the CO₂ laser for several seconds at the laser power of 0.4~1W (corresponding to the film temperature of 80~175 °C) to obtain the Ag-PVA nanocomposite film. The optical and morphological properties of the fabricated Ag-PVA nanocomposite films at the laser power of 1 W and 0.5 W are presented in Figs. 1(a) and 1(b). Clearly, not only the irradiation time but also the laser power strongly influences the optical property of the synthesized nanocomposite film. Namely, when the laser power is moderately high (1 W) only 10 sec

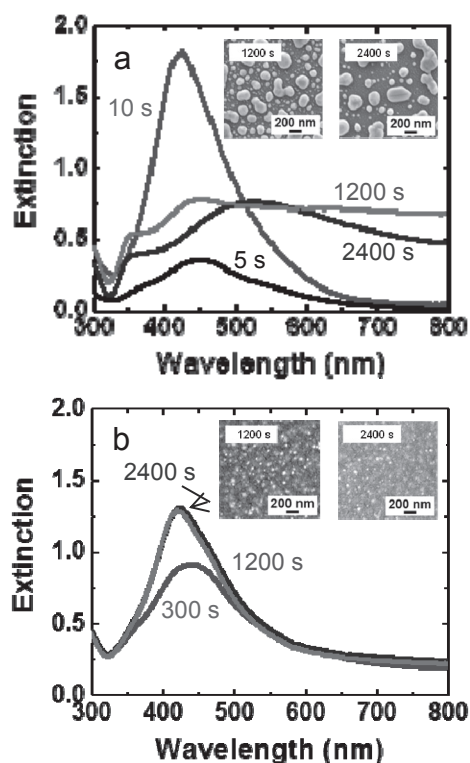


Fig. 1 Optical spectra of the synthesized Ag-PVA nanocomposite films by the various irradiation times at the laser powers of (a) 1 W and (b) 0.5 W. Insets in each panel show the SEM images. Concentration of AgNO₃ is 4.9 wt%

irradiation is sufficient to induce significant number of Ag nanoparticles in the polymer matrix, and the irradiation time longer than this results in the severe aggregation, as the broadening of the resonance width implies. The SEM images shown in the inset of Fig. 1(a) confirm this interpretation. When the laser power is low (0.5 W), however, the behavior is very different. The synthesis of Ag nanoparticles is slow at this laser power, and it takes as much as 1200 sec irradiation to complete the reduction. The irradiation time longer than this does not lead to the aggregation at this laser power, as we can infer from the optical spectra presented in Fig. 1(b). The SEM images in the inset of Fig. 1(b) confirm this interpretation. This is because the mobility of the synthesized small Ag nanoparticles is very low at the laser power of 0.5 W and hence they cannot meet another nanoparticles nearby to aggregate. Now we prepare the lower (1/4) concentration of AgNO₃ to prepare the AgNO₃-PVA

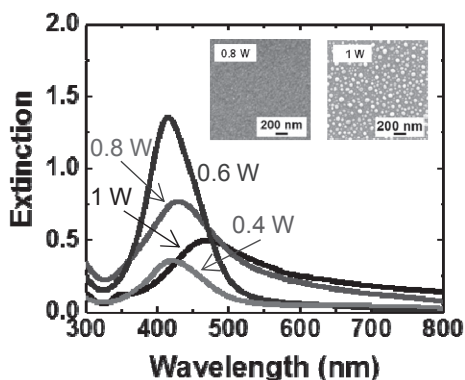


Fig. 2 Optical spectra of the synthesized Ag-PVA nanocomposite films by 1200 s irradiation at the laser powers of 0.4~1 W. Inset shows the SEM images. Concentration of AgNO_3 is 1.2 wt%, i.e., 1/4 of those used for Fig. 1.

films, and synthesized the Ag-PVA nanocomposite films by the 1200 sec irradiation at the various laser powers. The results are summarized in Fig. 2. Use of lower concentration of nanoparticle precursor results in the smaller nanoparticles even after the 1200 sec irradiation at the laser power of 1 W, because the synthesized small Ag nanoparticles cannot meet others to aggregate even under the high mobility at 1 W. The underlying mechanism for this is that the number density of synthesized Ag nanoparticles is significantly lower than the case of 4.9 wt% AgNO_3 concentration (Fig. 1(a)).

These results imply that the size-controlled synthesis of polymer-metal nanocomposite films is possible by the choice of not only the laser irradiation time but also the laser power and the concentration of nanoparticle precursor.

3. Tuning the surface plasmon resonance of laser-induced nanostructures in Ag films

Metallic nanostructures are frequently used to manipulate the interactions with light, and indeed they have proved their usefulness for biosensors, photovoltaic devices, energy harvesting, plasmonics, etc. In most cases surface plasmon resonance (SPR) plays an important role. Naturally, how to fabricate nanostructured metallic films is a very important issue, and many techniques have been developed for that. Recently we have demonstrated that the irradiation of a non-focused CO_2 laser beam with a power density of 4~6 W/cm^2 to a 5 nm Au film on a glass substrate for several seconds is sufficient to induce Au nanostructures. How it works for thin Ag films is an interesting question, since they are also frequently used for many applications. Recalling that the melting points and masses of Au and Ag are different we expect the different behaviors during the formation of laser-induced nanostructures. In Figs. 3(a) and 3(b) we show the optical spectra of 5 nm Ag films after the 5 sec~2 min irradiations at the laser power of 2 and 3 W, respectively. The shift of the SPR peak is

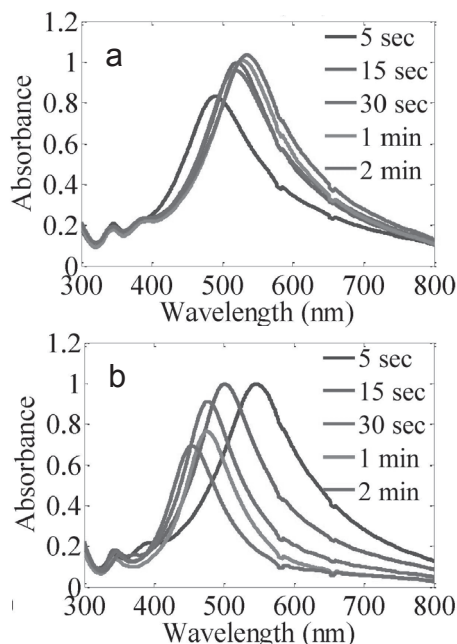


Fig. 3 Optical spectra of the 5 nm Ag films at the laser power of (a) 2 W and (b) 3 W.

more significant at the laser power of 3 W, and the resonance position shifts from 548 nm to 452 nm, i.e., tunability of 96 nm is easily obtained. In contrast when Au film is employed even the SPR is not visible at the laser power of 3W. Au film requires at least 4 W for the SPR to be visible. If we increase the laser power up to 5 W even more interesting phenomena are observed in 5 nm Ag films, and the results are summarized in Fig. 4. Very surprisingly, the irradiation center becomes almost transparent, and there are indeed almost no Ag nanoparticles left there. As it goes off from the irradiation center, however, more nanoparticles are observed up to some point where the laser power is sufficient to induce nanostructures. These puzzling results can be understood in terms of atomic diffusion once we recall that the mass of Ag is about half of Au and the melting point is about 100 °C lower than that of Au.

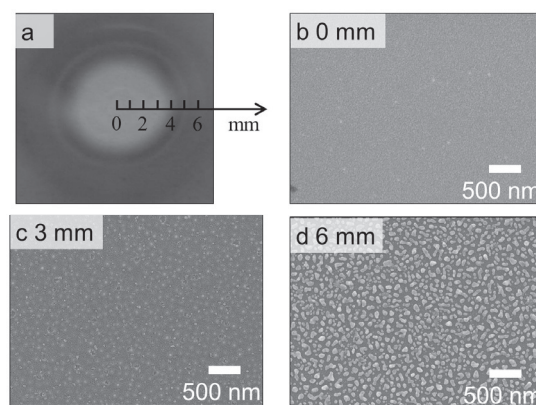


Fig. 4 (a) Photo of the irradiated 5 nm Ag film. SEM images of the film at (b) 0, (c) 3, and (d) 6 mm from the irradiation center. Laser power and irradiation time are 5 W and 10 min.

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Advanced Energy Structural Materials Research Section

A. Kimura, Professor
 K. Morishita, Associate Professor
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1. Introduction

Materials R&D is essential for safe and efficient operation of advanced nuclear energy systems in the near future. This section takes up a mission of materials R & D for advanced nuclear energy systems such as fusion reactors and Gen-IV nuclear systems. Current main researches are as follows:

(1) ODS steels R&D for ATF claddings: After Fukushima incident accident tolerant fuel (ATF) cladding R&D was proposed by DOE and the issues for materials R&D for ATF application have been discussed including resistance to corrosion/oxidation, strength and radiation tolerance. Among the candidate materials, FeCrAl-ODS steels were selected as most feasible material for ATF claddings and R&D of FeCrAl-ODS steels has been performed in this division as a national program to develop an innovative material with high performance.

(2) Structural materials integrity: Stress corrosion cracking susceptibility of structural materials in nuclear power plants has been examined for SUS316L and 310S by means of slow strain rate test in hydrogenated water (Fig.1). SUS310S is much more resistant to SCC indicating almost no occurrence of SCC, while SUS316L suffers a severe TGSCC in hot water dissolved with 1.4 ppm hydrogen at 340 °C.

(3) Multi-scale modeling: Radiation damage processes in nuclear materials take place at a wide variety of time and length scales. So-called the multiscale viewpoint is required to understand the processes. To do this, modeling effort has been made using several computational techniques complementarily such as molecular dynamics, ab-initio quantum calculations, kinetic Monte-Carlo, rate-equation theory analysis, FEM and CFD.

(4) Radiation damage mechanism of fission nuclear structural materials: For the sake of the highly efficient and safe operation of nuclear fission reactors, the mechanisms of irradiation embrittlement and stress corrosion cracking have been investigated. Small specimen test technique for evaluation of structural integrity has been developed towards extension of operation period of light water reactors.

2. Phase stability of oxide particles in ODS ferritic steels under ion-irradiation

Irradiation effects on hardness and phase stability were investigated for an FeCr(Y, Ti)-ODS ferritic steel strengthened by Y-Ti-O nano-particles after irradiation with 6.4 MeV Fe^{3+} at room temperature (RT) up to nominal damages of 2, 10 and 50 dpa. With increasing displacement damage up to 18 dpa, nano-sized oxide particles slightly shrank, while the corresponding number density drastically reduced by almost two orders of magnitude compared to that of before irradiation. It is considered that ballistic dissolution should be responsible for such reductions in the particle size and number density (Fig. 1). Dislocation loops consisting of $1/2\langle 111 \rangle$ type (> 80%) and $\langle 100 \rangle$ type were observed under weak beam dark field (WBDF) condition in the specimen irradiated to a nominal damage of 50 dpa. Although the oxide particles were almost completely dissolved, nanoindentation hardness measurements revealed that the hardening went up continuously with increasing displacement damage and estimated to be 1.63 ± 0.39 GPa by the Nix-Gao model at a nominal damage of 50 dpa.

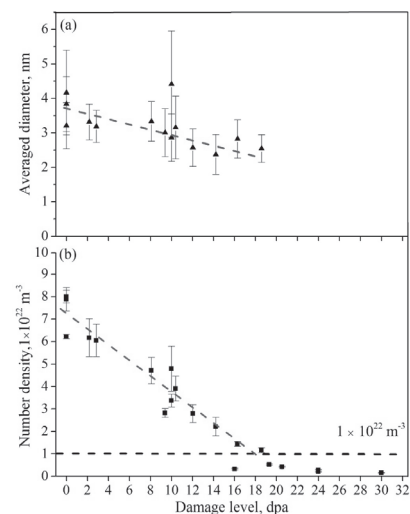


Fig. 1: Averaged diameter (a) and number density (b) of oxide particles as a function of dpa.

3. Structural integrity of a reactor pressure vessel using 3D CFD & FEM based probabilistic PTS analysis for optimizing maintenance strategy

The structural integrity of a reactor pressure vessel (RPV) is important for keeping the safety of a nuclear power plant. When the emergency core cooling system (ECCS) is operated and the emergent coolant water is injected into the RPV due to a loss-of-coolant accident (LOCA), the pressurized thermal shock (PTS) loading takes place. With the neutron irradiation, PTS loading may lead an RPV to fracture. Therefore, it is necessary to evaluate the performance of RPV during PTS loading to keep the reactor safety.

In the present study, optimization of RPV maintenance is considered, where two different attempts are made to investigate the RPV integrity during PTS loading by employing the deterministic and probabilistic methodologies. For the deterministic integrity evaluation, three-dimensional computational fluid dynamics (3D-CFD) and finite element method (FEM) simulations are performed, and stress intensity factors (SIFs) are obtained as a function of crack position inside the RPV. As to the probabilistic integrity evaluation, a practically more useful spatial distribution of SIF on the RPV is calculated. By comparing the distribution thus obtained with the fracture toughness included as a part of the master curve, the dependence of conditional failure probabilities on the position inside the RPV is obtained. The conclusion is as follows;

- (1) In the deterministic evaluation, the center of the cold plume has the largest KI value, which is 31.4% greater than the minimum value.
- (2) In the probabilistic evaluation proposed here, the cold plume cooling effect is considered by using 3D CFD and FEM to obtain the conditional failure probability. The failure probability thus obtained could be practically more useful than that obtained by the conventional 1D analysis.
- (3) Using the conditional failure probability as an index, the priority of the inspection and maintenance for RPV integrity can be optimized.

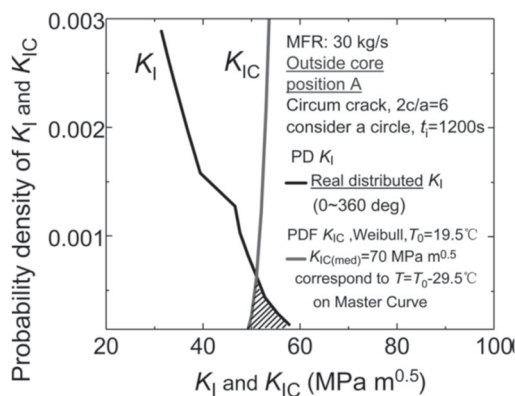


Fig. 3: An example of the probabilistic assessment considering plume cooling effect

4. Irradiation effects on a MoNbTaVW high entropy alloy

High-entropy alloys (HEAs) can be defined as solid solution alloys combined with more than five principal elements in equimolar or near equimolar percent. According to literatures, refractory high-entropy alloys (with bcc matrix) own superior high-temperature properties and have severer lattice distortion than the previous conventional alloys. Since much better high-temperature properties are required for the advanced nuclear systems, it is expected that they can be applied to the systems as a functional conversion material with unexpected high performance. However, few studies on the irradiation effects on HEAs has been reported and many issues of the irradiation effects on HEAs are still unknown. Recently, we focused on the ion-irradiation effects on MoNbTaVW alloy.

A HEA, MoNbTaVW, was produced with high purity (> 99.9%) elemental metals including tungsten, niobium, tantalum, vanadium and molybdenum by arc melting method. Ion irradiation was carried out using an ion accelerator, DuET (Fig. 3), in Kyoto University. After irradiation, the irradiation hardening was observed and the temperature dependence of irradiation hardening was clarified. Transmission electron microscope observation revealed that the irradiation hardening in MoNbTaVW alloy was due to the formation of a high number density of dislocation loops (Fig. 4).

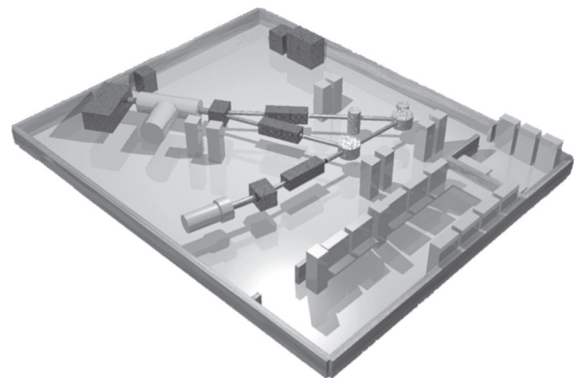


Fig. 3: Ion-accelerator (DuET)

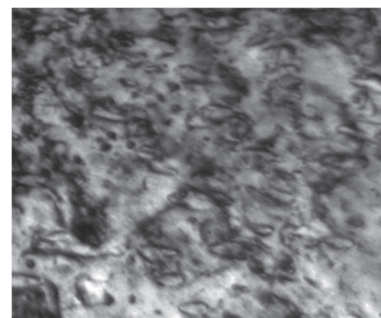


Fig. 4: A TEM micrograph of Fe-ion irradiated MoNbTaVW HEA upto 2 dpa at 773 K

Collaboration Works

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木村晃彦, FEI STU (スロヴァキア), IAEA-CRP, Pound robin test

木村晃彦, JRC European Commission- Petten, JRC-Institute for Energy and Transport, IAEA-CRP,

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木村晃彦, HZDR (ドイツ), IAEA-CRP, Pound robin test

木村晃彦, Karlsruhe Institute of Technology (KIT), Institute of Applied Materials (IAM) (ドイツ), IAEA-CRP, Pound robin test

木村晃彦, Australian Nuclear Science and Technology Organisation (オーストラリア), IAEA-CRP, Pound robin test

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Complex Plasma Systems Research Section

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1. Introduction

Magnetic nuclear fusion energy has some attractive features as a future option for the base-load electrical power source: (1) inherent safety features, (2) no long-life nuclear waste emission, (3) no greenhouse gas emission during the energy production, (4) huge energy density stored in the fuel source (~90 MWh/g for D-T fuel), (5) abundant source availability spreading all over the Earth, and (6) high nuclear proliferation resistance, in terms of both resources and weapons technologies. Among various issues to be overcome in physics and engineering fields, we have focused on the problems related to the plasma transport and magneto-hydrodynamics. Specifically, determination of a magnetic configuration that can efficiently confine high-density plasma at high temperature with a sufficiently long confinement time and developing diagnostics and control schemes for the high-temperature plasmas in such magnetic fields are regarded as crucial. In these respects, our research section investigates about heating and fuelling, confinement and diffusion mechanisms and their diagnostics in a magnetic plasma confinement device, named Heliotron J. Recent results of this section in FY2018 are as follows:

2. Application of Portable Near-Infrared Spectrometer to Heliotron J Plasma Diagnostics

The application of conventional passive spectroscopy to fusion plasma research differs depending on wavelength. In the vacuum ultraviolet (VUV) regime, there are many important impurity lines of highly charged states, but the complexity of these measurement systems typically implies a high cost. In addition, line blending of high-Z impurity sometimes causes problem in the quantitative analysis. In near-ultraviolet (NUV) to visible (VIS) regions, spectroscopic system utilizing a variety of optical components and detectors have been widely used to acquire spectra from hydrogen/deuterium or light impurities such as atomic helium. These species are particularly important in the divertor/edge region—emission from low principal quantum number (n) states i.e., H_α ($n = 2 - 3$; 656 nm), H_β ($n = 2 - 4$; 486 nm) for ionizing plasmas, and the emission from high- n Rydberg states for recombining plasma

(divertor detachment), where the series limit lies in the UV regime (360 nm @ H I, 345 nm @ He I 3D)^{1,2}. It may be difficult to perform these types of measurements in larger facilities because the transmittance of an optical fiber decreases rapidly below 400 nm.

In this respect, we have begun to apply a simple and portable monitoring system to acquire the near-infrared (NIR) spectra of Heliotron J plasmas in an attempt to survey the brightness of an unknown/unused line in the spectra acquired for the NIR region, and to investigate black-body radiation from the wall. Calibration of the VIS and NIR spectrometers were performed using the shorter and longer sides of the spectrum tungsten halogen lamp.

In the preliminary data, we have measured without considering the second-order diffraction component in the calibration factor – line spectra can be removed from the fitting region (see Fig. 1).

Characteristic continuum spectrum was observed in a certain plasma condition – electron cyclotron heated (ECH) plasma with relatively low line-averaged density of about $6 \times 10^{18} \text{ m}^{-3}$. The calibrated spectrum was well fitted by Planck's black-body radiation formula, and the temperature was determined to be about 2400 K as shown in Fig. 2. It was for the first time in Heliotron J identified that this spectrum was corresponded to the hot spot caused by super-thermal electrons accelerated by ECH.

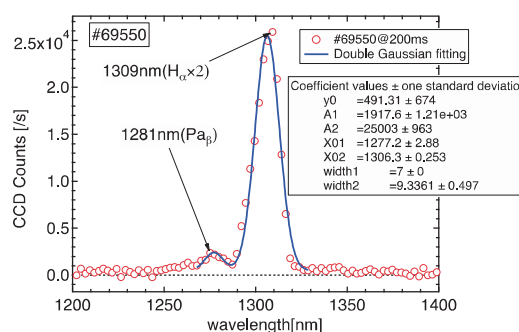


Fig. 1 Typical NIR line spectra. The second order Balmer-alpha line (656 nm) was detected side by side with the Paschen-alpha line (1281 nm) [1].

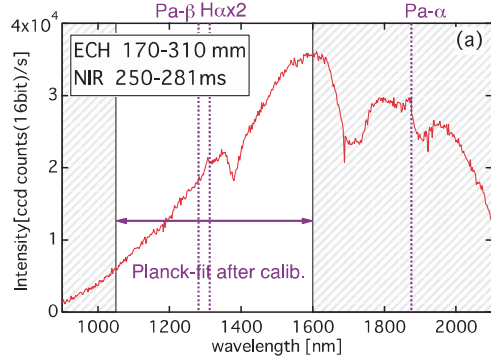


Fig. 2 Continuum spectra from #11.09 port appear in the latter period, 250–281 ms, of the ECH discharge in the interval 170 to 310 ms. [shot #69209]. After intensity calibration, the spectra was well fitted to the black-body radiation described by the Planck formula of about 2400 K. Wavelength of bright H I lines as indicated[1].

[1] Kado *et al.*, Rev. Sci. Instrum. 89, 10D129(2018).

3. Impact of ECH on fast-particle-driven MHD instabilities in Helical Plasmas

Fast particle (FP)-driven magnetohydrodynamics (MHD) instabilities enhance anomalous transport and/or induce the loss of fast particle including alpha particles in a D-T fusion reactor. Since redistribution and exhaust of alpha particles lead to reduction of fusion gain Q and damage of first wall, to establish methods of stabilization and/or control of FP-driven MHD instabilities is required for the D-T fusion reactor. However they have not been established yet. The electron cyclotron heating (ECH) and/or the electron cyclotron current drive (ECCD) are candidate methods to control the FP-driven MHD instabilities because ECH/ECCD may be an ideal tool to control the "modes" since they can provide highly localized EC waves with a known location and good controllability. FP-driven MHD instabilities such as energetic particle modes (EPMs) and Alfvén eigenmode (AEs), are observed in tangential NBI-heated plasmas of stellarator/heliotron devices such as Heliotron J, TJ-II and LHD. We studied ECCD effects on FP-driven MHD instabilities in above mentioned three devices based on the similarities and differences, e.g. magnetic shear, toroidal field period. In a low shear device, the increasing continuum damping of the modes by increase in magnetic shear due to EC-driven plasma current is effective. In a high shear device, the modification of shear Alfvén spectrum is more important effect than continuum damping.

The FP-driven MHD instabilities are also suppressed by both on- and off-axis ECH in the TJ-II plasmas. On the other hand, some FP-driven MHD

instabilities are stabilized and the others are destabilized by ECH depending on ECH power and deposition location in the Heliotron J and LHD plasmas.

In Heliotron J plasmas, we can scan heating power position and power. We observed both stabilization and destabilization of FP-driven MHD instabilities in the ECH power, deposition and magnetic configuration scan experiments. ECH injection power is changed from 114 kW to 282 kW and deposition is

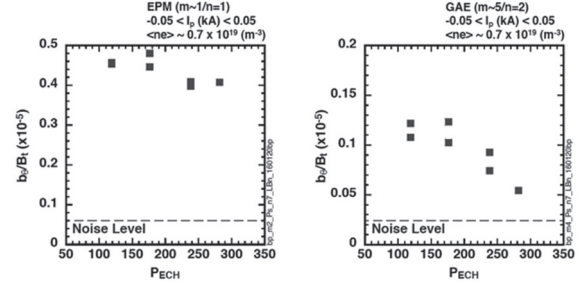


Fig. 3, Dependence of EPM and GAE amplitude on ECH injection power in Heliotron J plasmas.

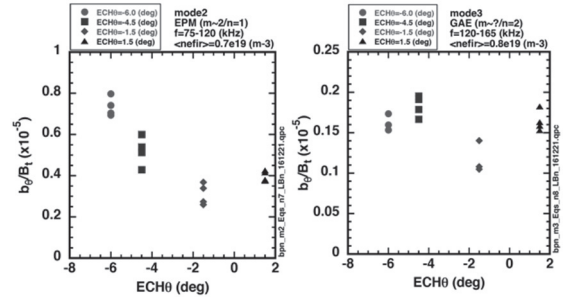


Fig. 4, Dependence of EPM and GAE amplitude on ECH deposition in Heliotron J plasmas.

adjusted to magnetic axis (on-axis), and the parallel refractive index N_{\parallel} is fixed to 0.0 for reduction of ECCD effect on the observed modes. Figure 3 shows the dependence of EPM and GAE amplitude on ECH injection power in Heliotron J. The EPM and GAE amplitude is slightly decreased and clearly decreased with increasing ECH power when on-axis ECH condition. According to linear theory of growth rate of mode, increasing electron temperature leads the increasing growth rate of mode due to the increasing fast ion beta $\langle \beta_f \rangle$. Since the local pressure gradient of fast ion can contribute the destabilization of FP-driven MHD instabilities, we scanned the ECH deposition location in Heliotron J, as shown in Fig. 4. Here, the deposition location is controlled by changing the injection angle of EC wave. The GAE amplitude decreases with increasing ECH power for on-axis ECH. When ECH deposition is close to the GAE location $r/a \sim 0.6$, the GAE amplitude is larger than that for on-axis ECH. These dependences indicate that both the change of fast ion profile by ECH through the change of electron density and temperature, and/or the collisional damping due to trapped fast electrons may affect the AE stability.

Collaboration Works

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Clean Energy Conversion Research Section

Ryuta Kasada, Visiting Professor
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1. Introduction

Beryllium is a very light metal with atomic number 4 and is known to have excellent properties such as high melting point, high rigidity, and high thermal conductivity. Currently, beryllium and its intermetallic compounds are used in a wide range of fields, such as structural materials in the aerospace industry, electronic components such as mobile phones, and X-ray transparent windows in medical equipment. In addition, in nuclear fusion reactors, which are expected as a new clean energy source, by utilizing excellent nuclear properties, they are used as plasma facing materials and neutron multipliers.

When beryllium compounds are used at high temperatures, the chemical stability at high temperatures is an important characteristic. When used in a fusion reactor, there is a concern about the generation of hydrogen that accompanies steam oxidation during a loss of coolant accident. Currently, beryllide which is a compound composed of beryllium and transition metal are being developed to suppress the high-temperature oxidation reaction. In the development of such new materials, microscopic observation with a scanning electron microscope and phase analysis by X-ray emission is one of the essential methods. However, conventional laboratory-level methods have made it difficult to analyze the X-ray emission spectrum in detail and to analyze the chemical state because light element beryllium has extremely low X-ray emission efficiency and low energy in soft X-ray range.

In this study, we analyzed beryllium, its intermetallic compounds, and their oxide films using a soft x-ray emission spectrometer (SXES) recently developed for electron probe microanalyzers (EPMA). Previously, the author successfully used this novel method to obtain the chemical state mapping of a simulated B₄C control rod after a severe accidental condition [1]. The paper of the present report has been just accepted as ref. [2].

2. Experimental procedure

The EPMA-SXES in IAE, Kyoto University, JEOL JXA-8500F with JS200N can measure low energy (100 to 112 eV) soft X-ray emission spectrum from beryllium with high energy resolution (Fig.1).

Beryllides, namely Be₁₂Ti and Be₁₂V, manufactured and processed by National Institutes for Quantum and Radiological Science and Technology (QST) [3] are used for the measurements. We

simulated the theoretical waveform of soft X-ray emission by electronic structure calculation based on density functional theory (DFT) and identified the emission peak.

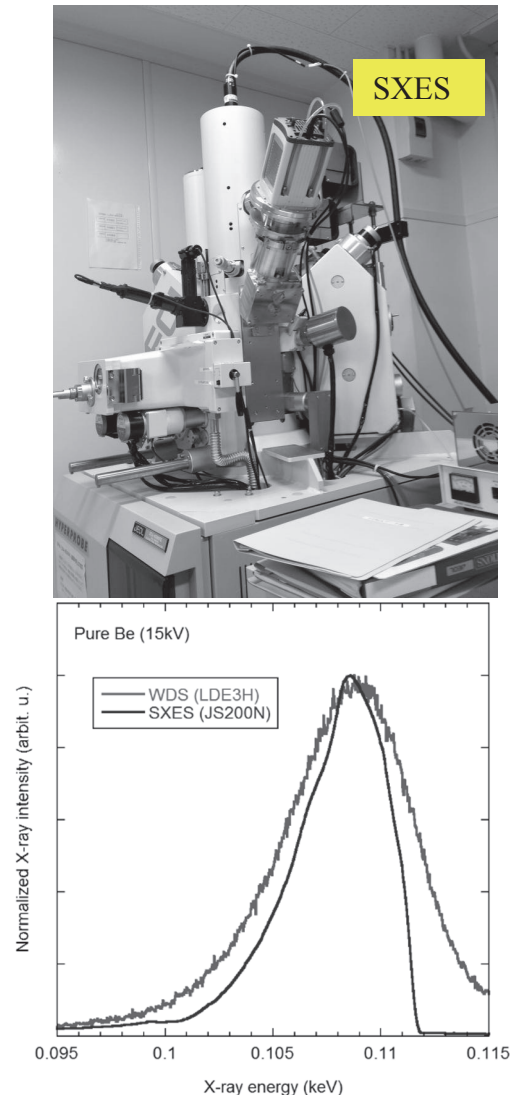


Fig.1 EPMA-SXES in N1 building of IAE and the obtained Be-K emission spectra.

3. Results and discussion

Figure 2 shows the experimental soft x-ray spectra of pure beryllium and beryllium compounds (Be₁₂Ti and Be₁₂V) and oxide phase (beryllia: BeO) obtained by EPMA-SXES. This is the first experimental result to observe the changes in the electronic state when beryllium becomes a compound with the transition metal. These soft X-ray emission spectra are in good agreement with the theoretical density of states

obtained in the electronic state calculation, indicating that the electronic structure has been changed by the hybridization with the transition metal's electron orbitals.

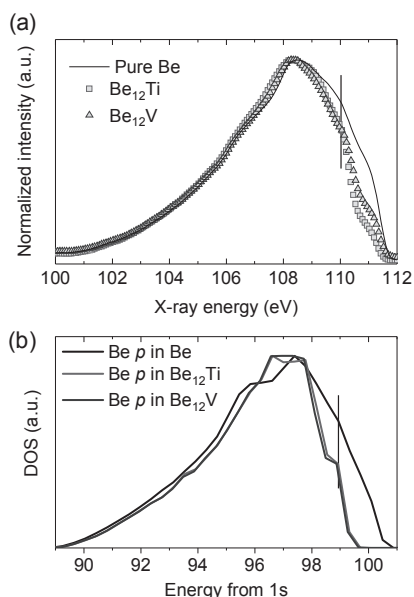


Fig. 2 Direct comparison of the Be-K spectra of Be, Be_{12}V , and Be_{12}Ti using the SXES with the convoluted DOSs of Be 2p by the DFT calculations. Black solid lines represent the shoulders of Be_{12}Ti and Be_{12}V [2].

It was also found that the beryllia formed as an oxide film when the beryllium compound is oxidized has its soft X-ray peak shifted to the lower energy side by about 4 eV as compared to the beryllide. Using this

large chemical shift and electronic structure information, we analyzed the chemical state distribution of steam oxidized beryllium compounds (Fig. 3). From the elemental and chemical state mapping, it can be confirmed that a thin oxide film is formed on the surface by steam oxidation of beryllium compound (Be_{12}V), which was single phase before the experiment, and a Be_2V phase containing a large amount of vanadium is formed.

4. Conclusion

This study clarified the valence electron structure of beryllium compounds and succeeded in analyzing the chemical state distribution. This approach is effective for other light elements such as lithium, beryllium and boron, and is expected to contribute in various fields that require micro analysis of light elements, especially energy materials. In future research, we hope to contribute to the development of more sophisticated beryllium compounds by both experimental and computational approaches.

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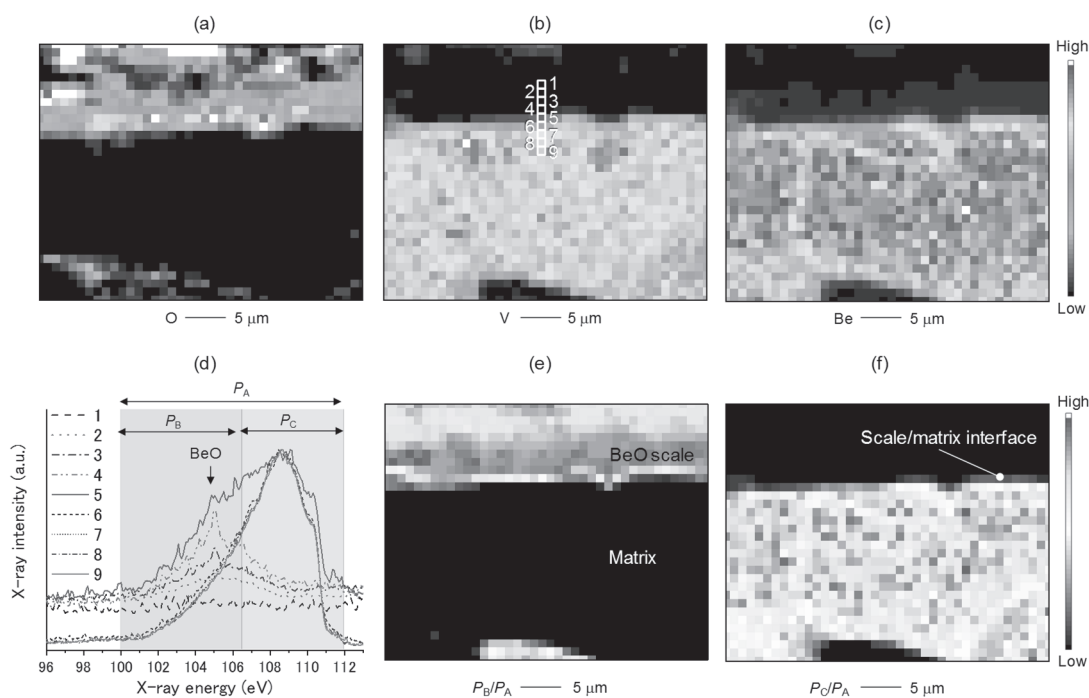


Fig. 3 SXES element mappings of (a) O, (b) V, and (c) Be from the steamed Be_{12}V specimen. (d) The Be-K spectra by the SXES from nine measuring area. Reconstructed images by calculating peak area ratio of (e) P_B/P_A and (f) P_C/P_A , showing chemical state mappings of BeO and Be_{12}V . In panel (d), nine SXES spectra were obtained from the area surrounded by white squares shown in panel (b) [2].

Clean Energy Conversion Research Section

Takeshi Mori, Visiting Associate Professor
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1. Introduction

Flow cytometry enables evaluation of the relative amount of antigen proteins in cells with single-cell resolution and has been used in the diagnosis of cancers as well as basic research in cell biology. Antigen proteins of interest are labeled by fluorophore-modified antibodies to detect the presence of antigen proteins on cells. Although flow cytometry is a useful technology for the detection of cellular antigens, it lacks sensitivity. For the fluorescence signal resulting from the fluorophore-modified antibody to exceed the autofluorescence signal of the cells, typically a few thousand antigen protein molecules per cell are required to be detected by flow cytometry.¹ However, antigen proteins of interest are often expressed at levels lower than the detection limit.

To improve the detection limit of flow cytometry, researchers have developed methods to increase the number of fluorophores per antigen on a cell. One of the representative approaches is based on amplification of the fluorescence signal via an enzymatic reaction.¹⁻³ This method is called catalyzed reporter deposition (CARD), in which horseradish peroxidase (HRP) modified on antibodies is used as an enzyme to covalently deposit tyramide-modified fluorophores to a cell. Using this method, antigens with low copy numbers that are difficult to detect by conventional fluorophore-modified antibodies were successfully detected.

2. CARP Method

If the signal amplification method can be expanded to other enzymes, it will allow the simultaneous detection of more than one antigen with low expression levels in a single cell. Herein, we describe our attempts to expand the signal amplification method to alkaline phosphatase (AP), which is another popular enzyme used in bioanalysis such as enzyme immunoassays and immunohistochemistry because of the inherent advantages of AP including its high stability and activity and small size. Detection mechanism is shown in Figure 1A. A fluorescent substrate for AP is composed of a hydrophobic alkyl chain, a hydrophilic phosphate, and a fluorophore. The antigen protein on the target cell surface is labeled with a ternary complex of antibody/streptavidin/AP, and then the substrate is dephosphorylated by AP to increase its hydrophobicity and cationic charge of the substrate. The plasma membranes of mammalian cells are known to have negative membrane potentials,

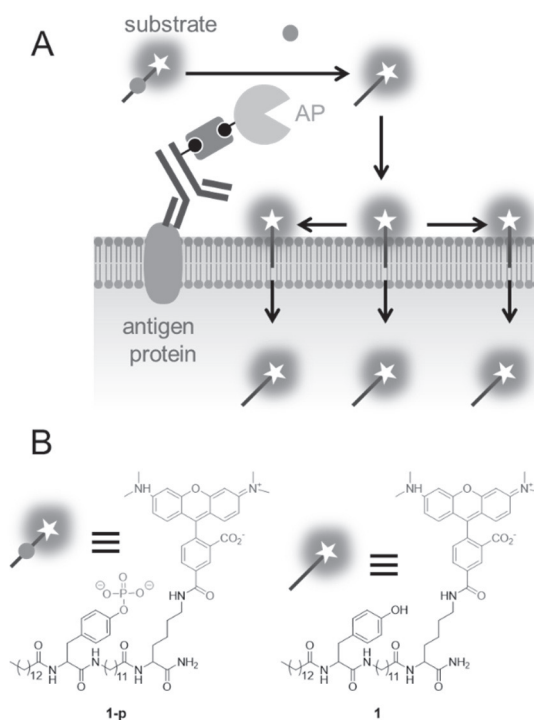


Fig.1: Mechanism of fluorescence signal amplification by CARP method (A), and the chemical structures of substrates (B).

which enable the penetration of hydrophobic and cationic molecules to accumulate in the cytosol. Thus, the dephosphorylated substrate penetrates the cell membrane to accumulate in the cytoplasm, which results in amplification of fluorescence signal of the target cell. We named our AP-based method the catalyzed reporter penetration (CARP) method. Figure 1B shows the structure of substrate 1-p, which contains a hydrophobic alkyl chain with a phosphorylated tyrosine in the middle and a membrane permeable fluorophore (tetramethyl rhodamine) on the terminus.

Because the substrate was designed to be hydrophobic, methyl β -cyclodextrin (M- β -CD) was used to assist distribution of the substrate from the aqueous phase to the cell membrane. M- β -CD is well known to solubilize hydrophobic molecules by the formation of inclusion complexes, which facilitates the transfer of the hydrophobic molecule from aqueous media to the cell membrane. We examined the effect of M- β -CD on the staining of cells with 1. As shown in Figure 2A, M- β -CD strongly enhances the staining of cells. Dephosphorylated substrate 1

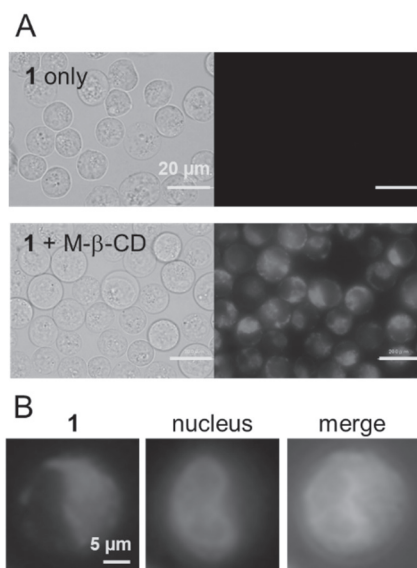


Fig.2: (A) Staining of K562 cells by **1** (5 μ M) with or without M- β -CD (5 mM). (B) Magnified image of a single cell stained by **1** with M- β -CD. The nucleus was stained by Hoechst 33342.

stained the cytoplasm except for the nucleus (Figure 2B), indicating the binding of **1** to the cytoplasmic membrane fraction.

On the surface of mammalian cells, endogenous APs are known to exist as membrane proteins. The activity of these endogenous APs must be suppressed to exclude the contribution of the endogenous APs in the dephosphorylation reaction of substrate **1-p**. We found that gentle fixation by using 4% paraformaldehyde/0.1% glutaraldehyde, which is reported by Luby-Phelps et al., was the most suitable condition to inactivate the cell surface APs.⁴ JY25 cells were strongly stained by **1-p** because of the dephosphorylation by the endogenous APs. However, the fixed cells displayed only a negligible fluorescence signal. Additionally, JY25 cells fixed using this method did not show loss of binding efficacy to the anti-CD20 antibody targeted to the cell surface antigen protein, CD20.

Finally, we demonstrated detection of the antigen proteins by using the CARP method. We selected CD20 as the target as is a representative biomarker of B cell-derived cancer cells. JY25 cells were chosen as the CD20 positive cells. After the inactivation of the endogenous APs by fixation or inhibition with pervanadate, each cell was labeled with a corresponding biotinylated antibody/streptavidin complex, and then the biotinylated AP was modified onto the antibody as depicted in Figure 1A. The resulting cell was stained with substrate **1-p** using the enzymatic reaction for 30 min at 37 °C and was subjected to the flow cytometric analysis. For comparison purposes, cells were also conventionally labeled using a fluorophore-modified antibody. Figure 3A shows the fluorescence images of JY25 cells

labeled using these two methods. The conventional labeling of JY25 cells with CD20 resulted in a fluorescence signal from the cell surface. In contrast, the CARP method resulted in the staining of the entire cytosol except for the nucleus. Figure 3B shows the flow cytometric detection of CD20. The fluorescence signal obtained by the CARP method was about five times higher than that from the conventional immunofluorescence method.

3. Summary

We successfully applied AP to the enzymatic amplification of the fluorescence signal from antigen staining of cells for flow cytometric analysis. Our fluorescent substrate **1-p** acquired membrane permeability in response to dephosphorylation leading to the staining of the entire cytoplasm. Treatment with pervanadate or gentle fixation of cells helped to inhibit endogenous APs to enable the dephosphorylation of the substrate specifically by the antibody-modified AP. Our AP-based CARP method is suitable for combination with the HRP-based CARD method to enable simultaneous detection of two independent antigens with low expression levels.

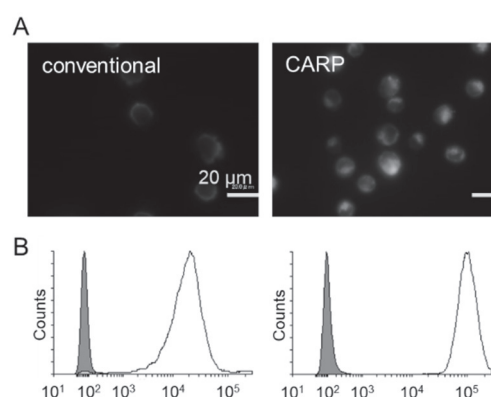


Fig.3: Detection of antigen proteins by using conventional immunofluorescence staining or the CARP method. Microscopic observation of JY25 cells expressing CD20 stained using two methods (A). Flow cytometric analysis of CD20 on JY25 cells (B) stained by immunofluorescence (left) and CARP method (right).

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Chemical Reaction Complex Processes Research Section

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1. Introduction

In this research section, we study on electrochemistry, materials science, genetic engineering and protein engineering. We also apply them to the developments of efficient solar silicon production processes, new secondary batteries and efficient bioethanol production processes.

In this fiscal year, we have researched an electrodeposition process of solar silicon, a potassium secondary battery using ionic liquids, and an efficient bioethanol production process using ionic liquids.

2. Production Process of Solar Silicon Using Molten Salt Electrodeposition

In the conventional industrial production process of crystalline Si solar cells, ingots of solar-grade Si (SOG-Si) are once prepared, and then they are sliced into wafers by diamond wire saws. This process has, however, several problems such as the large kerf loss and the complex process of cell production. If high-quality crystalline Si films are prepared directly on desired substrates at a low cost, a new production process of crystalline Si solar cells will be realized.

From this background, we proposed a new electrodeposition process of crystalline silicon [1]. In this process, molten KF–KCl is used as an electrolyte and SiCl₄ as a silicon source. We selected the molten KF–KCl because both KF and KCl are highly soluble to water. Thus,

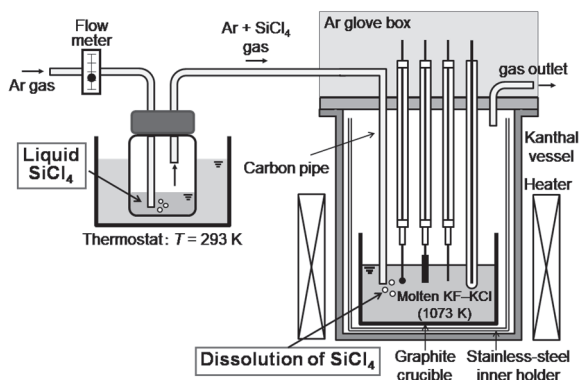


Fig. 1. Schematic drawing of the experimental apparatus for the introduction of SiCl₄ by a vapor transport method and electrodeposition of Si [2].

the adhered salt is easily removed by water washing. Moreover, high purity SiCl₄, which is commercially available at a low cost, is able to be used as a silicon source [1,2].

First, we checked if SiCl₄ gas reacts with F⁻ ions to produce SiF₆²⁻ ions by using the experimental setup shown in Fig. 1 [2]. After introduction of SiCl₄ into molten KF–KCl by a vapor transport method, the production of SiF₆²⁻ ions was confirmed by cyclic voltammetry. The dissolution efficiency of SiCl₄ was calculated to be 95% from the peak current density of Si deposition.

Fig. 2 shows surface and cross-sectional SEM images of a Si film obtained on a graphite plate at 45.6 mA cm⁻² for 60 min at 1073 K after the introduction of SiCl₄ (2.37 mol%). A dense and smooth crystalline Si film was obtained with nearly 100% current efficiency. A photoelectrochemical test at room temperature demonstrated that the Si film is a p-type semiconductor, indicating its applicability to photovoltaics.

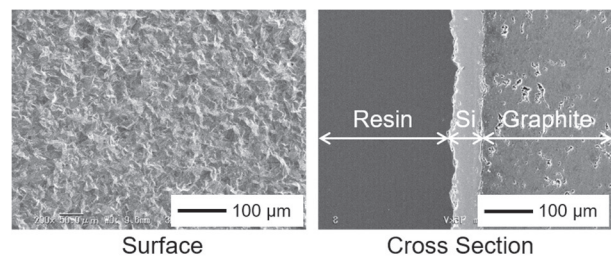


Fig. 2. SEM images of the Si film obtained on a graphite plate at 45.6 mA cm⁻² for 60 min in molten KF–KCl (KF:KCl=60:40 mol%) at 1073 K after the introduction of SiCl₄ (2.37 mol%).

3. Development of Ionic Liquid Electrolytes for Potassium Secondary Batteries

The demands for electrical energy storage devices are increasing due to the spread of renewable energies such as solar and wind power. Although conventional lithium-ion batteries exhibit high energy densities, the limited lithium and cobalt resources potentially lead to the price increase in the future, and the organic solvent-based electrolytes carry the risk of ignition accidents.

Under these circumstances, we proposed potassium secondary batteries with ionic liquid electrolytes as a novel battery system for the following reasons. Firstly, potassium resources are abundant in the crust and seawater as with sodium. Secondly, ionic liquids show high safety such as negligible volatility and non-flammability. Thirdly, for many kinds of ionic liquids (molten salts), the potassium-based electrolytes possess wider electrochemical windows than the lithium and sodium counterparts, which naturally leads to higher operating voltages for potassium secondary batteries.

We firstly selected FSA-based electrolytes (FSA = bis(fluorosulfonyl)amide) due to their high ionic conductivities, and investigated physicochemical properties of $M[\text{FSA}]-[\text{C}_3\text{C}_1\text{pyrr}][\text{FSA}]$ and $M[\text{FSA}]-[\text{C}_2\text{C}_1\text{im}][\text{FSA}]$ ionic liquids ($M = \text{K}, \text{Na}, \text{Li}$; $\text{C}_3\text{C}_1\text{pyrr} = N\text{-methyl-}N\text{-propylpyrrolidinium}$; $\text{C}_2\text{C}_1\text{im} = 1\text{-ethyl-3-methylimidazolium}$). As shown in Fig. 3, ionic conductivities of potassium-based electrolytes are higher than those of sodium-based ones and are comparable to those of lithium-based ones. The imidazolium-based electrolytes show higher ionic conductivities than those of pyrrolidinium-based electrolytes. Moreover, as the results of electrochemical measurements, potassium-based electrolytes possess wider electrochemical windows than those of lithium and sodium counterparts. Therefore, $\text{K}[\text{FSA}]-[\text{OCat}][\text{FSA}]$ ($\text{OCat} = \text{C}_3\text{C}_1\text{pyrr}$ or $\text{C}_2\text{C}_1\text{im}$) ionic liquids are good candidates as electrolytes of potassium secondary batteries.

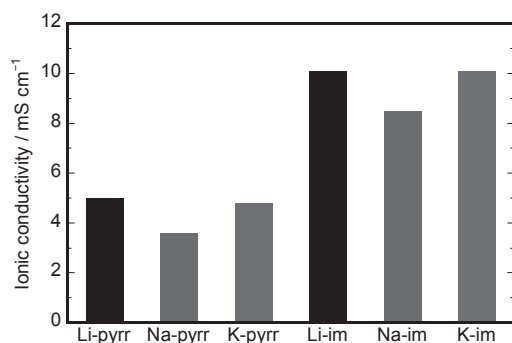


Fig. 3 Ionic conductivities of $M[\text{FSA}]-[\text{OCat}][\text{FSA}]$ ($M = \text{Li}, \text{Na}, \text{K}$; $\text{OCat} = \text{C}_3\text{C}_1\text{pyrr}$ or $\text{C}_2\text{C}_1\text{im}$) at 298 K. Molar fraction of $M[\text{FSA}]$ is 0.20 [3].

4. Efficient Bioethanol Production from Cellulose Using Ionic Liquid

Cellulose is the most abundant natural compound among woody biomass and expected to be a source for biofuel such as bioethanol. However, rigid crystal structure of cellulose makes it difficult to hydrolyze to glucose. Recently, pretreatment with ionic liquid was found to be effective for hydrolysis of cellulose by cellulase.

In this fiscal year, bagas was used as a cellulose containing biomass. At first, bagas was hydrolyzed with cel-

lulase and xylanase after treatment of ionic liquid, 1-Butyl-3-methylimidazolium Chloride ($[\text{Bmim}]\text{Cl}$) or Choline acetate ($[\text{Cho}][\text{OAc}]$). Then, a recombinant xylose-fermentation yeast strain (named AA) or a pentose phosphate pathway enhanced AA strain (named 4P) was used to ferment hydrolyzed solution of bagas. As shown in Figs. 4 and 5, ethanol was fermented under all of the conditions although fermentation efficiency and rate was slightly different between each of the ionic liquids and the strains.

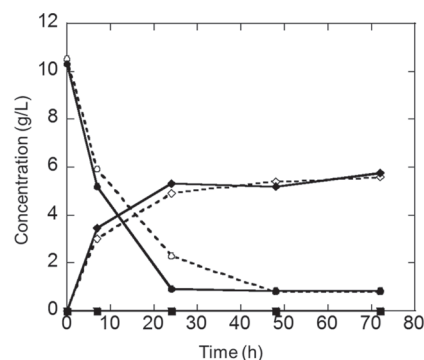


Fig. 4. Ethanol fermentation of hydrolyzed solution treated with $[\text{Bmim}]\text{Cl}$. AA: dashed line, 4P: solid line, glucose: circle, xylose: square, ethanol: rhomboid.

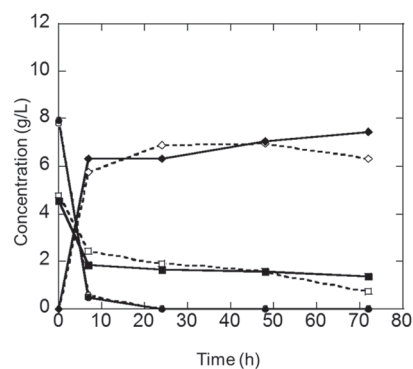


Fig. 5. Ethanol fermentation of hydrolyzed solution treated with $[\text{Cho}][\text{OAc}]$. AA: dashed line, 4P: solid line, glucose: circle, xylose: square, ethanol: rhomboid.

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Molecular Nanotechnology Research Section

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1. Introduction

Nanotechnology is essential for highly efficient energy use. Our group studies the basics of assembling small molecules into the advanced materials and devices in energy sector with high efficiency. We have already developed several unique techniques which are totally new molecular assembling methodology such as 'electro-chemical Epitaxial Polymerization' and 'Two-Zone Chemical Vapor Deposition (2Z-CVD)' which enable to produce molecular wires on metal surface from small molecules. By using these techniques, organic electronic devices such as field-effect transistors and organic solar cells will be developed.

Recently, we demonstrate a new concept of 'conformation-controlled surface catalysis'; the two-zone chemical vapor deposition of the 'Z-bar-linkage' precursor, which represents two terphenyl units are linked like a 'Z', exhibiting flexible geometry that allows it to adopt chiral conformations with height-asymmetry on a Au(111) surface, results in the efficient formation of acene-type graphene nanoribbons (GNRs) through optimized cascade reactions. These cascade reactions on surface include the production of self-assembled homochiral polymers in a chain with a planar conformation, followed by efficient stepwise dehydrogenation via a conformation-controlled mechanism. Our proposed bio-inspired concept analogous to the biological catalyst, enzyme, is useful for the fabrication of new nanocarbon materials.

Main research achievements in Molecular Nanotechnology Research Section in 2018 are described below.

2. Production of wider graphene nanoribbons produced by inter chain fusion of polyphenylenes via 2-Zone CVD

Graphene nanoribbons (GNRs), quasi-one-dimensional graphene strips, have shown great potential for electronics, optoelectronics, and photonics. These properties strongly depend on width and edge structure of them. Therefore, precisely controlled width and edge structure are required for desired properties. Bottom-up synthesis of GNRs is a

one of suitable method to satisfy these requirements because of definition of their edge structures and widths by the shape of precursors. Atomically precise synthesis of armchair-edged GNRs have already been achieved under ultra-high vacuum (UHV) condition. However, given GNRs in this method were low yield and density was still low. Therefore, it was difficult to develop organic electronic devices with them. To develop devices, high-yield fabrication of assembled GNR films, isolation, and device fabrication are required.

We have developed 2Z-CVD to produce densely-packed, parallelly-aligned self-assembled GNRs on Au(111) under low vacuum condition from halogenated polycyclic aromatic hydrocarbon (PAH) precursors. This technique successfully produced a series of armchair-edged GNRs in high yield. Attractive features of this method originate from an independent temperature-control of radical-generation process (zone 1) and the growth process (zone 2), which afforded GNRs in high yield without using UHV conditions. The precursor was sublimated to the Au(111) substrate in zone 2 by passing through zone 1 in a quartz tube. The mechanism is supposed to involve radical generation in zone 1, polymerization of the radicals on the Au(111) substrate in zone 2, and subsequent dehydrogenation to form GNRs.

On the other hand, according to theoretical calculations, armchair-edged GNRs (AGNRs) with widths less than 10 nm should have a suitable bandgap for semiconducting devices due to quantum confinement. However, most GNRs prepared by bottom-up synthesis reach widths less than 2 nm, because in general, the fabrication of wide GNRs using a bottom-up method requires high-molecular weight precursors which have disadvantages such as high sublimation temperature and low solubility. Moreover, it is difficult to produce GNRs with width less than 10 nm via top-down method because of limitation of electron beam focusing in lithography process.

Recently, we succeeded in producing wide graphene nanoribbons (GNRs) with the width of up to 7.2 nm fabricated via 2Z-CVD using 4,4-dibromo-*p*-terphenyl as the precursor. Densely packed arrays of poly(*p*-phenylene) produced on

Au(111) using this method could be converted into wide GNRs via interchain fusion by thermal annealing.

3. Graphene clusters from a quaterphenyl-branched Z-bar-linkage precursor via 2-Zone CVD

In the previous study, the biradical form of terphenyl-branched precursor might favor asymmetric conformations and could be converted to acene-type GNRs via homochiral polymerization and cyclodehydrogenation.²⁾ Whereas, the quaterphenyl-branched one might favor symmetric conformations which led to the molecular arrays of fused precursors at 400 °C via intramolecular dehydrogenation and graphene clusters via intermolecular dehydrogenation at temperature over 450 °C. Steric hindrance of the symmetric conformations is presumed to prohibit polymerization due to the strong affinity of the biradical to Au(111). The different adsorption conformations on Au(111) might account for the divergent reaction pathways. This study of ‘conformation-controlled surface catalysis’ is conducive to the rational design of precursor in the on-surface synthesis.

4. Skeletal rearrangement of polycyclic aromatic hydrocarbons with strain-induced surface reaction

Strain-induced rearrangements of aromatic carbon rings have been observed in graphene structures. As a typical example, a mechanical stress in graphene triggers a Stone-Wales rearrangement, a typical reaction of carbon allotropes that yields a defect composed of two heptagonal and two pentagonal rings fused together. Such defects play an important role in the formation of curved graphene and fullerenes. Therefore, it is crucial to control the rearrangements of sp²-carbon skeletal structures in order to synthesize nanocarbon materials. For macromolecules such as graphene intramolecular rearrangements feasibly occur because such local reactions do not strictly affect the total energy of the huge systems. For small polycyclic aromatic hydrocarbons (PAHs), on the other hand, it has been difficult to induce skeletal rearrangements in conventional organic synthesis. The preceding mechanochemical procedures for aromatic compounds cannot induce unimolecular reactions but can induce sp³-hybridized polymerizations because of the enormous increase in intermolecular interactions. Other synthetic methods under severe conditions, such as flash vacuum pyrolysis, are required to undermine the aromaticity in the transition states and to obtain intramolecularly rearranged PAHs. Therefore, the exploration of PAH reaction schemes will be a significant step towards under-

standing the mechanisms underlying the reaction and repair of defects in carbon allotropes, and towards designing and fabricating further functional nanocarbon materials.

Recently, we demonstrate a reaction scheme for the skeletal rearrangement of PAHs on a metal surface using high-resolution noncontact atomic force microscopy (AFM). We produced a well-designed PAH-diazuleno[1,2,3-cd:10,20,30-fg] pyrene (DAPH)-adsorbed flatly onto Cu(001), in which two azuleno moieties are highly strained by their mutual proximity by a combination of organic synthesis and on-surface cyclodehydrogenation. This local strain drives the rearrangement of one of the azuleno moieties into a fulvaleno moiety, which has never been reported so far. Our proposed thermally driven, strain-induced synthesis on surfaces will pave the way for the production of a new class of nanocarbon materials that conventional synthetic techniques cannot attain.

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Biofunctional Chemistry Research Section

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1. Introduction

A transition to renewable energy technologies requires new chemistry to learn from nature. Nature has found fantastic solutions to convert solar energy to produce chemicals and to utilize them in the exceptionally efficient manners for almost 3 billion years. It is our challenge to understand the efficient bioenergetic processes of nature and to construct bio-inspired energy utilization systems. The research interests in our group focus on the design of biomacromolecules and their assemblies for molecular recognition, catalysis and signal transduction in water, the solvent of life. We take synthetic, organic chemical, biochemical and biophysical approaches to understand the biological molecular recognition and chemical reactions. Proteins and protein/nucleic acids assemblies are explored to realize biomimetic function of biological systems, such as visualization of cellular signals by fluorescent biosensors, directed self-assembly of peptides and proteins to build up nanobiomaterials, tailoring artificial receptors and enzymes based on the complex of RNA and a peptide or a protein, and reconstitution of the functional assemblies of receptors and enzymes on the nanoarchitectures. Followings are main research achievements in fiscal year 2018.

2. DNA Binding Adaptors to assemble protein of interest on a DNA scaffold

Proteins are particularly interesting class of molecules to assemble on DNA scaffold because of their huge functional variability. Various methods to assemble POIs on the DNA scaffold have been reported to date, but much remain to be established. Further development in the method for locating POIs with controlling not only the positions, but also the number of molecules, stoichiometry, and the orientation is necessary to explore the chemistry of spatially assembled proteins and enzymes, such as the cascade reaction consisting of multiple enzymes. The orthogonal modular adaptors are one of the promising methods to construct well-defined protein assemblies, with the spatial and orientational control of enzymes

on the DNA scaffold *in vitro*, and possibly in the cell. Recently, we proposed a general strategy to construct a set of orthogonal modular adaptors by investigating the kinetic aspects of cross-linking reactions between modular adaptors and the substrate modified DNAs. In this year, based on the strategy, we constructed the sequence modular adaptor, which consist of the same self-ligating protein tag and the different types of sequence-specific DNA binding proteins. These design principle is useful for expanding the variation of sequence-specific modular adaptors. By using the modular adaptors that forms the covalent bond between the DNA address and modular adaptor exclusively controlled by the sequence-specific DNA binding, the snap-shot of spatially assembled cellular multi-enzyme system would be constructed *in vitro*. By taking advantages of DNA nanotechnology and reliable chemistry of the site specific location of proteins on DNA, an attractive function of spatially organized proteins and enzymes is now exploring.

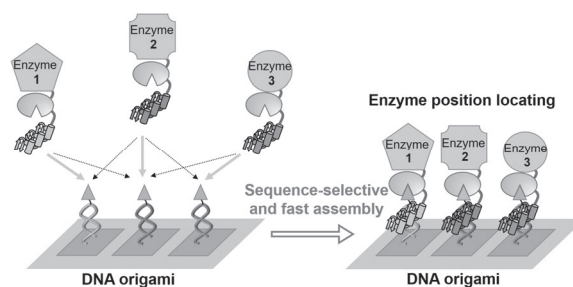


Figure 1 A schematic illustration of the sequence specific modular adaptor for locating POI on a DNA scaffold.

3. Highly selective dual sensing of ATP and ADP by fluorescent ribonucleopeptide sensors

Specific detection and quantification of a given target molecule by fluorescent biosensor is one of the general and powerful methods to elucidate the mechanism of chemical reaction and to apply for the diagnostic and therapeutic purposes. We have developed a method for construction of ribonucleopeptide (RNP) receptor-based fluorescent sensors. Rev pep-

tide-RRE RNA complex was utilized as a scaffold of RNA-oriented RNP library constructed by introducing randomized RNA sequences into the RNA subunit. RNP receptors that specifically binds to the given target molecule can be selected from the RNP library by applying in vitro selection method. Fluorescent RNP sensors that exert fluorescence intensity changes upon binding the substrate of the parent RNP receptor were constructed by introducing a fluorophore at the N-terminal of Rev peptide in RNP. We have also reported rational modular design of RNP sensors by fusing the Rev-binding RNA sequence (RRE) to the RNA aptamer of interest and successively forming a complex with fluorophore-modified Rev. In this design, RNA aptamer is utilized for the binding module and fluorophore-modified RNP for the reporter module. Based on the plausible secondary structure of RNA aptamer, we designed aptamer-conjugated RNPs by linking RRE RNA and RNA aptamers through a stem structure. As the further development of this strategy for practical use, we also developed the method for construction of the covalently-linked RNP complex. Covalently-linked RNP sensors were applied for simultaneous detection of the multiple target ligands in a solution.

In this study, we applied the method as shown above to construct the respective highly selective ATP and ADP sensors for the simultaneous detection. Dual sensing of ATP and ADP would be helpful for the accurate detection of various enzymatic reactions of metabolic pathway relating ATP production or consumption. We applied the modular strategy to replace the stem-loop (SL) region of ATP-selective aptamer that reported by Sazani *et al.* (*J. Am. Chem. Soc.*, **2004**, 126, 8370) to RRE RNA (Fig. 2). Three modular RNPs were designed by appending the RRE RNA sequence to SL1 or SL2 of ATP-selective aptamer (sATP) that reported by Sazani *et al.* (*J. Am. Chem. Soc.*, **2004**, 126, 8370). In modifying SL2, the RRE sequence was appended in either of the polarity of RRE sequence to afford sATPRRE-I and sATPRRE-II. Modification at SL1 gave an RRE appended aptamer sATPRRE-III. All F-sATPRRE-RNPs showed measurable fluorescence intensity changes upon addition of ATP with each F-sATPRRE-RNP showing different affinity to ATP and the relative fluorescence intensity change (I/I_0). Furthermore, sATPRRE-II and sATPRRE-III were converted into covalently-linked RNP sensors (c-sATPRRE-II and c-sATPRRE-III). ADP-selective RNP also constructed by applying modular design strategy by using ADP-selective aptamer reported by Srinivasan *et al.* (*Chem. Biol.*, **2004**, 11, 499). The ADP-binding RNP sensor showed the apparent fluorescent change both in the noncovalent (sADPRRE) and covalent types (c-sADPRRE).

These sensors, c-sATPRRE-II and c-sADPRRE

were utilized for the simultaneous detection of ATP and ADP in a solution. They showed the similar fluorescent responses as in the single usage without any interference from each other. These two sensors also utilized for time-course monitoring of enzymatic reaction catalyzed by creatine phosphokinase (CPK). The reaction of CPK was started in the presence of 1 mM ADP and 2 mM phosphocreatine. The time-course increase in the fluorescence intensity of ATP sensor was observed with decrease in that of ADP RNP sensor. HPLC analyses provided essentially the same time-dependent concentration changes to the results obtained by using the ATP and ADP sensors, indicating the binding kinetics of the ligand to the sensor was fast enough to realize the real-time monitoring of the reaction.

Application of two types of covalently-linked RNP sensors enabled a facile and quantitative analysis of the target chemical reaction. Our modular strategy to construct fluorescent sensors from RNA aptamers provides powerful detection & analytical tools for targets, for which appropriate sensors are otherwise unavailable.

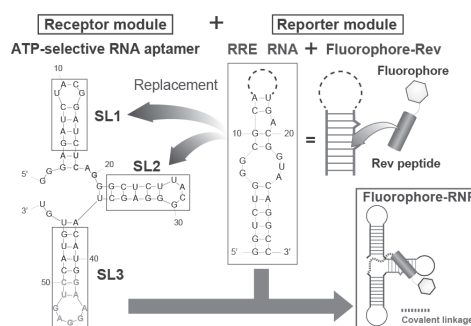


Figure 2 A scheme illustrates the modular strategy to construct ATP-selective fluorescent RNP sensors from the ATP-selective RNA aptamer. The consensus nucleotide sequence of ATP-selective RNA aptamer reported by Sazani *et al.* is showed in bold and its two regions were colored by red and light blue, respectively.

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Collaboration Works

森井孝, Nanyang Technological University (シンガポール), RNP 分子認識の 1 分子計測

森井孝, 国立シンガポール大学 (シンガポール), イノシトール誘導体の生理活性評価

森井孝, Ghent University (ベルギー), クロスリンク反応性を内在する機能性生体高分子によるケミカルバイオロジーの開拓

森井孝, Seoul National University (大韓民国), 特定空間に配置された酵素複合体の構築

森井孝, 中田栄司, Rajendran Arivazhangan, Ewha Womans University (大韓民国), 小分子による酵素機構の解明

森井孝, 仲野瞬, POSTECH (大韓民国), 蛍光性バイオセンサーの構築

森井孝, 仲野瞬, POSTECH (大韓民国), RNA 分子センサーの構築

森井孝, 中田栄司, Rajendran Arivazhangan, Vanderbilt University School of Medicine (アメリカ), Topoisomerase 反応の可視化

Financial Support

1. Grant-in-Aid for Scientific Research

森井孝, 新学術領域研究, 活性酸素種による翻訳後修飾を検出する蛍光バイオセンサー

森井孝, 挑戦的萌芽研究, トリプレットリピート病の鍵を握る RNA 凝集体の直接観察と検出法の開発

森井孝, 基盤研究 (A), 人工代謝経路を内包するナノ空間「複合触媒コンパートメント」の創出

中田栄司, 新学術領域研究, 分子コンビナートによる非天然化合物合成システムの創製

中田栄司, 挑戦的萌芽研究, 組成比を制御したヘテロ多量体調製技術による人工フィコビリソームの創製

仲野瞬, 若手研究, 生成物解離を制御した RNA-ペプチド複合体リセプター酵素の創製

2. Others

森井孝, 科学技術振興機構, 細胞内環境測定多元同時センサーの開発

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Structural Energy Bioscience Research Section

M. Katahira, Professor
 T. Nagata, Associate Professor
 T. Mashima, Assistant Professor

1. Introduction

We explore the way how biomolecules such as proteins (involving enzymes) and functional nucleic acids (DNA and RNA) work at atomic resolution based on structural biology with NMR. We determine both static and dynamical structures with the aid of our own development of the new methodology and elucidate the underlying mechanism of functions of these biomolecules. Structural biological approach is also applied to analyze enzymes involved in degradation of wood biomass at atomic resolution. The analysis is useful to develop the way to extract energy and valuable materials that can be used as starting materials of various products from the wood biomass. Thus, we pursue to contribute to the paradigm shift from oil refinery to biorefinery. Followings are main research achievements in the year of 2018.

2. Classification and characterization of two new fungal glucuronoyl esterases from *Ceriporiopsis subvermispora* and *Pleurotus eryngii*

The lignin-carbohydrate complex (LCC) found in the recalcitrant woody biomass is a complex of lignin and hemicellulose. Fungal glucuronoyl esterases (FGEs) catalyze cleavage of LCC at the ester bond formed between an alcohol group of lignin and the xylan-bound 4-Omethyl-D-glucuronic acid of glucuronoxylans. Here, we built a phylogenetic tree from about 400 putative FGEs obtained on BLAST analysis and defined six main clades. We then found that FGEs of *C. subvermispora* and *P. eryngii* belong to clades V and II, respectively, and that FGEs of these clades have not been studied yet. We developed high-yield *Pichia pastoris* expression systems of the catalytic domains of FGEs of *C. subvermispora* (CsGE) and *P. eryngii* (PeGE). We then used benzyl glucuronic acid to confirm the activities of these FGEs. Firstly, we developed the improved protocol to accurately measure the activity. We successfully quantified the hydrolyzed product, glucuronic acid, spectrophotometrically with higher accuracy using our new protocol. It turned out that PeGE exhibits the highest activity among FGEs reported so far. Then, we demonstrated that PeGE exhibits high tolerance toward various denaturing agents, which may make it a potentially more applicable enzyme.

3. Structural and functional studies of a serine-type glutathione S-transferase of *Ceriporiopsis subvermispora*

Glutathione (GSH) S-transferases (GSTs) are enzymes that catalyze the reactions involved in detoxification and metabolic pathways. We previously developed high-yield *E. coli* expression systems of two GSTs of *C. subvermispora*, CsGST63524 and CsGST83044, and characterized their activities. Here, we solved the crystal structures of the CsGST63524 in ligand-free and GSH-bound forms at 2.45 and 2.50 Å resolutions, respectively. It was found that the residue located closest to the sulfur atom of glutathione for hydrogen bonding is Ser21, which indicated that CsGST63524 is a serine-type GST. Functional mutagenesis unexpectedly showed that Ser21 is not essential for the enzymatic activity, but interestingly revealed that non-canonical amino acid residues, Asn23 and Tyr45, are enzymatically important. We have also identified the putative substrate binding site, which comprises mostly hydrophobic residues, of CsGST63524 (Figure 1). This is reasonable because many of the substrates that CsGST63524 targets are hydrophobic. Additionally, relatively large GSH-bound pocket of CsGST63524 rationally explains its substrate-preference.

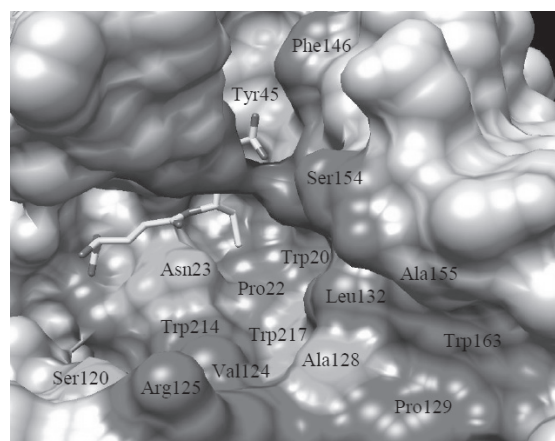


Figure 1. Close-up surface representation of the putative substrate-binding site of CsGST63524 located near the GSH-binding site.

4. Interaction of carbohydrate-binding module from *Trichoderma reesei* Cel7A with cellohexaose and lignins from Japanese cedar and *Eucalyptus globulus*

Lignocellulosic biomass, which comprises cellulose, hemicelluloses, and lignin, is the most abundant renewable carbon resource. The production of bio-based fuels and value-added chemicals from lignocellulosic biomass is attractive, because it has a potential of partial replacement of fossil resources and to overcome environmental issues. Saccharification of lignocellulosic biomass using cellulolytic enzymes is ideal regarding isolation of the components intact. However, nonproductive binding of lignin to cellulolytic enzymes has been problematic and need to be avoided. It has been known that carbohydrate-binding modules (CBMs) of cellulolytic enzymes strongly bind to lignin, but the adsorption mechanism at molecular level is still remained elusive. Here, NMR-based identification of binding sites on CBM1 of cellobiohydrolase I (Cel7A) from a hyper-cellulase-producing fungus, *Trichoderma reesei*, toward cellohexaose and lignins from Japanese cedar (C-MWL) and *Eucalyptus globulus* (E-MWL) was carried out. Firstly, we developed *E. coli* expression system of TrCBM1, and preparation method to obtain properly folded and stable isotope-labeled TrCBM1. Chemical shift perturbation analyses revealed that TrCBM1 adsorbs cellohexaose highly specifically using two subsites, flat plane surface and cleft, which were located on the opposite side of the protein surface. On the other hand, MWLs, which exhibited higher affinity than cellohexaose toward TrCBM1, were adsorbed using multiple binding sites, including the subsites. Of the residues belonging to the flat plane surface, Gly6 and Gln7 were involved in lignin

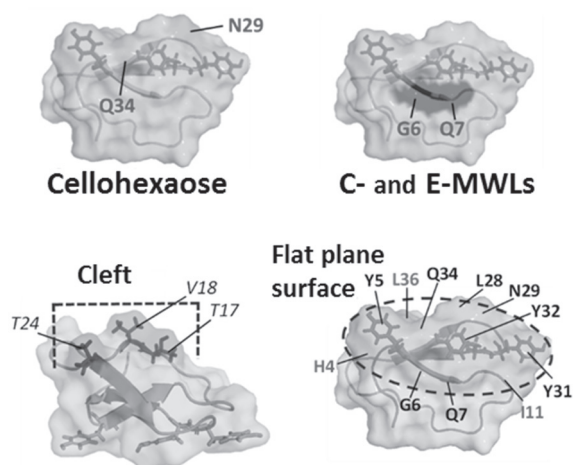


Figure 2. Mapping of the binding sites on the TrCBM1 model structure. (Top) Binding sites for cellohexaose (left), and C- and E-MWLs (right), respectively. (Bottom) Common binding sites for cellohexaose, and C- and E-MWLs are shown from different directions.

binding, while Asn29 and Gly34 in cellohexaose binding (Figure 2). It turned out that much larger surface area was used in TrCBM1 to bind with C-MWL than E-MWL. This indicates that the mechanisms of adsorption toward hardwood and softwood lignins are quite different.

5. The mechanism by which the deaminase activity of human APOBEC3F, which depends on the length of single-stranded DNA, is affected by the concentrations of APOBEC3F and single-stranded DNA

APOBEC3F (A3F), a member of the human APOBEC3 (A3) family of single-stranded (ss) DNA cytidine deaminases, acts as an anti-human immunodeficiency virus 1 (HIV-1) factor by deaminating deoxycytidines to deoxyuridines in the complementary DNA of the viral genome. Previous studies on A3F were mainly focused on its interaction with an accessory protein of HIV-1 known as a viral infectivity factor, while a full understanding of the deamination behavior of A3F awaits further investigation. Here, we investigated the ssDNA-length-dependence of the deaminase activity of the C-terminal domain (CTD) of A3F. The use of the N214H mutant of A3F-CTD, which exhibits higher deaminase activity than the wild-type, facilitated tracking of the reaction on the real-time NMR time scale. It turned out that A3F-CTD efficiently deaminates the target deoxycytidine in long ssDNA with a low ssDNA concentration ($[A3F-CTD] \gg [ssDNA]$), while the target deoxycytidine in short ssDNA is deaminated efficiently by A3F-CTD with a high ssDNA concentration ($[A3F-CTD] \ll [ssDNA]$). This property of A3F is quite different from that of the previously studied A3 family member, A3B. In the case of A3B, deamination of the target deoxycytidine in short ssDNA is more efficient than that in long ssDNA; the concentrations of the protein and ssDNA had no effect. This unique property of A3F is rationally interpreted on the basis of its binding characteristics as to ssDNA.

6. Identification of the mode of the interaction between telomeric i-motif DNA and cyclic tetraoxazole compound

We determined how cyclic tetraoxazole compound (**1**) interacts with telomeric i-motif DNA by NMR in combination with CD, mass spectroscopy, and gel-electrophoretic mobility shift analysis. It was revealed that two molecules of compound (**1**) bind cooperatively to the i-motif structure. Chemical shift perturbation indicated that the most preferred binding site is comprised of the first loop and the third loop of telomeric i-motif and their neighboring region. The binding causes slight distortion of the C:C base pair. When the second compound (**1**) binds to the secondly preferred binding site, two other C:C base pairs were also distorted.

Collaboration Works

片平正人, Nanyang Technological University (シンガポール) & University of Bordeaux (フランス) iモチーフ 4 重鎖 DNA と低分子化合物の相互作用様式の解明

Financial Support

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片平正人, 新学術領域研究, ヒト生細胞の分子夾雑環境における核酸の構造と相互作用の解明

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1. Introduction

The DNA topoisomerases (Topos), especially the human DNA topoisomerases, have been identified as the potential targets of a variety of therapeutics including anticancer drugs. The DNA topology such as overwinding or underwinding that arises due to the intertwined nature of the DNA double helices are regulated by the Topo enzymes.^[1] Also, these enzymes play major roles in various biological processes such as replication, transcription, recombination, and chromosome condensation and segregation. If the DNA overwinding problem that arises during the replication and transcription is not relaxed, it eventually stops the functions of the enzymes involved in these processes. Topos control the topological conditions by transiently cleaving the phosphodiester bond, which generates a Topo-DNA cleavage complex. Once the winding stress is resolved, the enzyme-mediated DNA break is resealed. This process is critical for the healthy cells to survive and function normally, and failure to reseat the DNA break can ultimately lead to cell death. Topos are classified into two types based on the number of strands cleaved in one round of action: i) Type I: cuts one strand of DNA, topological changes happen, and then reanneal the cleaved strand; and ii) Type II: cuts both the strands of one DNA duplex, topological stress is released, and then reseals the cleaved strands. Topos involve in step-by-step processes such as binding of Topo to DNA, ATP driven strand passage, strand cleavage by Topo, formation of Topo-DNA cleavage complex, religation of cleaved DNA, and catalytic cycle after DNA cleavage/enzyme turnover. All these steps are of great interest as potential targets for the development of anticancer drugs.^[2] Despite the development of various Topo-inhibitors, the progress towards understanding how these inhibitors interact with these enzymes is impeded by the drawbacks in the traditional methods. For instance, it is not well understood at which step of the enzyme reaction is inhibited by a particular drug molecule. Thus, to understand the Topos reaction and the mechanisms of the inhibitors, it is necessary to develop a versatile

method.

2. Fabrication of topologically-interlocked DNA structures inside a DNA origami frame and applications for protein and drug analysis

Since the Topo enzymes target the topologically-constrained DNAs, the interlocked DNA structures such as catenane and rotaxane can be used as the potential targets to investigate the Topos functions and their inhibitors.^[3] The fabrication of the duplex DNA catenanes and rotaxanes inside the relatively larger and complex DNA nanostructures such as DNA origami has not yet been realized. These molecular assemblies have potential applications such as the functional components for molecular switches and motors, novel platforms for the investigation of the function of proteins, analysis of protein inhibitors, and so on. I have been collaborating with the research groups of Prof. Takashi Morii of IAE, Kyoto University and Prof. Youngjoo Kwon of Ewha

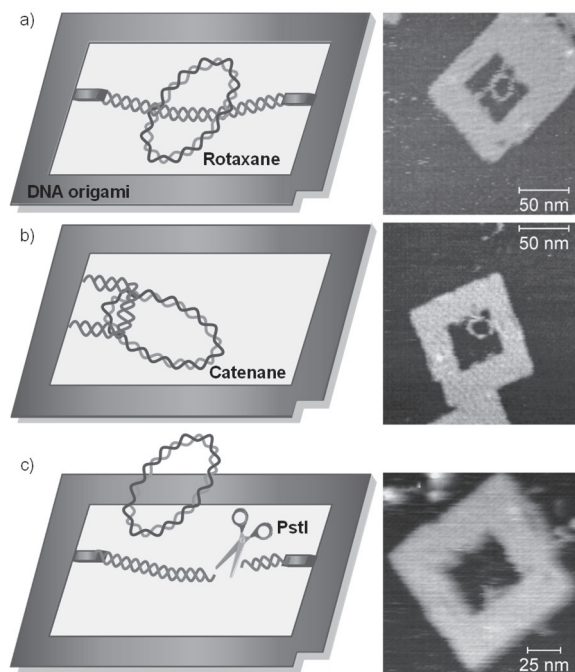


Figure 1. Schematic illustrations (left) and AFM images (right) of (a) the DNA rotaxane-, (b) catenane-like structures inside a DNA origami frame. (c) The restriction enzyme PstI reaction on the rotaxane-like structure.

Womans University, South Korea for the preparation of the topologically-interlocked supramolecular assemblies inside a DNA origami nanostructure.

Here, we have developed an elegant method by the combination of scaffolded DNA origami – a method to self-assemble DNA into the arbitrary two- and three-dimensional structures as templates,^[4-6] and high-speed atomic force microscopy (HS-AFM)^[7-12] for the screening of Topo-inhibitors. As for the target structures for the Topo reactions, we have constructed topologically-interlocked DNA catenane- and rotaxane-like structures inside a DNA origami frame. The formation of the DNA origami frame and the insertion of the catenane- and rotaxane-like structures were successfully characterized by agarose gel electrophoresis and HS-AFM imaging (Figure 1a,b). We could successfully fabricate the rotaxane- and catenane-like structures with the yield of about 30 and 60%, respectively. To increase the stability of these functional structures, the nicks in these structures were sealed by using T4 DNA ligase. The ligation was also confirmed by the thermal treatment of these structures, where the ligated samples were stable at high temperature treatment while the unligated samples failed to keep the folded structures. The experimental conditions such as the amount of salt, annealing temperatures, concentration of the DNA strands were optimized. The purification and quantification methods to get rid of the excessive staples and unbound catenane/rotaxane rings were also established. Further, we have investigated the stability of the DNA origami frame and the catenane/rotaxane ring structures in the presence of various kinds of Topo inhibitors. Both the origami and the DNA ring were stable against the Topo inhibitors for several hours at room temperature. This indicated that the DNA origami based analysis of Topo inhibitors could be successfully carried out.

After successful fabrication of the interlocked structures, we have performed the enzymatic reactions on them. The restriction enzyme PstI has the scission site in the linear duplex of the rotaxane-like structure and XbaI cuts the ring of both rotaxane- and catenane-like structures. After the restriction enzyme treatment, the structures were analyzed by both agarose gel electrophoresis and AFM imaging. After the overnight reaction, the yield of the interlocked structures were significantly decreased to 4% (PstI for rotaxane), 8% (XbaI for rotaxane) and 21% (XbaI for catenane), indicating the success of the reaction (Figure 1c).

We are now investigating the TopoII α reactions on these interlocked functional structures. After successful investigation of the Topo reactions, these

structures will be used for the screening of Topo inhibitors. Such a screening will be carried out by the direct and real-time characterization methods such as HS-AFM and fluorescence imaging. Apart from the Topo reactions and inhibitor screening, the fabrication of the topologically interlocked structures within a DNA origami nanostructure is also promising in the fields of molecular switches, motors, sensors, and logic devices.^[13] Topologically interesting structures such as Borromean rings, catenanes, and knots have already been prepared by using DNA.^[13] Also, the complexity of the catenane^[14] and rotaxane^[15] structures were increased by constructing them by the DNA origami method.^[4-6] However, for the first time we have fabricated the duplex DNA catenanes and rotaxanes inside the relatively larger and complex DNA nanostructures such as DNA origami and applied for the enzymatic reactions and drug analysis.

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Self-Assembly Science Research Section

M. Kinoshita, Professor

1. Introduction

A variety of self-assembly and ordering processes in biological systems, which occur at molecular levels, are sustaining life. Biopolymers, a great diversity of molecular and ionic species, or water is simply *material* when each of them is separately present. However, the complicated correlations among these material constituents can lead to *life*. We are elucidating those correlations, uncovering the mechanism of the biological processes, and clarifying the roles of water by developing special theories based on statistical mechanics and hydration thermodynamics. The achievements will provide important bases of nanobiotechnology. The current subjects are hydrophobic and hydrophilic hydrations, behavior of confined liquids, folding/unfolding mechanisms of proteins, molecular recognition, prediction of the native structure of a protein, enhancement of the thermal stability of membrane proteins, and functioning of ATP-driven proteins.

(1) Physical Origin of Thermostabilization by a Quadruple Mutation for the Adenosine A_{2a} Receptor in the Active State [1-3]

The G protein-coupled receptors (GPCRs) form a large, physiologically important family of membrane proteins and are currently most attractive targets for drug discovery. We investigate the physical origin of thermostabilization of the adenosine A_{2a} receptor (A_{2a}R) in the active state, which was experimentally achieved by another research group using the four point mutations. The investigation is performed on the basis of our recently developed free-energy function (FEF) which has been quite successful for thermodynamics of GPCRs in the inactive state. The experimental condition for solving the wild-type and mutant crystal structures was substantially different from that for comparing their thermostabilities. Therefore, molecular dynamics (MD) simulations are necessitated, which also allows us to account for the structural fluctuations of the membrane protein. We show that the quadruple mutation leads to the enlargement of solvent-entropy gain upon protein folding. The solvent is formed by hydrocarbon groups constituting nonpolar chains within the lipid bilayer and the entropy is relevant to thermal motion of the hydrocarbon groups. From an energetic point of view (e.g., in terms of protein intramolecular hydrogen bonds), the mutation confers no improvement upon the structural stability of A_{2a}R. The reliability of our FEF and the crucial importance of the solvent-entropy effect have thus been demonstrated for a GPCR in the active state. We are now ready to identify thermostabilizing mutations of GPCRs not only in the inactive state but also in the

active one. (We already developed a reliable method for the identification for GPCRs in the inactive state.)

(2) Universal Effects of Solvent Species on the Stabilized Structure of a Protein [4]

We investigate the effects of solvent specificities on the stability of the native structure (NS) of a protein on the basis of our FEF. We use CPB-bromodomain (CBP-BD) and apoplastocyanin (apoPC) as representatives of the protein universe and water, methanol, ethanol, and cyclohexane as solvents. The NSs of CBP-BD and apoPC consist of 66% α -helices and of 35% β -sheets and 4% α -helices, respectively. In order to assess the structural stability of a given protein immersed in each solvent, we contrast the FEF of its NS against that of a number of artificially created, misfolded decoys possessing the same amino-acid sequence but significantly different topology and α -helix and β -sheet contents. In the FEF, we compute the solvation entropy using the morphometric approach combined with the integral equation theories, and the change in electrostatic (ES) energy upon the folding is obtained by an explicit atomistic but simplified calculation. The ES energy change is represented by the break of protein-solvent hydrogen bonds (HBs), formation of protein intramolecular HBs, and recovery of solvent-solvent HBs. Protein-solvent and solvent-solvent HBs are absent in cyclohexane. We are thus able to separately evaluate the contributions to the structural stability from the entropic and energetic components. We find that for both CBP-BD and apoPC, the energetic component dominates in methanol, ethanol, and cyclohexane, with the most stable structures in these solvents sharing the same characteristics described as an association of α -helices. In particular, those in the two alcohols are identical. In water, the entropic component is as strong as or even stronger than the energetic one, with a large gain of translational, configurational entropy of water becoming crucially important, so that the relative contents of α -helix and β -sheet and the content of total secondary structures are carefully selected to achieve sufficiently close packing of side chains. If the energetic component is excluded for a protein in water, the priority is given to closest side-chain packing, giving rise to the formation of a structure with very low α -helix and β -sheet contents. Our analysis, which requires minimal computational effort, can be applied to any protein immersed in any solvent and provides robust predictions that are quite consistent with the experimental observations for proteins in different solvent environments, thus paving the way toward a more detailed understanding of the folding process.

(3) Mechanism of Protein-RNA Recognition: Analysis Based on Statistical Mechanics of Hydration [5]

We investigate the RBD1-r(GUAGU) binding as a case study using all-atom models for the biomolecules, molecular models for water, and currently the most reliable statistical-mechanical method. RBD1 is one of the RNA-binding domains of mammalian Musashi1 (Msi1), and r(GUAGU) contains the minimum recognition sequence for Msi1, r(GUAG). We show that the binding is driven by a large gain of configurational entropy of water in the entire system. It is larger than the sum of conformational-entropy losses for RBD1 and r(GUAGU). The decrease in RBD1-r(GUAGU) interaction energy upon the binding is largely cancelled out by the increase in the sum of RBD1-water, r(GUAGU)-water, and water-water interaction energies. We refer to the increase as “energetic dehydration”. The decrease is larger than the increase for the van der Waals component, whereas the opposite is true for the electrostatic component. We give a novel reasoning for the empirically known fact that protein residues possessing the side chains with positive charges and with flat moieties frequently appear within protein-RNA binding interfaces. A physical picture of general protein-RNA binding mechanism is then presented. To achieve a sufficiently large water-entropy gain, shape complementarity at the atomic level needs to be constructed by utilizing the stacking and sandwiching of flat moieties (aromatic rings of the protein and nucleobases of RNA) as fundamental motifs. To compensate for electrostatic energetic dehydration, charge complementarity becomes crucial within the binding interface. We argue the reason why the RNA recognition motif (RRM) is the most ubiquitous RNA binding domain.

(4) Statistical Thermodynamics for Unexpectedly Large Difference between Disaccharide Stereoisomers in terms of Solubility in Water [6]

We unravel the physical origins of the large difference between cellobiose and maltose, which consist of two β -1,4 and α -1,4 linked D-glucose units, respectively, in terms of the solubility in water. We construct a thermodynamic theory where the chemical-potential difference between disaccharides in water and in vacuum is identified as the key FEF. Its energetic and entropic components are calculated for cellobiose and maltose by statistical-mechanical theories for solute hydration. The disaccharide structures are taken into account at the atomic level and a molecular model is adopted for water. MD simulations are used to account for the conformational fluctuation of a disaccharide molecule, which also enables us to estimate the conformational entropy. We show that the cellobiose/maltose solubility ratio calculated is in good agreement with the experimental value. The solubility becomes much lower for cellobiose due to conformational-entropy and water-entropy effects. The former effect is relevant to higher stability of the

intramolecular hydrogen bond between oxygen atoms in the six-membered ring and in the neighboring hydroxyl group. The hydration alters the fluctuation of a molecular conformation to a larger or less regular one, but the degree of this alteration is smaller. The latter effect is attributed to more separation of two hydroxymethyl groups in a molecule, causing lower probability of the overlap of excluded volumes generated by the groups for water molecules. We suggest that physicochemical properties of disaccharides in water become variable depending on the stereoisomerism through hydration effects and the origins of the variety are entropic.

(5) Statistical Thermodynamics for Large Difference between Thermophilic Rhodopsin and Xanthorhodopsin in terms of Thermostability [7]

Though thermophilic rhodopsin (TR) and xanthorhodopsin (XR) share the high similarity in amino-acid sequence and almost the same structure, TR is much more thermostable than XR. We investigate physical origins of this difference on the basis of the change in our improved FEF upon protein folding. Since the energetics within the transmembrane (TM) region is substantially different from that within the water-immersed (WI) regions, we determine the TM and WI portions of XR or TR by analyzing the distribution of water molecules using MD simulations. The energetic component of the FEF change consists of a decrease in energy arising from the formation of intramolecular HBs and an increase in energy caused by the break of protein-water HBs referred to as “energetic dehydration penalty”. The entropic component is a gain of the translational, configurational entropies of hydrocarbon groups within the lipid bilayer and of water molecules. The entropic component is calculated using the integral equation theory combined with our morphometric approach. The energetic one is estimated by a simple but physically reasonable method. We show that TR is much more stable than XR for the following reasons: The decrease in energy within the TM region is larger, and the energetic dehydration penalty within the WI regions is smaller, leading to higher energetic stabilization; and tighter packing of side chains accompanying the association of seven helices confers higher entropic stabilization on TR.

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High Temperature Plasma Equipment Engineering Research Section

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1. Introduction

The major subjects are to study fast-ion confinement in plasma confinement devices and to investigate interactions between fast-ions and materials, such as a first wall and a vacuum vessel. The fast-ion confinement is a critical issue for the fusion reactor since the alpha particles produced in the D-T reaction should be utilized to heat plasma efficiently. Fast-ion profile and velocity distribution are investigated using ion cyclotron range of frequency (ICRF) minority heating in Heliotron J with special emphasis on the effect of the toroidal ripple of magnetic field strength ('bumpiness'). In fusion reactors, fuel must be supplied since fuel particles decrease via the fusion reactions and escape continuously from the core plasma. Fueling using hydrogen-ice pellet is also our subject to generate high-density plasmas. This method is considered to have an advantage for core-plasma fueling. A small-size and slow-speed injector has been developed for plasmas in Heliotron J and the operation for fueling begins.

2. Study of Fast-ion Generation by Combination Heating of ICRF and NBI in Heliotron J

Main purpose of this study is to optimize fast ion confinement by using ICRF heating in a helical-axis heliotron device, Heliotron J on the basis of results of several helical devices. For the research of the fast ion confinement in a three dimensional magnetic field, fast ions are generated by ICRF minority heating in combination with NBI heating in Heliotron J ($R_0 = 1.2$ m, $a = 0.1$ - 0.2 m, $B_0 \leq 1.5$ T). The energy range is extended from the injection energy of the NBI beam E_0 , 25 keV, to 60 keV during the ICRF pulse in the newly attempted low- ε_t configuration and medium density operation (1×10^{19} m $^{-3}$). This configuration is better in the fast ion generation and confinement than the high bumpiness configuration which is the best among the bumpiness scan. Here, the toroidicity and the bumpiness normalized by the helicity for the low- ε_t and the high bumpiness configurations are (0.77, -1.04) and (0.86, -1.16) in Boozer coordinates, respectively. They are key parameters in $1/\nu$ regime of helical devices. The low- ε_t configuration is expected to have good

confinement from the neo-classical theory. The Monte-Carlo calculation shows the advantage of the low- ε_t configuration for the generation and confinement of fast ions.

Using Monte-Carlo method with the experimental magnetic field and plasma parameters, the numerical calculation including orbit tracing, Coulomb collisions and ICRF acceleration of NBI particles has been performed in order to estimate the averaged behavior in whole torus for various configurations. The birth position of the NBI particles (hydrogen) was fixed at the one point and no divergence of the NB is included in the last year. For more realistic simulation of fast ions in the experimental conditions, we plan to use NFREYA code for the calculation of the birth point of the NBI particles.

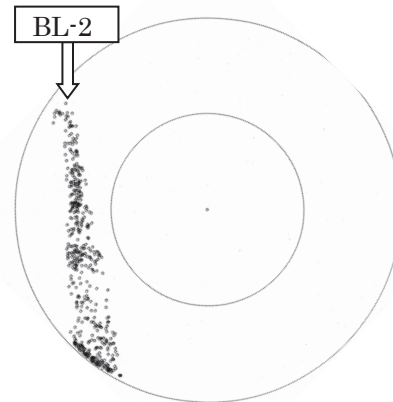


Fig.1 Ionization points of injected beam particles in the top view of Heliotron J.

The ionization points of the beam particles from the unit, 'BL-2'. Measured high-energy particle flux with a charge exchange neutral particle analyzer (CX-NPA) is originated from beam-injected ions and accelerated by ICRF heating. In this calculation of Fig. 1, injection energy of NBI is 27 kV and the component ratios are 0.6 for H, 0.3 for H $_2$, and 0.1 H $_3$, respectively. The line-averaged electron density is 1×10^{19} m $^{-3}$, center electron temperature is 250 eV, center ion temperature is 170 eV, and the magnetic configuration is standard. The beam is diverged and

reaches the vacuum chamber wall. In Fig. 2, radial profiles are shown for three components of the beam. The radial profiles are almost identical. These position and velocity data will be used as the input parameter of the Monte-Carlo simulation for ion acceleration by ICRF heating.

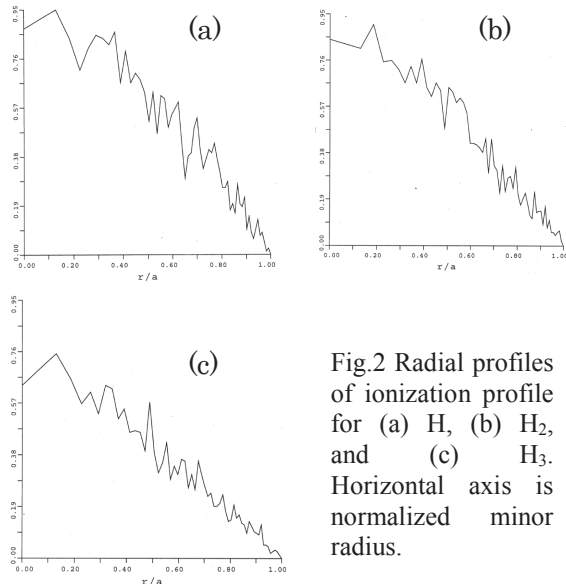


Fig.2 Radial profiles of ionization profile for (a) H, (b) H₂, and (c) H₃. Horizontal axis is normalized minor radius.

3. Study of Density Control Using Hydrogen Ice-Pellet Injection

The ice-pellet injection system has been developed for the new particle supply method following the supersonic molecular beam injection (SMBI) under the bilateral collaboration program in Heliotron J. This method is considered to be effective specially to supply particles into the plasma core region. The conditions of the pellet injector are; injection speed is less than 300 m/s, and the diameter is less than 1 mm

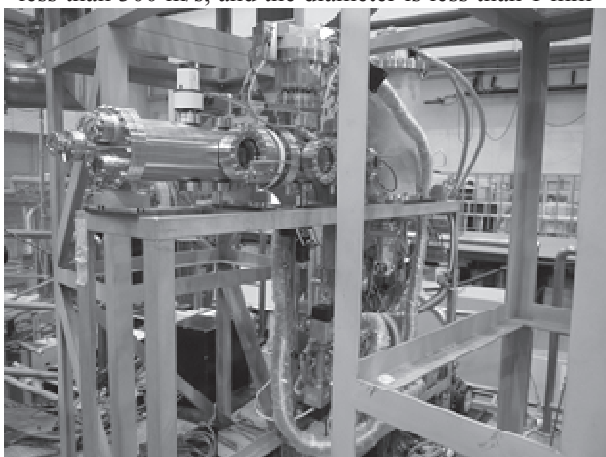


Fig. 3 Ice hydrogen pellet generator and injector installed in Heliotron J. An ice pellet is produced by means of cryogenic technique. Injection is performed by high-pressure helium gas.

for the plasma parameters of Heliotron J. Installed pellet injector is shown in Fig. 3. The pellet injection method is pneumatic propulsion using high-pressure helium gas. The injection test has been successfully done for hydrogen pellet and deuterium pellets. Injected pellets are monitored using H α array detector located at the same poloidal cross-section as the pellet injection as shown in Fig. 4. A pellet is injected from the outer port on the right side in the figure and 32-channel array detector observed the H α emission light from the pellet flying in the plasma.

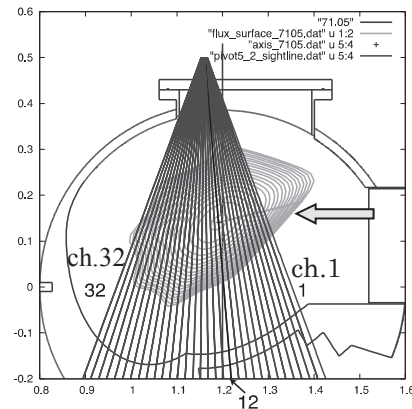


Fig.4 The arrangement of the line of sight of the H α array detector and a pellet path. A pellet is injected from the right port in the figure. The chord which include the plasma center is No. 12.

The measured H α emission signal is shown in Fig. 5 for ECH+NBI plasma. From this measurement, the pellet penetration depth can be estimated. The vertical axis is the channel number shown in Fig. 4. In this shot pellet ablation is completed before the plasma center. This length is almost expected from the numerical calculation code, ABLATE.

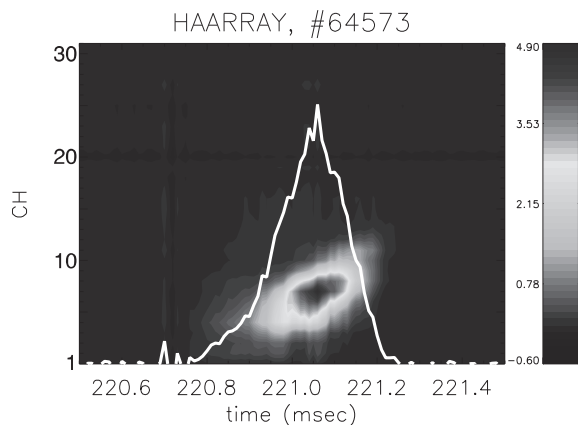


Fig.5 Time evolution of Ha array detector signal. The vertical axis corresponds to the channel number of the detector. White line denotes the sum signal of the total channels.

Collaboration Works

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Environmental Microbiology Research Section

T. Hara, Program-Specific Professor

Y. Takatsuka, Program-Specific Associate Professor

1. Introduction

There is a very close relationship between the consumption of energy resources and environmental protection, which is becoming an important issue for developing a sustainable society. We still rely heavily on fossil energy, and there is concern that emitted greenhouse gases break the harmony of the global environment. In addition, we need a great deal of energy to fix environmental pollution that continues to be the shadow of the civilization's progress due to the energy consumption of fossil fuels. As one of the solutions, we will develop a practical method using 'enzymes' derived from environmental microorganisms with high efficiency of energy utilization in catabolism. In 2018, our research section has been established as a donation department and works with biotechs and university start-ups to aim for networking of researches toward social implementation of our technologies.

2-1. Two-compositely microbial catalyst efficiently degraded polychlorinated biphenyls.

Polychlorinated biphenyls (PCBs) are organochlorine compounds that theoretically contain the 209 analogues of different chlorine substituents and had been used in various industrial applications. However, since PCBs, like dioxins, have proven to be serious endocrine disrupters for humans, the abolition of their use

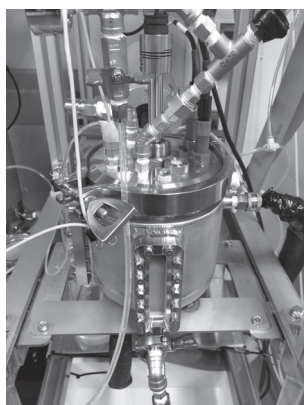


Figure 1. The composite BDOs-microbial catalyst was evaluated in the dedicated experimental bioreactor with the device of oxygen microbubble generation.

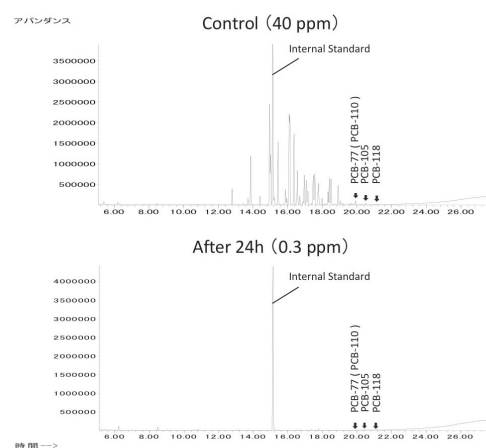


Figure 2. The data from gas chromatograph quadrupole mass spectrometer showing the PCBs degradation by the composite BDOs-microbial catalyst.

and production has been promoted worldwide. Biphenyl dioxygenase (BDO) plays a crucial role in the degradation of PCBs. BDO catalyzes the incorporation of two oxygen atoms into the aromatic ring of PCB, which induces the aromatic ring cleavage. We developed the composite type of catalytic enzyme with two BDOs that having different substrate specificity and the bioreactor for generating oxygen microbubbles that enhance the enzymatic activity of BDOs (Figure 1). As a result, we succeeded in constructing a practical system combining catalytic enzymes and microbubbles, and it degraded 99.3% of 40 mg L⁻¹ of major commercial PCB (Kenechrol KC-300 and KC-400) in 24 hours (Figure 2). This result achieved the waste disposal standard defined by the Ministry of the Environment of Japan.

2-2. Several bacterial species associated with PCBs dechlorination were genetically identified on PCBs contaminated site.

In order to further extend the composite degrading reaction of PCB, we have tried to create a unique artificial enzyme that dechlorinates PCBs by two-electron reduction. Here, we collected fresh-water sediments from the PCBs contaminated site in Osaka area and investigated whether the bacteria associated with PCBs dechlorination exist. It has resulted in finding

Dehalobacter sp. and *Desulfitobacterium* sp. by 16S rRNA gene phylogenetic analysis. It was reported that ‘*Dehalobacter*’ dechlorinates *Penta-/Hexa*-chlorinated biphenyls^[1] and ‘*Desulfitobacterium*’ dechlorinates *Tetra*-chlorinated biphenyls hydroxylated at the para position^[2]. Moreover, we succeeded in preparing the media for growing these particular bacterial species and its cultivation method. These results suggested that it can be acquired new activity capable of degrading PCB congeners which could not be degraded oxidatively by BDO so that the cocktail containing multiple PCB dechlorinating bacteria with different substrate specificities can be easily prepared. We are actually investigating the properties of the dechlorinating reaction of PCBs using this bacterial cocktail preparation. These results were reported at the 70th SBJ Annual meeting (2018) Osaka.

3-1. The biological enzymatic pesticide may become new pesticide with new sterilizing mechanism to replace the organic synthetic chemicals.

Many plant diseases are generally caused by either ascomycetes or basidiomycetes that belonging to filamentous fungi. ‘Filamentous fungi’ is hypha, and it proliferates to mycelia. The cell wall is a peculiar composite material. It incorporates a mix of cross-linked fibers and matrix components. The fibrous components of the cell wall are glucan, chitin, and mannan, and these sugar chains contribute to form a supple and solid filiform microfibril wall. Glycosidase is one of the hydrolases that catalyzes the hydrolysis of glycosidic bonds in complex sugars. We are developing a new bio-macromolecular type of fungicide utilizing the hydrolysis reactions of glycosidases against fungal microfibril wall. Currently, our composite type of bacterial catalyst composed of 5 strains from class *Bacilli*, which produce and secrete various glycosidases, controlled 99.3% of a tomato-*Pestalotia* disease with *Pestalotiopsis* sp. (Figure 3). Glycosidases are classified into approximately 130 families, and their catalytic reactions are roughly divided into

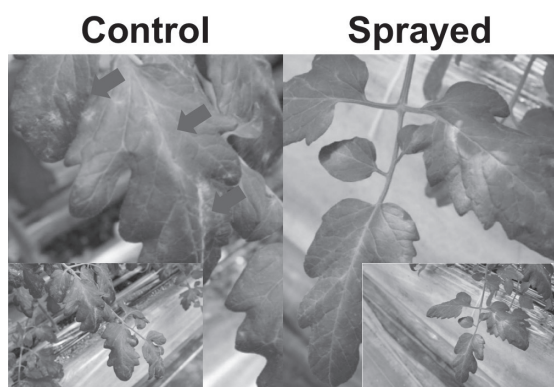


Figure 3. The glycosidase secreted type of the composite microbial catalyst inhibited tomato-*Pestalotia* disease.

anomeric inversion and/or anomer retention, and exoglycosidase or endoglycosidase. Hence, the classification of glycosidase can be understood diverse, and we consider that it is possible to digest fungi cell wall efficiently, by compositely capably using these diversities of enzyme activities.

3-2. Phytopathogenic filamentous fungi that secrete various glycosidases kill hostile phytopathogenic filamentous fungi for their survival.

We investigated the fungicidal properties of glycosidases produced by a phytopathogenic filamentous strain belonging to basidiomycetes. This filamentous strain secretes enzymes when grown in bran medium and exhibits various glycosidase activities. The crude enzyme fraction showing such composite glycosidase activity digested 3 out of 6 wet-rice-specific epidemically filamentous fungi (Figure 4). There are not so

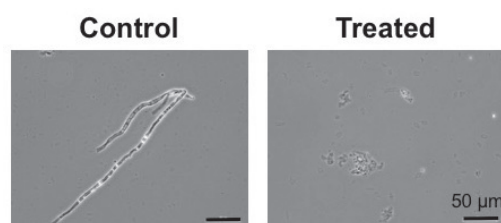


Figure 4. The crude enzyme fraction secreted from the phytopathogenic filamentous fungus digested a wet-rice specific epidemically filamentous fungal strain.

many enzymes showing high digesting activity against multiple strains of phytopathogenic filamentous fungi. Single glycosidase activity, however, digested only 2 strains. These results suggest that composite glycosidase activity have highly fungicidal activity rather than the single glycosidase activity. In fact, we try to purify this crude enzyme. In the near future, we will be able to clarify the effectively fungicidal mechanism that this crude enzyme shows by knowing the type of the enzyme(s), the amount of the secretion, and the specific activity.

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Collaboration Works

原富次郎, 高塚由美子, 東京農業大学, バチルス・サブチリス YAZ51 株由来の新規リポペプチドの構造解析と機能解明

Financial Support

1. Grant-in-Aid for Scientific Research

原富次郎, 挑戦的萌芽研究, 嫌気的自然環境で起こる有機汚染物質の脱塩素化反応を好気条件下で実現させる

高塚由美子, 挑戦的萌芽研究, 嫌気的自然環境で起こる有機汚染物質の脱塩素化反応を好気条件下で実現させる

2. Others

原富次郎, 日本医療研究開発機構, 新メソッドによる薬用ニンジンの品質評価を軸とした伝統的栽培法数値化と効率的生産法の開発

原富次郎, オーガニック・テックファーム (株), 微生物由来タンパク質を用いた植物の病害防除に関する指導

原富次郎, オーガニック・テックファーム (株), 微生物農業資材の研究開発

原富次郎, ワケンホールディングス (株), 環境微生物に関する研究のため

原富次郎, 東洋ガラス (株), エネルギー応用環境微生物学研究部門

原富次郎, (株) 竹中工務店, エネルギー応用環境微生物学研究部門

Presentations

高塚由美子, 原富次郎, 平野竜行, ポリ塩化ビフェニル類汚染地下水に棲息する嫌気性微生物に関する調査, 第 70 回日本生物工学会大会, 関西大学千里山キャンパス, 2018.9.6

3-2. AWARD

The 14th Annual Meeting of the Atomic Energy Society of Japan of Kansai Branch.

Quantum Radiation Energy Research Section
Siriwan Krainara (D3)

A research presentation of the 14th Annual Meeting of the Atomic Energy Society of Japan of Kansai Branch was held on 31st August 2018 at Osaka Science & Technology Center (OSTEC) in Osaka for university students, graduate students, and young researchers in the Kansai region. This opens an opportunity for students and young researchers to present their works, to discuss with others and to receive suggestions from the experts.

In this meeting, Siriwan Krainara, Ph.D. student attended and made an oral presentation on the topic of “Mitigation of the space charge effect for improving the performance of THz-CUR source”. She presented the methods and the simulated results on the manipulation of transverse and longitudinal laser distributions in order to mitigate a space-charge effect for improving the quality of electron beams. Eventually, an enhancement of the radiated power of the THz coherent undulator radiation (THz-CUR) generated from a compact linear accelerator based THz-CUR source at Kyoto University could be achieved. Finally, she was awarded the Presentation Award of “Achieved Excellent Results”.



Poster Award in the Workshop on “Radiation Effects on Materials (2018)”

Advanced Energy Structural Materials
Research Section
Jin Gao (Postdoc fellow)

This workshop is an annual program organized by Radiation effects on Materials Organization, which started from 1978 for organization of workshop for discussion of irradiation hardening and embrittlement towards keeping better integrity of nuclear structural components. Institute of Advanced Energy, Kyoto University has been hosting the workshop for these three years as a core of the community after Institute for Materials Research, Tohoku University.

In this poster presentation, ion-irradiation effects on welded ODS ferritic steels were reported. A larger irradiation hardening was observed for the welded part of the ODS steel than base metal, which was attributed for the higher number density of fine dislocation loops.



Poster Award in the Workshop on “Radiation Effects on Materials (2018)”

Advanced Energy Structural Materials
Research Section
Peng Song (Postdoc fellow)

This workshop is an annual program organized by Radiation effects on Materials Organization, which started from 1978 for organization of workshop for discussion of irradiation hardening and embrittlement towards keeping better integrity of nuclear structural components. Institute of Advanced Energy, Kyoto University has been hosting the workshop for these three years as a core of the community after Institute for Materials Research, Tohoku University.

In this poster presentation, ion-irradiation effects on ODS steels were reported. Most of interesting was that oxide particles in ODS ferritic steel were dissolved by the 6.4 MeV iron-irradiation at room temperature. Radiation tolerance of the oxide particles in different steels were investigated.



Poster Award in the Workshop on “Radiation Effects on Materials (2018)”

Advanced Energy Structural Materials
Research Section
Toshiki Nakasuji (D3)

The Irradiation Materials Annual Meeting is a good place that irradiation materials researchers can discuss the fundamental questions and concerns in the irradiation effect. This meeting was supported by the "Joint Usage/Research Program on Zero-Emission Energy Research, Institute of Advanced Energy, Kyoto University" and held in November, 2018. Mr. Nakasuji made a good presentation on their effort on “Risk-based Integrity Assessment of Reactor Pressure Vessel”, and received the Student Poster Session Award for their valuable unique ideas. His future success is greatly anticipated.



Poster Award in the Workshop on “Radiation Effects on Materials (2018)”

Advanced Energy Structural Materials
Research Section
Daniel Morrall (D3)

This workshop is an annual program organized by Radiation effects on Materials Organization, which started from 1978 for organization of workshop for discussion of irradiation hardening and embrittlement towards keeping better integrity of nuclear structural components. Institute of Advanced Energy, Kyoto University has been hosting the workshop for these three years as a core of the community after Institute for Materials Research, Tohoku University.

In this poster presentation, mechanical properties, corrosion behavior and radiation effects on mechanically alloyed austenitic stainless steel were investigated. The developed ODS steel showed a higher strength more than 3 times in comparison to the conventional steels, SUS304L.



Poster Award in the Workshop on “Radiation Effects on Materials (2018)”

Advanced Energy Structural Materials
Research Section
Yen-jui Huang (Postdoc fellow)

This workshop is an annual program organized by Radiation effects on Materials Organization, which started from 1978 for organization of workshop for discussion of irradiation hardening and embrittlement towards keeping better integrity of nuclear structural components. Institute of Advanced Energy, Kyoto University has been hosting the workshop for these three years as a core of the community after Institute for Materials Research, Tohoku University. In this poster presentation, the effects of water chemistry of stress corrosion cracking (SCC) of austenitic stainless steel were reported. The susceptibility to SCC was evaluated by means of slow strain rate test method in a variety of environment such as hot water and supercritical pressurized water with dissolved oxygen and dissolved hydrogen.



Student Award in IAE, Kyoto University (2018)

Advanced Energy Structural Materials
Research Section
Peng Song (Postdoc fellow)

This award is conferred annually for excellent students of the institute of advanced energy, Kyoto University, who gained superior achievements in their research under supervision of professors in the institute.

I studied on helium effects on the ODS ferritic steels utilizing dual ion beam irradiation facility (DuET) to understand material integrity in the fusion related environment where both irradiation damage and high concentration of helium are introduced. It was made clear that helium bubbles were not correlated with the ion-irradiated hardening, while the hardening was due to fine dislocation loops and unfolded dislocation loops based on the results of nanoindentation tests and high resolution TEM works.



Student Award in IAE, Kyoto University (2018)

Advanced Energy Structural Materials
Research Section
Daniel Morrall (D3)

This award is conferred annually for excellent students of the institute of advanced energy, Kyoto University, who gained superior achievements in their research under supervision of professors in the institute.

I studied on mechanically alloyed austenitic stainless steel that is developed for application to so-called accident tolerant fuel claddings of light water reactors. The yield stress of the newly developed alloy is more than three times higher in comparison to the conventional SUS316L and corrosion resistant in supercritical pressurized water (773K, 25 MPa) is much better than SUS316L. These high performance properties of the alloy is due to fine grains about two order of magnitude smaller than SUS316L.



Molten Salt Prize (Molten Salt Committee, The Electrochemical Society of Japan)

Chemical Reaction Complex Processes
Research Section
Toshiyuki Nohira (Professor)

Professor Toshiyuki Nohira was awarded Molten Salt Prize from the Molten Salt Committee of the Electrochemical Society of Japan on January 28th, 2019. The Molten Salt Prize is annually given to a researcher who has achieved outstanding academic results in the field of molten salts. He was awarded this prize on the achievements of “Novel Electrochemical Reactions in Molten Salts and Their Applications”.

In his award lecture, which was held on January 28th, 2019 at Kobe University, he presented several new electrochemical reactions in molten alkali halides and alkali earth halides, e.g., a new production method of solar grade silicon, electrodepositions of Si, Ti and W, and a new electrochemical synthesis method of diamond.



Young Researcher's Award in the 3rd Kansai Electrochemistry Workshop

**Chemical Reaction Complex Processes
Research Section
Tomonori Kato (M2)**

The 3rd Kansai Electrochemistry Workshop, which was sponsored by the Kansai Branch of the Electrochemical Society of Japan, was held on 1st December, 2018 at Kobe University. This event provides young researchers and students in the field of electrochemistry and its surrounding area an opportunity to present their works.

Tomonori Kato (M2) attended and made a poster presentation on the topic of "Electrodeposition of crystalline silicon film from KF-KCl molten salt aiming at the development of a new production process of silicon solar cells".

He received the Young Researcher's Award from the Kansai Branch of the Electrochemical Society of Japan.



Young Researcher's Award in the 3rd Kansai Electrochemistry Workshop

**Chemical Reaction Complex Processes
Research Section
Yuanjia Ma (D1)**

The 3rd Kansai Electrochemistry Workshop, which was sponsored by the Kansai Branch of the Electrochemical Society of Japan, was held on 1st December, 2018 at Kobe University. This event provides young researchers and students in the field of electrochemistry and its surrounding area an opportunity to present their works.

Yuanjia Ma (D1) attended and made a poster presentation on the topic of "Precipitation of silicon from liquid Si-Zn alloy in molten chlorides aiming at the development of a new production process of solar-grade silicon".

She received the Young Researcher's Award from the Kansai Branch of the Electrochemical Society of Japan.



**The 25th Young Researcher's Award in
139th Meeting of The Surface Finishing
Society of Japan.**

**Chemical Reaction Complex Processes
Research Section
Yutaro Norikawa (D2)**

The 139th Meeting of The Surface Finishing Society of Japan was held on 18–19th March 2019 at Kanagawa University.

In this meeting, Mr. Yutaro Norikawa made a poster presentation on the topic of “The Effect of Temperature on Electrodeposition of Ti in Fluoride–Chloride Mixture Molten Salt”. He presented the effect of temperature on the electrochemical behavior of Ti(III) ions and the deposited Ti. The diffusion coefficient of Ti(III) ions became higher according to the temperature increase. Rapid diffusion of Ti(III) ions was advantageous to obtaining smooth Ti films. However, Ti films with smooth surface were obtained at lower temperature. This result means the crystal growth due to temperature is dominant for electrodepositing smooth Ti films. Finally, he was awarded the The 25th Young Researcher's Award.



4. JOINT USAGE/RESEARCH PROGRAM



Joint Usage/Research Center Program “Zero Emission Energy Research”

It is an urgent task to find out the best solutions against the energy and environmental problem for ensuring the sustainable society on the earth. The new energy system for this purpose has to be an environmentally friendly or ecological one. Here, we should consider not only the energy sources but also the efficiency in the each phase of energy usage. The former should have good quality and enough quantity. The latter should be considered including the so-called “three Rs (Reduce, Reuse and Recycle)” in the energy system;

- Reduce of energy consumption, environmental pollutant such as greenhouse gas, waste-heat, hazardous waste, etc.
- Reuse of waste heat/energy, etc.
- Recycle of fuel, etc.

In order to realize them, only the extension of the present technology is not enough. Interdisciplinary studies with innovative ideas are indispensable to realize the energy system for next generation.

We propose a new concept of Zero Emission Energy as a typical model of Advanced Energy. IAE Zero Emission Energy Research aims at the realization of environmentally friendly energy system for sustainable society with minimum emission of environmental pollutants and with maximum utilization of energy and resources. Since FY2011, we had operated a project, “Joint Usage/Research Program on Zero Emission Energy”, which is the program authorized by the MEXT. We have started the second term of the Program from FY2016. Here, we aim to (1) promote interdisciplinary joint usage/research studies for

Zero Emission Energy Science & Technology, (2) promote education & practical training for young researchers and (3) explore future horizon of Advanced Energy System for sustainable development. IAE provides many unique & attractive facilities for the Joint Usage/Research not only in the field of advanced plasma & quantum energy but also in the field of soft energy.

Many researchers have participated in this program. In FY2018 Joint Usage/Research collaborations of total 98 subjects (including two workshops) on Zero Emission Energy were performed with more than 294 visiting participants from 56 all-Japan Universities and Institutions including graduate/undergraduate students. Researchers from five foreign Universities also participated in the program. The results of these collaborations are summarized in a report “IAE Joint Usage/Research Program on Zero Emission Energy 2018. Some of them were reported and discussed in a Research Summary Meeting of FY2018 held at Uji Campus on March 7, 2019. If you have interest to this collection, please contact to the Office of Zero Emission Energy Research.

In addition to the Joint Usage/Research collaborations, we organized "The 9th International Symposium of Advanced Energy Science -Interplay for Zero-Emission Energy-" on September 3–5, 2018 at Uji Obaku Plaza, Kyoto University. This symposium consists of oral and poster sessions, panel discussion, parallel seminars and satellite meeting. About 402 scientists and students including four foreign and five domestic invited speakers were participated in the symposium. In addition, several informal seminars and/or internship on Zero Emission Energy were also organized. (http://www.iae.kyoto-u.ac.jp/zero_emission/calendar/)

We are also operating “Zero Emission Energy Network” to share the knowledge of Advanced Energy and Zero Emission Energy with researchers in the fields of energy science and technology, since world-wide activities for Zero Emission Energy Research are indispensable for the realization of sustainable society.

In FY2018, the intermediate examination by MEXT was conducted for all the Joint Usage/Research Center Programs. Our program was given "A" evaluation. We will continue the effort to keep this high evaluation with the researchers of the related communities.

The 9th International Symposium of Advanced Energy Science
-Interplay for Zero-Emission Energy-

Sept. 3-5, 2018

Venue: Uji Obaku Plaza, Kyoto University Campus, Kyoto, Japan

Organized by: IAE, Zero Emission Energy Research, Kyoto University

Invited Speakers:

- Kazuo Ohgura (Kyoto Univ.)
- Yukihiro Ueda (Kyoto Univ.)
- Paul Walker (University of Cambridge)
- George M. Rice (University of California)
- Shirley Meng (Tsinghua Univ.)

List of Zero Emission Energy Joint Usage/Research Subjects in FY 2018

(Subject, Principal Researcher, IAE Key Person)

Elucidating Hopping Conduction Mechanism of Hydronium Solvate Ionic Liquids using NMR

A. Kitada, M. Katahira

He and Heavy ion synergism on hydrogen isotope behavior in tungsten at higher temperature

Y. Oya, T. Hinoki

Effects of Magnetic Field and Metal Nanoparticles on Photocurrents of Dye-Metal Nanoparticle Composite Films

H. Yonemura, H. Sakaguchi

Recovery of Silicon Deposits from Liquid Si-Zn alloy for the Production of Solar-grade Silicon

K. Yasuda, T. Nohira

Development of anode/electrolyte interface for advanced Na-ion battery

H. Sakaguchi, T. Nohira

Study on development of compound-based anode for K-ion battery and on compatibility with molten salt electrolyte

Y. Domi, T. Yamamoto

Study of interaction between dislocation and irradiation defects for evaluation of material degradation in nuclear structural materials

K. Fukumoto, A. Kimura

Characterization and application of biomass originated from indigenous bacteria of activated sludge

M. Takeda, M. Katahira

Study on chemical stability elucidation method of Li based oxide for advanced tritium breeding material by EPMA-SXES analysis

K. Sasaki, K. Mukai

R&D of standard for ion-irradiation fields

R. Kasada, K. Yabuuchi

Photoenergy Conversion System Based on Hybrid DNA/Dye Nanomaterials

K. Yamana, T. Morii

Combined effect of high-temperature irradiation with heavy ion and helium on hydrogen permeation behavior in functional coating for fusion reactor blanket

T. Chikada, K. Yabuuchi

Development of the energy functionality through selective phonon-mode excitation by mid-infrared free-electron laser

K. Hachiya, H. Ohgaki

Electrodeposition of Si films in molten salts for low-cost manufacturing of solar cells

X. Yang, T. Nohira

Development of PALS evaluation method using a TEM-disk-size miniature specimen.

M. Akiyoshi, T. Hinoki

Influence of high temperature irradiation on hydrogen isotope retention and permeation in first wall and divertor materials for fusion reactors

Y. Hatano, T. Hinoki

Analysis of high-reactive structure in lignin for advanced biomass utilization

K. Fukushima, M. Katahira

High-Fluence Irradiation Behavior of Reduced Activation Fusion Reactor Materials

H. Tanigawa, T. Hinoki

Development of pollution drainage-zero emission system using hybrid nanofibers containing enzyme and photocatalyst

T. Waku, T. Morii

Development of a tool that detects trace amounts of proteins

Y. Katsuda, T. Morii

Development of Organic-Inorganic Hybrid Film toward High-Performance Organic Thin-Film Solar Cells

T. Akiyama, H. Sakaguchi

Design and development of functional organic materials for energy conservation-directed light-emitting devices

M. Shimizu, H. Sakaguchi

Chemical state analysis in oxidation reaction of advanced neutron multiplier for fusion reactor blanket

M. Nakamichi, K. Mukai

Photoinduced electron-transfer reactions of metal complexes as photosensitizers bound to the active site of enzyme

H. Takashima, E. Nakata

Mechanism of Radiation Resistance of Advanced Tungsten Alloys

A. Hasegawa, A. Kimura

Verification of a new theory on MHD relaxation from axisymmetric to helical axis toroidal plasma
S. Masamune, K. Nagasaki

Effects of chromium and titanium concentration on low-temperature ductility of high-purity low-activation vanadium alloys
T. Nagasaka, A. Kimura

Irradiation-assisted Ostwald ripening of oxide particles in oxide dispersion strengthened (ODS) alloys
N. Oono, A. Kimura

Modeling and Experimental Study on Damage Rate Effects on Bubbles/Voids Formation in Fusion Reactor Structural Materials
T. Yamamoto, A. Kimura

In Situ Measurement of Oxide Precipitation in Al-Added ODS Alloy Powders
N. Iwata, A. Kimura

Mechanical Property of Ion-irradiated RAFMs by Ultra Micro-tensile Test
M. Ando, A. Kimura

Evaluation of the stability of irradiation induced point defect clusters during annealing
S. Jitsukawa, A. Kimura

Investigation of hydrogen isotope retention mechanism in tungsten based materials under divertor plasma exposure in fusion reactors
Y. Ueda, A. Kimura

Improvement of Radiation Measurement Method for the Detection of special nuclear materials with IEC Device
T. Misawa, K. Masuda

Study on Pulse Shape Discrimination for Neutron Energy Distribution Measurements using Scintillators
Y. Takahashi, K. Masuda

Interaction analysis between cellulase carbohydrate-binding module and lignin by ultra-high sensitivity NMR for biorefinery
T. Watanabe, M. Katahira

Towards an innovative micro-grid for Rural Electrification in Cambodia
V. Vai, H. Ohgaki

Synergistic effects of electronic excitation and displacement damage in oxide/nitride ceramics
K. Yasuda, A. Kimura

Confirmation of the process of internalization by using ultrasound-enhanced cell-internalization
T. Otsuki, E. Nakata

A small-molecule-based technology for live-cell imaging of energy metabolism.
S. Sato, T. Morii

Influence of Spacer Wire on Natural Convection Heat Transfer from Vertical Rod Bundle in Liquid Metal
K. Hata, T. Nakajima

Development of functional peptides that bind to RNA
T. Sakamoto, T. Nagata

Supramolecular assembling regulation of bacterial cell division protein FtsZ on DNA nanostructures
A. Onoda, E. Nakata

Suppression of wall erosion by vapor shielding during transient heat loads at fusion reactor
K. Ibano, S. Konishi

Development of the improved RNA mutagenesis technology for regulating an energy system in the cell
M. Fukuda, T. Morii

Suppression of MOX fuel used in LWR swelling caused by development of gas bubble resulted from He accumulated during long-term storage.II
H. Serizawa, T. Hinoki

Irradiation effect of mid-infrared free electron laser on melanoma
T. Kawasaki, H. Zen

Development of photo-functional atomic layer heterostructures
Y. Miyata, Y. Miyauchi

Production and transport control of reactive radicals with atmospheric pressure plasma
H. Matsuura, S. Kado

Study of electron bunch length by measuring coherent synchrotron radiation with narrow-band detectors
N. Sei, H. Ohgaki

Improvement of Mechanical Properties on the ODS Stainless Steels for Advanced Nuclear and Thermal Power System Components
S. Noh, A. Kimura

Microstructural evolution and change in thermal conductivity of heavy ion-irradiated Fe-based composite materials
N. Hashimoto, A. Kimura

Clarification on formation mechanism of ion radiation-induced defects for silicon carbide materials
B. Tsuchiya, T. Hinoki

Highly efficient photochemical reactions induced by optimal laser pulses
Y. Ohtsuki, T. Nakajima

Structural studies on hierarchical molecular architectures created in microfluidic device
M. Numata, E. Nakata

Studies of ballooning mode using high-speed soft X-ray camera in Heliotron J
Y. Takemura, S. Yamamoto

Observation of Phase Transition Precursor in Prussian Blue Related Compounds Under Mode Selective Excitation of Bridging Molecules"
M. Kitaura, H. Zen

Development of single-electron irradiation technique for microscopic track structure study
Y. Uozumi, H. Ohgaki

Effect of high density neutral particles on peripheral plasma during SMBI
N. Nishino, H. Okada

Analysis of reaction mechanism of haloacid dehalogenase
T. Nakamura, T. Morii

Development of innovative solar cell devices based on the synergy between layered material and nitride semiconductor
S. Mouri, K. Matsuda

Development of HeI image reconstruction technique using neural network in Heliotron J
H. Kawazome, S. Kado

Effect of hydrogen on surface hardness in ion-irradiated tungsten
K. Sato, A. Kimura

Analysis of radiation induced nano-clusters in RPV steels
H. Watanabe, A. Kimura

Effects of microstructure evolution on the surface by ion irradiation and evaluation of residual elastic strain
T. Shibayama, T. Hinoki

Iontronic devices using multifunctional microparticles
N. Yonekura, T. Nakajima

Effect of external stress on radiation damage in explosion bonded Cu/steel joint
S. Ohnuki, A. Kimura

Impact of high energy ion irradiation on thermal and particle loading properties of plasma facing materials
K. Tokunaga, A. Kimura

Development of nucleic-acids-based enzyme containing G-quadruplex structures.
H. Masaki, T. Morii

Real-time NMR analysis of the continuous degradation process of azo dyes using azoreductase in cooperation with the NADPH regeneration system.
M. Horiuchi, T. Nagata

Physical properties of heterostructures of 2D materials
S. Okada, K. Matsuda

Digital Imaging Spectrometry for Visible Spectra in Fusion Plasma
M. Irie, S. Kado

High temperature oxidation/corrosion of SiC/SiC composites
K. SHIMODA, T. Hinoki

Local measurement of the recycling flux in the Heliotron J plasma using high wavelength-resolution spectroscopy of a helium atom near-infrared emission line
T. Shikama, S. Kado

Phase measurement of vacuum-ultraviolet pulse and control of electronic states
R. Itakura, T. Nakajima

Computer simulation study for development of an irradiation correlation technique
Y. Watanabe, K. Morishita

Observation of fine temperature structure by using digital ECE
S. Inagaki, K. Nagasaki

Development of intracellular thermosensors for the understanding of energy production in mitochondria
R. Sakaguchi, T. Morii

Study of atomic layered materials toward efficient and high-performance energy conversion
S. Konabe, Y. Miyauchi

Accelerated CO₂ reduction reaction achieved by accumulation of solute in nanoporous carbon electrode
K. Fukami, M. Kinoshita

Development of multi-channel spectroscopic system for turbulence measurement
A. Fujisawa, S. Ohshima

Optimization study on high energy ion confinement in advanced heliotron configuration
M. Yoshikawa, S. Kobayashi

Study on Rural Electrification by Renewable Energy in Sarawak and its Impact on QOL
N. Abd Rahim, H. Ohgaki

Study on the hydrothermal corrosion of irradiated SiC and underlying mechanisms
S. Kondo, K. Yabuuchi

Effect of temperature distribution on integrity of a reactor pressure vessel during emergency core cooling
Y. Yamamoto, K. Morishita

Design and construction of external stimuli-responsive protein materials
Y. Suzuki, E. Nakata

Fabrication of large-scale mock-up samples of precipitate/matrix interface for in-depth analysis of irradiation-induced precipitate dissolution in nuclear materials
Y. Matsukawa, A. Kimura

Development of high-efficiency ultrashort-pulse ring beam converter with axicon mirrors
G. Miyaji, K. Matsuda

Saturation of an infrared semiconductor detector and pulse structure of a light source
Y. Ikemoto, H. Zen

Study on emission process of scintillation material using the one electron beam
S. Kurosawa, H. Ohgaki

Study of carbon-based materials and bio-photoreaction using infrared free electron laser"
Y. Hayakawa, H. Ohgaki

Boundary diagnostics using field corresponding double probe in Heliotron J
K. Uehara, S. Ohshima

Statistical analysis on edge turbulence fluctuation data in a toroidal plasma
Y. Nagashima, S. Ohshima

Study for polarization control of coherent THz undulator radiation
S. Kashiwagi, H. Zen

Capacity Recovery Mechanism on Al-doped Alpha Fe₂O₃
S. Takai, T. Morii

Search for nonlinear effects using KU-FEL
A. Irizawa, H. Zen

A3 (Japan, Korea, China) Symposium on Emerging Materials: Nanomaterials for Electronics and Energy
H. Ago, K. Matsuda

Future prospects of high energy particle irradiation research on zero-emission energy structural materials (Zero-emission energy workshop)
R. Kasada, A. Kimura

5. COLLABORATION WORKS IN THE LABORATORY FOR COMPLEX ENERGY PROCESSES

Collaboration Works in The Laboratory for Complex Energy Processes

1. Introduction

The laboratory was established for research on advanced energy by the collaborative projects among the researchers in the Institute . to concentrate all our knowledge and wisdom to find solutions to these interdisciplinary energy/environmental problems. From such a viewpoint, the research targets of the laboratory are focused on two specific fields, (i) "advanced studies of science and technology on plasma energy and quantum energy" and (ii) "innovative studies of nano-bio functional materials for power generation". Therefore, two sections (A2 and A3 mentioned below) are founded. In addition, A1 section promotes international or domestic collaborative research and assists activities such as academic meetings and seminars.

In order to perform the research objectives of the Institute of Advanced Energy, it is essentially necessary to organize the cooperative research program with much close connection between related research fields in the institute. The laboratory takes charge of organizing and promoting the cooperative research project as a center of research activity in the Institute. The research staffs in the institute participate in specific projects to carry out their subjects. The scientists of other faculties in Kyoto University can also participate in the cooperative project to enhance the progress of research and educational activities. The laboratory also manages various functions such as symposium and seminar for related topics on energy field. The cooperative research activities will be published in a publication edited in the laboratory at the end of the year. Management of the technical staffs for large scale equipment are also under the responsibility of the laboratory.

A1 Division of International and Industrial Partnership

This division promotes international collaborative research on advanced energy to lead the field of energy science and technology as a worldwide pioneer. For this purpose, the symposium and the workshop organized by institution member are supported. This section also promotes young researcher/student exchange, coopera-

tive research activities and multi-lateral collaborative research with industries. Establishment of infrastructure and human resource development are also supported.

A2 Division of Plasma and Quantum Energy Research

This section promotes studies on advanced plasmas and quantum energy for realizing future energy systems, integrating plasma energy science and advanced energy material research. In particular, based on the results obtained in our related group, we aim at extending the research fields and contributing to human society by utilizing the existing key devices such as Heliotron J, DuET, MUSTER and inertial electrostatic confinement (IEC) device, which have been developed in IAE.

A3 Division of Soft Energy Science Research

This division promotes studies on emergent materials and systems for realizing next generation soft energy system. In particular, functional nano- and bio-materials to efficiently utilize solar energy and bio-energy are studied by integrating laser science, nanotechnology, and bio-technology. We aim at extending our research fields by utilizing the existing devices such as System for Creation and Functional Analysis of Catalytic Materials, SEMs, SPM, Solar Simulator, KU-FEL and various laser systems.

2. The cooperative research program

A brief summary of the cooperative research subjects carried out in FY2018 are shown next pages, which were proposed by researchers of IAE and selected by the program committee of the Laboratory.

The framework of the cooperative researches in the section A2 and A3 are changed in this year. The financial resource is focused to a small number of project proposals under the leadership of the chairs of three divisions who review the proposals from IAE researchers and arrange the accepted ones.

As a result, the research themes of 5 were applied and applications of 5 were accepted. The number of research subjects is listed in Table 1 according to the project categories.

Table 1 Number of the accepted research subjects according to the standard project theme

The whole sum 5

Category			Total
A1	A2	A3	
5	2	2	9

The individual research subjects are as follows

A1

“Supporting Activities on International and Industrial Collaborative Research”

“A3 (Japan, Korea, China) Symposium on Emerging Materials; Nanomaterials for Electronics and Energy”

- K. Matsuda Y. Miyauchi (Inst. Adv. Energy, Kyoto Univ.)
- Y.H. Lee (SKKU)
- F. Wei (Tsinghua Univ.)
- R. Saito (Tohoku Univ.)
- S. Iijima H. Shinohara Y. Ohno R. Kitaura (Nagoya Univ.)
- S. Maruyama (Tokyo Univ.)
- S. Saito (Tokyo Institute of Technology)
- H. Kataura (National Institute of Advanced Industrial Science and Technology)
- H. Gogoh T. Fujigatani (Kyusyu Univ.)
- M. Noda (Waseda Univ.)

“Holding the Workshop on technology and application of the next generation nondestructive assay using quantum beam and travel fee support for student presenters”

- H. Zen H. Ohgaki (Inst. Adv. Energy, Kyoto Univ.)
- M. Katoh, T. Ohigashi (UVSOR, IMS)
- M. Ito (JAMSTEC)

“International Workshop on Magnetic Configuration Optimization in Helical Systems”

- K. Nagasaki, S. Yamamoto, S. Ohshima, T. Mizuuchi, T. Minami, H. Okada, S. Kado, S. Kobayashi (Inst. Ad. Energy, Kyoto Univ.)
- Y. Nakamura, A. Ishizawa (Grad. Sch. of Energy Sci., Kyoto Univ.)
- S. Murakami (Faculty of Engineering Kyoto Univ.)
- M. Yokoyama, Y. Suzuki, M. Nakata, S. Okamura, A. Shimizu (National Inst. Fusion Sci.)
- A. Bader (University of Wisconsin Madison, USA)
- J. Proll (Eindhoven University of Technology, Netherland)
- C. Zhu (Princeton Plasma Physics Laboratory)

“NMR training of the structure-function correlation studies on woody biomass and functional biomacromolecules, and information exchange at the Yokohama NMR meeting”

- T. Nagata, Y. Yamaoki, K. Kondo, K. Kanba (Inst. Ad. Energy, Kyoto Univ.)
- T. Nagashima, T. Yamazaki, N. Kobayashi, K. Tsuda (RIKEN Yokohama, RSC)
- N. Nishida (Tokyo Univ.)
- G. Kawai (Chiba Institute of Technology)

“Seminar on development and application of ultrafast electron diffraction system in MeV and keV energy range”

- H. Zen. H. Ohgaki, T. Kii, K. Masuda (Inst. Adv. Energy, Kyoto Univ.)
- J. Kyu Ha (KAERI, Korea)

A2**“Influences of three dimensional magnetic field on a diverter plasma in a torus device”**

- S. Ohshima, T. Minami, S. Yamamoto, S. kado, S. Kobayashi, H. Okada, K. Nagasaki, S. Konoshima, (Inst. Adv. Energy, Kyoto Univ.)
- R. Matoike (Grad. Sch. Energy Sci., Kyoto Univ.)

“Production of MeV-class electrons by stochastic Landau-acceleration using non-resonant microwaves and its application to novel plasma initiation”

- S. Kobayashi, K. Nagasaki, H. Ohgaki, T. Kii, H. Zen, K. Masuda, T. Minami, S. Yamamoto, S. Kado, S. Ohshima, H. Okada, T. Mizuuchi, S. Konoshima (Inst. Adv. Energy, Kyoto Univ.)
- S. Torsten, H. Laqua (Max-Planck Institute for Plasma physics)
- M. Preynas (Ecole polytechnique federale de Jausanne)

A3**“Development of time-resolved fluorescent polarization system for measuring kinetic process of recognition and/or reaction and its application ”**

- E. Nakata, T. Morii, K. Matsuda (Inst. Adv. Energy, Kyoto Univ.)

“Development of defect-free graphene nano ribbons with MIR-FEL”

- T. Kojima, H. Sakaguchi, H. Ohgaki, T. Kii, H. Zen (Inst. Adv. Energy, Kyoto Univ.)

THE LABORATORY SEMINARS

Laboratory Seminars

The Laboratory promotes topical academic seminars in order to strengthen the research activities in each research section and to enhance the mutual cooperation among a lot of academic fields. The Laboratory also had a symposium on April 5, 2019 for discussions of the cooperative research results in FY2018

In FY2018 seminars were held with following themes.

1. Topical Seminars

(1) April 11, 2018

S. Fujiyoshi

“Nanometer-precision cryogenic fluorescence microscopy: towards molecular-level optical imaging”.

Tokyo Institute of Technology

(2) Jun. 25, 2018

Gunsu S. Yun

“Plasma Physics and XFEL activities in POSTECH”.

Department of Physics, POSTECH

(3) July 9, 2018

Sudip. Sen

“Partnership and Interdisciplinary Research at the Consortium of Modelling and Simulation at National Institute of Aerospace in Virginia”.

National Institute of Aerospace and William & Mary, Virginia, USA

(4) November 1, 2018

Gary S. Was

“Ion Irradiation as a surrogate for Reactor Irradiation: The Expected and The Surprises”.

Michigan University USA

Sergei L. Dudarev

“Elastic Fields and Interaction between Self-Interstitial Atom Defects in Bcc Metals”.

United Kingdom Atomic Energy Authority

(5) February 1, 2019

D. Shibata

“Considering Agriculture from the Aspect of Energy-Relations with Paris Agreement, Bioeconomy, SDGs-”.

Inst. Adv. Energy, Kyoto Univ.

(6) February 20, 2019

T. Lhendup

“Analysis of Building Energy Performance: Current and Future Trend in Bhutan”.

Matsumae International Foundation Fellow

K. Sakaue

“Interdisciplinary Research on Quantum- Opt Beams : from Laser-Compton Gamma-ray to Laser Processing”

Waseda Institute for Advanced Study

(7) March 25, 2019

W. Chaiwat

“Study on Propensity to Spontaneous Heating of Torrefied Biomass Under Dry Air and Water Vapor at Over 100°C using TG-DSC”.

Mahidol University

2. Colloquium

(1) September 20, 2018

T. Kojima

“On-Surface Bottom-Up Synthesis with Biomimetic Approach”.

Inst. Adv. Energy, Kyoto Univ.

(2) October 5, 2018

T. Kii

“Current Path in Superconductor”.

Inst. Adv. Energy, Kyoto Univ.

(3) October 18, 2018

Y. Miyauchi

“Nanomaterials Science on Heat to Light Energy Conversion”.

Inst. Adv. Energy, Kyoto Univ.

(4) November 2, 2018

K. Masuda

“Development and Applications of Nuclear Fusion –Based Compact Neutron Generators”.

Inst. Adv. Energy, Kyoto Univ.

(5) November 22, 2018

T. Nakajima

“Real-Time Monitoring of Nano bubbles using a Laser”.

Inst. Adv. Energy, Kyoto Univ.

(6) December 19, 2018

K. Yabuuchi

“Lattice Defects in Advanced Energy Structure Materials”.

Inst. Adv. Energy, Kyoto Univ.

(7) December 20, 2018

T. Nagata

“Energy Structural Life Science Approach for the Effective Utilization of Biomass”.

Inst. Adv. Energy, Kyoto Univ.

(8) January 17, 2019

T. Hinoki

“Development of Ceramic Matrix Composites for the Use in Steam Environment Up to 1600°C”.

Inst. Adv. Energy, Kyoto Univ.

(9) January 25, 2019

T. Minami

“Formation of Electron Internal Transport Barrier and Nd:YAG Thomson Scattering Measurement in Heliotron J”.

Inst. Adv. Energy, Kyoto Univ.

(10) February 1, 2019

T. Kodaki

“Efficient Production of Energetic Materials from Biomass”.

Inst. Adv. Energy, Kyoto Univ.

(11) February 8, 2019

E. Nakata

“Development and Applications of Targeting Technique Based on the Regulation of Dynamic Equilibria”.

Inst. Adv. Energy, Kyoto Univ.

(12) February 15, 2019

S. Nakano

“Construction of Receptor-Based Sensors and Catalysts by Using the Library of RNA-peptide Complex”.

Inst. Adv. Energy, Kyoto Univ.

(13) February 22, 2019

T. Yamamoto

“Development of Ionic Liquid Electrolytes for Potassium Secondary Batteries”.

Inst. Adv. Energy, Kyoto Univ.

(14) March 1, 2019

A. Rajendran

“Topologically-Interlocked DNA Structures inside a DNA Origami Nanostructure”.

Inst. Adv. Energy, Kyoto Univ.

(15) March 8, 2019

K. Morishita

“System Main technology for Advanced Safety of Nuclear Energy Plants”.

Inst. Adv. Energy, Kyoto Univ.

(16) March 28, 2019

J. Yagi

“High Temperature Liquids for Fusion Engineering”.

Inst. Adv. Energy, Kyoto Univ.

6. PROJECTS WITH OTHER UNIVERSITIES AND ORGANIZATIONS

Innovative strategy for highly efficient utilization of solar energy

"Exploring novel principles for highly efficient utilization of solar energy"

The MEXT special budget project in its final year of the six-years program pursued three main research topics including efficient conversion of solar energy to electricity, production of solar fuels, and efficient conversion of biomasses to useful chemicals.

1. Efficient conversion of solar energy to electricity

Helical nanopore formation caused by chiral symmetry breaking in metal-assisted chemical etching of silicon. Porous silicon is formed not only by anodic polarization of a silicon wafer in HF but also by accelerated local corrosion at the interface between silicon and metal nanocatalysts in etchant that contains an oxidant and HF. This type of porosification is so-called metal-assisted chemical etching of silicon. When using Pt as the nanocatalyst, helical nanopore is obtained. Prof. Fukami studied the mechanism of helical nanopore formation in detail. His group has clarified that an instability observed in the silicon anodization is the clue to understand the chiral symmetry breaking and the steady growth of helical nanopore into silicon.

Electrodeposition of Si, Ti and W from Water-Soluble KF-KCl Molten Salts. It is well known that refractory metals and Si can be electrodeposited from fluoride-based molten salts like LiF-KF and LiF-NaF-KF. One of the problems in the previous studies employing fluoride-based molten salts was the difficulty in removing the salt adhered to the deposits, because the solubility of LiF and NaF in water is very low. Prof. Nohira has recently proposed a new electrodeposition process of Si and Ti using eutectic KF-KCl (45:55 mol%) system. Since both KF and KCl are highly soluble in water, the adhered salt can be removed easily by washing with water. This year, Prof. Nohira's group investigated the electrodeposition of Si, Ti and W in molten KF-KCl.

Further improvement of photovoltaic performance of polythiophene/antimony sulfide planar solar cells. Prof. Sagawa investigated incorporation of interfacial layer of SrTiO₃ between TiO₂ and Sb₂S₃ interface to decrease the interfacial barrier for easy electron extraction and declination of charge recombination in the planar solar cells composed of glass/F-doped SnO₂/TiO₂/Sb₂S₃/poly[(3-hexylthiophene)-2,5-diyl]/poly[3-(3-carboxypropyl)thiophene-2,5-diyl]/Au. Through the optimization in terms of the interfacial contact, increase of the open circuit voltage was not only achieved but the short circuit current density and the fill factor in addition to the enhancement of the power conversion efficiency as compared with the device without the SrTiO₃ layer.

Novel Light-matter Interaction in Low-dimensional Materials toward Light Energy Applications. Prof. Matsuda's group has investigated toward the efficient light energy utilization using extremely low-dimen-

sional materials such as carbon nanotubes, nano-graphene, and transition-metal dichalcogenides. These novel extremely low-dimensional materials have attracted a great deal of attentions from view point of fundamental physics, material science and also potential applications. The studies of atomically-thin layered materials such as transition-metal dichalcogenides called as "beyond graphene", have emerged, and drastically accelerated, because of novel optical phenomena and its usefulness for light energy applications. Novel optical properties and functionalities in these extremely low-dimensional materials were investigated.

Energy Material Research in KU-FEL. Prof. Ohgaki's group carried out research on applications of KU-FEL on energy materials at Institute of Advanced Energy, Kyoto University. The Mid-Infrared FEL facility, KU-FEL, has been offering FEL beams to the research on the energy material, such as wide-gap semiconductors.

Rapid in-situ synthesis of metal-polymer nanocomposites using a mid-IR laser. Prof. Nakajima demonstrated a rapid in-situ fabrication of metal-polymer nanocomposite films using a mid-IR laser, and characterized the optical and morphological properties. The required laser power and irradiation time were only 0.8-1W and 10-30 sec, respectively. Interestingly, the properties of the fabricated films depended on the various factors such as the concentrations of polymer and precursor of nanoparticles in the solution, not to mention the laser power and irradiation time. The morphological and optical properties of metal-polymer nanocomposite films through those parameters were successfully controlled.

2. Production of solar fuels

Significance of the reaction by spatially organized enzymes. One of the intriguing challenges for the efficient usage of solar energy tackles sequential chemical reactions driven by the visible light that realize the artificial photosynthesis. The research topics in Prof. Morii's group have been focused on the sequential enzymatic reaction by spatially arranged enzymes, the "dark reaction" of artificial photosynthesis system. Protein-based adapters were developed to locate multiple enzyme types to defined positions in an orthogonal manner on nanoscale scaffolds made by DNA origami. This strategy enables reconstitution of the natural enzyme cascades outside the cell.

Nature-Inspired Surface Science for Energy. Nature autonomously produces the complex-structured biological systems according to the self-organization principles, where individual molecular precursors are built into larger units (machines) based on the chemical interactions and molecular recognition principles. In the history of evolution, nature has utilized such systems to convert energy sources into chemical energy with minimizing

losses. Such energy utilization systems can be seen on photosynthesis and metabolism. Hence learning from nature can serve as a new paradigm to produce the unique materials for artificial energy-conversion. Additionally, surface science, called 'catalysis' plays a decisive role in producing the functional materials in modern society. Prof. Sakaguchi's group has been working on the 'nature-inspired surface science'. Cutting edge researches on surface polymerization to produce the functional materials on the basis of nature-inspired strategy, by the use of chirality, self-assembly and spatial patterns have been carried out.

3. Efficient conversion of biomasses to useful chemicals

Heterologous expression and characterization of enzymes of wood rotting fungi to be used for utilization of woody biomass. The first step to utilize woody

biomass for the production of high valued-added materials is degradation of three major components, cellulose, hemicellulose and lignin. Lignocellulose degradation enzymes of wood rotting fungi can be effectively used for this purpose. Prof. Katahira's group expressed, purified and characterized the following representative enzymes; lytic polysaccharide monoxygenases (LPMOs) for degradation of cellulose, manganese peroxidases (MnP) and glutathione S-transferases (GSTs) for degradation of lignin, and glucuronoyl esterases (GEs) for degradation of lignin-carbohydrate (lignin-hemicellulose) complexes. Some of these enzymes exhibited either very high or unique activity, which are advantageous for the application. Crystal structures of some of these enzymes are also resolved, giving a basis to elucidate the structure-function correlation.

NIFS Bilateral Collaboration Research Program on Heliotron J

Since FY2004, the Heliotron J group at IAE, Kyoto University has joined the Bilateral Collaboration Research Program by National Institute for Fusion Science (NIFS), an Inter-University Research Institute. This unique collaboration program promotes joint researches bilaterally between NIFS and research institutes or research centers of universities that have unique facilities for nuclear fusion research. Under this collaboration scheme, the facilities operated in the different universities are open to all fusion researchers just as joint-use facilities of NIFS.

The main objective of the research in our Heliotron J group under this joint research program is to investigate experimentally/theoretically the transport and stability of fusion plasma in advanced helical-field, and to improve the plasma performance through advanced helical-field control in Heliotron J. Picked up in FY2018 are the following seven key-topics; (1) transport study concerning field configuration control and relating plasma structure formation control, (2) ECH/EBW heating mechanism study, (3) high-density NBI plasma generation and high-beta plasma confinement, (4) edge-plasma study in an advanced helical device, (5) suppression of MHD instabilities by configuration control, (6) plasma current control in an advanced helical device, (7) development of new technology in experiment and analysis.

Only some results from this collaboration in FY2018 are shortly reported below. Annual report for all of the collaboration subjects in this program will be published by NIFS.

Configuration dependence of isotope effects on turbulence system in Heliotron J [1]: The hydrogen/deuterium (H/D) isotope effect on fluctuations and its configuration dependence are studied in a helical device, Heliotron J. The isotope dependence of a toroidally symmetric fluctuation in a low frequency range of ~ 4 kHz, which is considered as a zonal flow, is observed in low-density ECH plasmas in Heliotron J. The fluctuation with long-range toroidal correlation becomes stronger and the correlation is enhanced in D dominant plasmas in standard configuration of Heliotron J, which shows that the confinement of turbulence transport should be improved in D plasmas. Interestingly, however, the opposite dependence on isotope ratio is observed in the magnetic configuration tagged here “low-bumpiness”. It is likely that impurities and radial electric field, which can also be influenced by isotope mass, have no significant influences on the zonal flow behavior in this experimental condition. The configuration dependence can be one of factors to explain the dif-

ference in isotope effect between tokamaks and helical devices.

Effect of magnetic field structure on electron internal transport barrier and its role for the barrier formation in Heliotron J [2]: Electron internal transport barrier (eITB) has been observed in various helical devices, such as, CHS, LHD, TJ-II and W7-AS. In Heliotron J experiments, the eITB formation is determined not only by the neoclassical transport to produce the positive radial electric field but also by the existence of a low-order rational surface. The low-order rational surface expands the improved confinement region generated by the eITB, and the power threshold to form the eITB for the plasma without the eITB is also reduced. Because a magnetic island can be formed on this rational surface, it is necessary to consider the effect of the magnetic island on the eITB formation.

Control of fast-ion-driven MHD instabilities by using electron cyclotron current drive [3]: Fast-ion-driven MHD instabilities sometimes cause enhancement of anomalous transport and loss of energetic particles like fusion oriented alpha particles. Therefore, the control of these instabilities is important to improve efficiency of output power of fusion reactor. Electron cyclotron current drive (ECCD) has good controllability by changing reflective index (N/ℓ) and absorption location via injection path change. We have demonstrated that FP-driven MHD instabilities including energetic particle modes (EPMs) and Global Alfvén eigenmodes (GAEs) can be controlled by means of magnetic shear modified by EC-driven plasma current. The $m/n=2/1$ mode of EPM is suppressed by increasing toroidal current in the co- and counter directions in the experiment in Heliotron J. The $m/n=4/2$ mode of GAE has same tendency.

References

- [1] S. Ohshima, et al., “The Configuration Dependence of Isotope Effects on Turbulence System in Heliotron J”, 27th IAEA FEC (22-27 Oct. 2018, Gandhinagar, India), EX/P3-3.
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7. HOW TO GET TO THE IAE

