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Institute of Advanced Energy
Kyoto University

ANNUAL REPORT 2023

京都大学エネルギー理工学研究所
Institute of Advanced Energy, Kyoto University

ANNUAL REPORT

2023

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Kyoto University

Gokasho, Uji, Kyoto 611-0011
Japan

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FOREWORD

The Institute of Advanced Energy (IAE) was founded in May 1996 to explore the energy systems for the next-generation by going back to the fundamental principles of nature, and to create new energy theories for the next generation and advanced technologies to guide and implement these theories. At present, the faculty members belonging to the Faculty Consort of Advanced Energy in the Natural Science Platform are engaged in 14 research sections in three divisions, each of which investigates one of the following three basic processes of energy: generation, conversion, and utilization. The Laboratory for Complex Energy Processes supports and stimulates collaborative research to address issues related to complex energy processes. The Integrated Research Center for Carbon Negative Science (ICaNS) was established in 2022. Through extensive collaboration with researchers in the Graduate Schools of Energy Science and Engineering, the Center is actively developing new concepts, academic foundations, and science and technology for the effective use of carbon dioxide to realize a carbon-neutral society.

The two core research areas of the Institute are “Plasma and Quantum Energy Science” and “Soft Energy Science”. The former aims to realize nuclear fusion to generate solar energy on Earth. The latter aims to achieve highly efficient energy utilization and conversion based on the principles of materials science and energy utilization by living organisms that have built the biosphere on Earth with solar energy. It also actively promotes the internationalization of research and the transfer of research results to society through cooperation between industry, academia and government.

Certified as a “Zero-Emission Energy” Joint Usage/Research Center by the Ministry of Education, Culture, Sports, Science and Technology (MEXT) in 2011, the Institute is entering its third phase of operation and continues to contribute to the zero-emission energy research community. As a Zero-Emission Energy research center, we collaborate with domestic and overseas researchers in a wide range of academic fields and promote the shared use of cutting-edge research equipment to strengthen the foundation of academic research and to accelerate new scientific research.

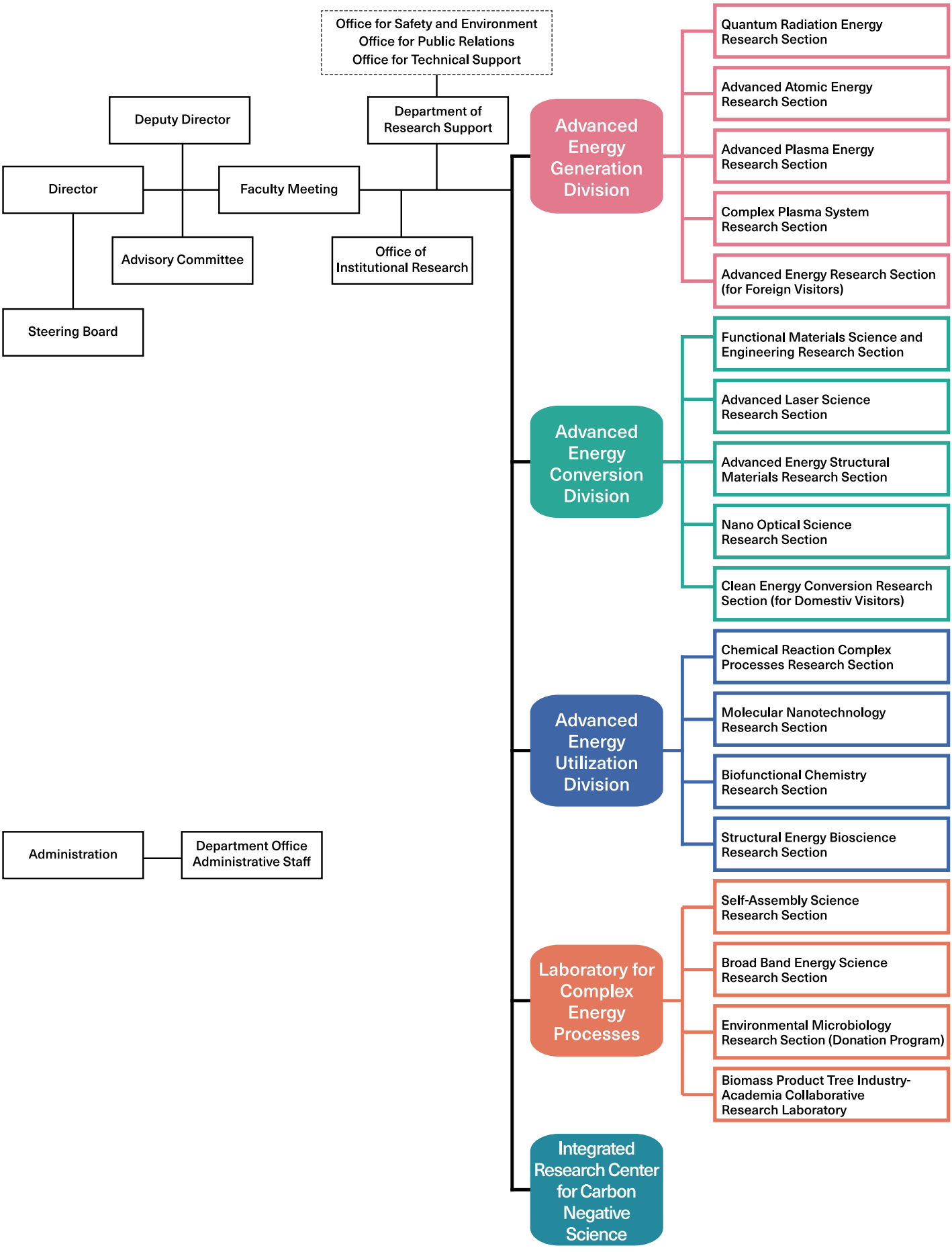
Japan has also set a goal of “virtually eliminating greenhouse gas emissions by 2050,” and carbon neutrality is now a goal for societies worldwide. The IAE is committed to a wide range of research into zero emission energy, which is certain to play an increasingly important role in achieving carbon neutrality and providing a variety of new energy technology options.

This annual report summarizes the major research achievements of each of IAE’s research divisions for FY2023 (April 2023-March 2024) to represent IAE’s research activities. I hope you will enjoy our Institute’s ongoing research in a wide range of scientific disciplines, which will surely provide innovative solutions to meet the demands of achieving carbon neutrality.

March 2024

Takashi MORII
Director
Institute of Advanced Energy
Kyoto University

2. ORGANIZATION CHART



3. RESEARCH ACTIVITIES

3-1. RESEARCH ACTIVITIES IN 2023

Quantum Radiation Energy Research Section

H. Ohgaki, Professor
T. Kii, Associate Professor (concurrent)
H. Zen, Assistant Professor
Jordi Cravioto Caballero, Program-Specific Assistant Professor

1. Introduction

Coherent-radiation energy with a wide wavelength tunability and a high power is an indispensable tool for exploiting cutting-edge science. The research in this section aims at generating and application of new quantum-radiation energy. Free-electron laser (FEL) is one of such radiation. We have been developing a mid-infrared FEL, KU-FEL. To extend study field wider wavelength region, a coherent A compact THz source, high Tc undulator for X-ray generation, and Laser Compton Gamma-ray (LCS) for isotope imaging have been carried out. Transdisciplinary research on renewable energy has also been promoted through international collaborations.

2. Free-electron Laser

FEL is a next generation light source because of its wide wavelength tunability where the conventional lasers cannot reach, potential high efficiency, and high peak 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, a high Tc undulator, etc.

2.1 KU-FEL

The target wavelength of KU-FEL is MIR (Mid infra-red) regime, from 5 to 20 μm, with high-power and tunability for basic research on energy materials. 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 60 mJ in a 2-μs macro-pulse at the wavelength of 9.8 μm. The FEL is routinely operated and opened for internal and external users.

For increasing the peak power of the KU-FEL, the photocathode operation of the 4.5-cell thermionic RF gun has been established. Under the photocathode operation, the micro-pulse energy of 100 μJ and the world highest extraction efficiency (9.4%) of the oscillator-type FEL has been achieved. Then the micro-pulse duration was shortened down to 150 fs (~4.2 cycles at 11 μm). In addition, Nonlinear compression of 8.6-μm FEL pulse has been achieved and the pulse duration was compressed from 146 to 106 fs (from 5.1 to 3.7 cycles) by passing through a 30-mm thick Ge plate.

For further increase of the peak power of KU-FEL, newly fabricated 1.6-cell RF gun has been installed at the upstream side of the accelerator tube. The initial commissioning of the new RF gun was successfully finished and FEL lasing with the electron beam generated from the gun has been achieved.

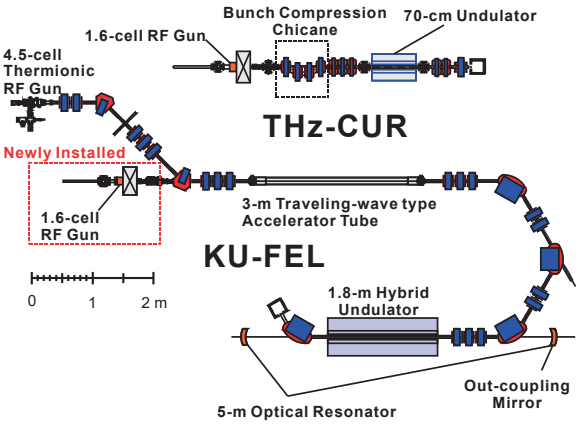


Fig. 1 Schematic drawing of the KU-FEL and THz-CUR

2.2 THz Coherent Undulator Radiation Source

A new compact terahertz coherent undulator radiation source (THz-CUR in Fig. 1) 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. 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.

The 1.6 cell RF gun used for the THz-CUR was replaced with an energy chirping cell attached RF gun for improving its performance under collaboration with Dr. Sakaue, Tokyo University. The gun utilizes a velocity bunching scheme for generating ultra-short electron bunch. A commissioning experiment has been done and the saturation of THz peak power due to the space charge effect can be success-

fully suppressed.

The polarization control method of the THz-CUR has been developed under collaboration with Dr. Kashiwagi, Tohoku University. The polarization state of the THz-CUR can be easily controlled from linear to left-handed circular and right-handed circular without significant power loss.

2.3 Application of MIR-FEL and THz-CUR

Many application researches of MIR-FEL and THz-CUR have been performed under the Joint Usage/Research Center for Zero Emission Energy Research of our Institute. In JFY2023, 17 external user groups used KU-FEL.

3. Bulk SC Staggered Array Undulator

An undulator with strong magnetic field will play an important role in future synchrotron light sources and FELs. We have developing a new undulator which consists of stacked bulk high critical temperature superconductors array and a solenoid magnet. The magnetic field strength is about three times higher than that of conventional permanent magnet undulators. (Fig.2)

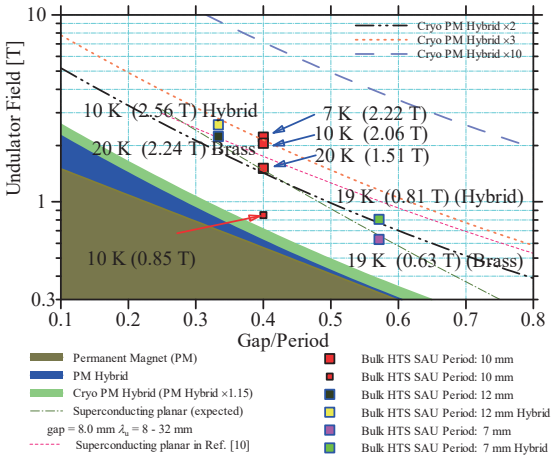


Fig. 2 Performance comparison

4. Isotope Imaging for Nuclear Safety and Security

Multi-isotope imaging method has been developed at BL1U beamline in UVSOR, Institute of Molecular Science. The enriched $^{206, 207, 208}$Pb and natural Pb target rods of 8 mmϕ was used for 1-D imaging experiment. The NRF gamma-rays emitted from the witness target consisted of enriched $^{206, 207, 208}$Pb rods were measured with two Ge detectors. The flux of the incident LCS gamma-ray beam (maximum energy of 5.53 MeV) with 2 mmϕ beam size was monitored by a plastic scintillator detector and whole absorption was measured by a $LaBr_3$(Ce) detector. The scanning step was 4 mm. As a result, two isotopes ($^{207, 208}$Pb) image was clearly obtained, but failed for ^{206}Pb whose NRF reaction rate is one order smaller than that of $^{207, 208}$Pb. Flat-LCS and standard LCS have been used for the measurement, and Flat-LCS enhanced lower energy (5.0-5.3 MeV) NRF peaks.

5. Social aspects of energy use

In 2023, more than 775 million people in the world are still without electricity. Recently, reports show that this figure has increased for the first time in decades. In Southeast Asia, almost 31 million people remain without access, but the study is insufficient compared to regions such as Africa and South Asia. Moreover, research focuses on economic, technological and institutional aspects of electrification, but studies focusing on social barriers and implications are still scarce. Therefore, our group investigates the social effects of electrification with a quality-of-life perspective by comparing experiences of rural electrification projects in Southeast Asia (Fig. 3). Applying mixed methods from the social sciences, we have found that solar systems can improve the education of children in rural households, reduce dependence on expensive and dangerous energy sources, and improve social interaction. However, economic disparities in the community can be exacerbated and concerns about changing lifestyles and limited system capacity are crucial aspects for successful projects. Our group also analyses how household roles affect efficient appliance purchasing in urban contexts and topics related to energy justice.

Fig. 3 Rural electrification survey sites 2016-2022

Acknowledgment

All our research works have been supported by the KAKENHI, Q-LEAP(MEXT), JASTIP(JST), UVSOR Collaboration Research, CSEAS DASU (Kyoto University), and the Laboratory for Complex Energy Processes Collaboration Research (IAE).

Collaboration Works

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Advanced Atomic Energy Research Section

K. Nagasaki, Professor (concurrent)
J. Yagi, Associate Professor
K. Mukai, Assistant Professor

1. Introduction

Main objective of our research division is to realize advanced energy systems for the sustainable development under global environmental constraints. We have shown 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 we now propose an innovative Negative emission scenario to isolate CO_2 in the atmosphere by a carbonization process. Our research section focuses on development of hydrogen isotopes fuel circulation system, breeding blankets, fusion material R&D, feasibility study for fusion-biomass hybrid power system, conversion of biomass waste, and fusion neutron generation/measurement. The following are main research achievements in the fiscal year of 2023.

- Accomplishment of the highest efficiency for fusion fuel extraction from lead lithium eutectic alloy using the droplet system in the fusion study field.
- Electrochemical purification of nitrogen in liquid lithium using chloride molten salt.
- Elucidation of corrosion behavior on reduced activation steel F82H.
- Development of the water-cooling system for the cathode in the glow discharge type of fusion neutron source.

2. Fusion fuel (hydrogen isotope) recovery system development from liquid lead lithium droplets

Lead lithium eutectic alloy (Pb-17at%Li, Pb-Li) is a promising liquid material for the efficient fuel (hydrogen isotope) breeding on a fusion reactor. Effective recovery of the bred fuel is a key issue of liquid blanket fusion reactor.

We developed the vacuum sieve tray method, fusion fuel recovery from liquid Pb-Li droplets falling in vacuum. This fiscal year, on a collaboration work with National Institute for Fusion Science (NIFS), the continuous fuel recovery campaign was performed. We obtained fuel extraction efficiencies between 0.6 and 0.7 (Fig. 1). The long blue line shows proof-of-principle results performed in our division in 2013 [1]. Red circles show the results performed at NIFS this year. The two results are almost identical, showing the consistency of this method. This is the highest efficiency record in the fusion field.

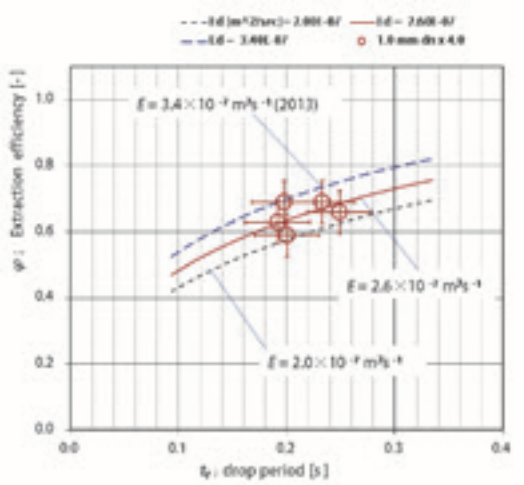

Fig.1 Obtained extraction efficiencies as a function of the droplet falling period. Blue long dash line shows a proof-of-principle result obtained in 2013 [1]. Red circles are results in 2023. Both are almost identical, showing the consistency of this recovery method.

3. Electrochemical purification of nitrogen impurities in liquid lithium using chloride molten salts

Fusion-relevant neutron sources, such as Advanced Fusion Neutron Source (A-FNS), are necessary for neutron irradiation experiments for the fusion material development. Liquid lithium is the flowing target of A-FNS, and easily absorbs nitrogen impurities which may cause corrosion of the structure material. Therefore, nitrogen extraction technology is essential for the A-FNS development.

We adapted an electrochemical method using chloride molten salt to extract nitrogen. In this ex-

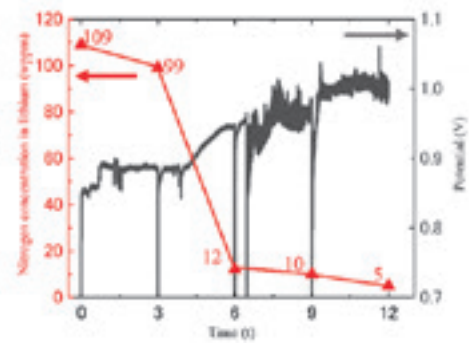

Fig.2 Temporal change of N concentration in liquid Li and the required potential for 2mA current.

periment, an electrochemical cell filled with chloride molten salt (LiCl 58.5 mol% – KCl 41.5 mol%) was prepared, and Li supported by a stainless-steel tube was placed in the chloride molten salt as the counter electrode. The working electrode was coil-shaped nickel wire. The temporal change of nitrogen concentration in liquid lithium was monitored at a constant current of 2mA (Fig. 2). This purification system sufficiently extracted nitrogen impurities.

4. Corrosion of reduced activation steel F82H steel by solid breeder material (LTZO) pebble

JA-DEMO plans to adapt lithium zirconate titanate ($Li_{2+x}TiO_{3+x}$+Li_2ZrO_3; LTZO) pebbles as the solid blanket breeder material, and reduced activation ferritic/martensitic (RAFM) steel F82H as the blanket structure material. The corrosion characteristics of F82H by LTZO pebbles are crucial because corrosion on F82H may degrade the strength of the structure. We experimentally investigated the formation of the corrosion layer on F82H to find the activation energy, which is required to predict corrosion behavior.

The corrosion on F82H by the LTZO pebbles was induced at 693, 833, and 993 K under sweep gas (Ar + 0.1% H_2) flow. The temperature dependence of the diffusion coefficient is shown in Fig.3. ① is plotted based on the corrosion layer formed up to 380 hours, while ② is based on the corrosion layer formed up to 190 hours. The activation energies in the cases of ① and ② are calculated to be 1.67 eV and 0.94 eV, respectively. The red line in Fig.3 is the result of a similar study that investigated corrosion between Li_2TiO_3+excess Li_2O and EUROFER (another type of RAFM steel) [2]. The difference between ① and ② will be due to the "breakaway behavior" which is also reported by the work [2]. The activation energies in the present study are higher than that of the prior study on EUROFER. This may be due to the difference in the contact area between the solid breeder specimen and the structural material, and the supply rate of the Li_2O vapor. Therefore, it is expected that the mechanism of corrosion and diffusion of Li and O that contribute to corrosion is not significantly different among the different types of solid breeder materials and structural materials.

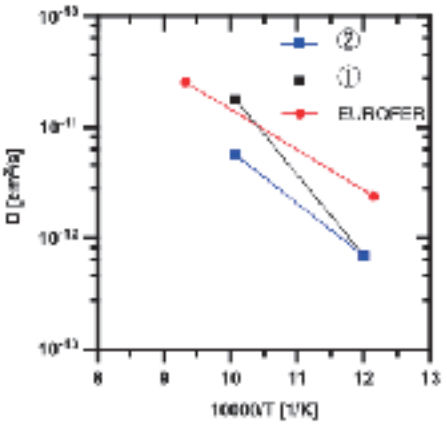

Fig.3 Temperature dependence on the diffusion coefficient of the corrosion layer on F82H or EUROFER.

5. Upgrading of the glow discharge type fusion neutron source by cathode cooling

The fusion neutron source of glow discharge type emits neutrons by inducing nuclear fusion reactions between deuterium and/or tritium. Fusion reactions in this device mainly occur on electrodes, especially on a cathode. This neutron source is expected to be used not only for fusion research but also for industrial applications and medical applications.

The device generates ions by applying an electric input (several tens of kilovolts and several tens of milliamperes) to induce a glow discharge. Although a neutron production rate (NPR) has a positive correlation with a current, an NPR tends to stagnate at a high current operational regime. This stagnation of NPR is caused by the decrease of deuterium concentration on a cathode due to deuterium desorption.

We constructed the water-cooling feedthrough system to solve the issue caused by deuterium desorption. The present study aims to evaluate the cathode cooling effect on NPR. The diamond-like carbon (DLC)-coated cathode was employed in the neutron production experiment. Fig.4 shows that the cathode cooling prevents the stagnation of NPR in the high current regime (> 30 mA) and enhance the NPR. This effect means the cooling system surpasses deuterium concentration on the cathode. At 50 kV and 60 mA (the maximum electric input of this experiment), the NPR in the case using the water-cooling system achieved more than twice as high as the NPR in the case without the water-cooling system. The water-cooling system is expected to expand applications of fusion neutron sources.

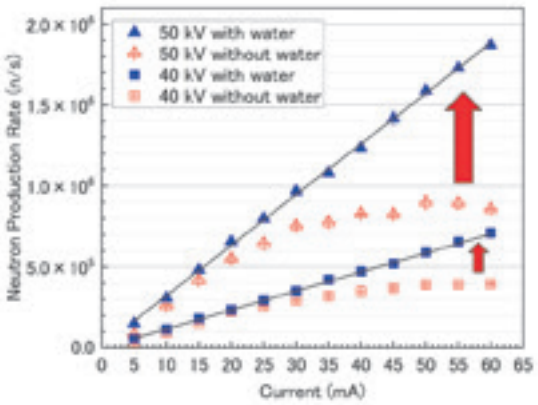

Fig.4 Comparison of NPRs between the cases with/without the water-cooling system.

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Advanced Plasma Energy Research Section

K. Nagasaki, Professor
S. Kobayashi, Associate Professor

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 optimizing the helical-axis heliotron configuration are in progress under collaboration with other groups of international/national institutes and 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 FY2023 is reported focusing on transport characteristics regarding fast ion induced magnetohydrodynamics (MHD) instabilities, especially in response of energetic particle (EP) driven MHD instability to modulated ECH in Heliotron J. Several techniques have been demonstrated to mitigate EP-driven MHD instabilities. Electron cyclotron heating and current drive (ECH/ECCD) represent potent methods for stabilizing these MHD instabilities. This study focuses on assessing the influence of ECH on suppressing EP-driven MHD modes in Heliotron J to reveal intricate interactions between ECH and EP-driven modes.

2. Response of energetic particle driven MHD instability to modulated ECH in Heliotron J[1]

In our preliminary modulation trial, the NBI power was set at a modest level of 90 kW for co-injection, whereas the modulation amplitude of the 2nd-harmonic ECH scanned systematically. The modulation frequency is set at 50 Hz, with 10 ms duration for both the maximum and minimum power levels. The maximum power of the ECH modulation is 192 kW, while the minimum power varies from 158 kW to 113 kW. An EP-driven mode (EPM) is observed in the frequency range 95-103 kHz with some delay after the modulated ECH power reaches its minimum amplitude [1]. In subsequent trials, we raised the NBI power to roughly 100 kW for co-injection and 450 kW for counter-injection. In the case that the maximum power of the ECH modulation changed to 247 kW with its minimum power from 228 kW to 113 kW, an EPM of 100 kHz is also observed at the lower power level. Additional instability with $f = 85$ is excited when the NBI power is increased (see Fig. 1). Figure 1 illustrates the temporal evolution of EPM observed in modulated ECH plasmas.

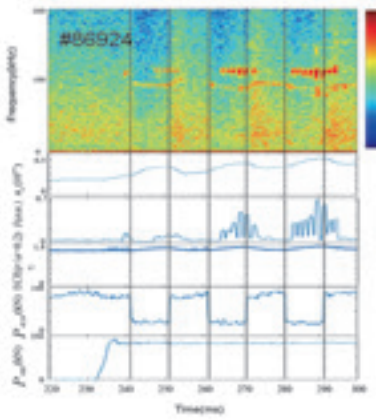

Fig. 1. Time evolution of EP-driven mode in Heliotron J.

The electron cyclotron emission (ECE) data is depicted, serving as an indicator of the core electron temperature, given the optical thickness in the core region is approximately 2. A noticeable increase in the ECE signal accompanies the escalation of ECH power, contrasting with the decline in averaged electron density measured using a microwave interferometer. Additionally, the onset of the mode occurs with a delay of 6.0 ms following the reduction in ECH power. Subsequently, after a brief delay of 1.5 ms, the mode vanishes and is effectively suppressed upon the resumption of ECH power increase. Analysis based on hybrid EP-MHD simulations conducted by MEGA [2] and

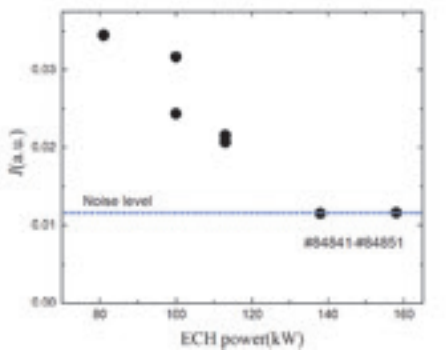

Fig. 2. Dependence of mode amplitude on ECH power.

the shear Alfven continua derived from STELLGAP developed by D. Spong (2003), along with prior experimental findings in the same magnetic configuration, suggest the observed mode is identified as an EPM with m/n=1/2, where m and n represent the poloidal and toroidal mode numbers, respectively.

The amplitude of the observed mode exhibits a clear correlation with the ECH injection power. As the ECH power is increased, the suppression of the mode becomes evident, as depicted in the experiment. When the minimum ECH power level is set at 100 kW, the mode is clear. It is noteworthy that once the ECH power surpasses the threshold one, the mode experiences effective suppression as shown in Fig. 2[1].

The threshold range lies within 110 to 138 kW. These findings underscore the pivotal significance of ECH power in regulating and alleviating the identified mode. Defining this range for mode suppression offers valuable perspectives for enhancing the operational efficiency of the Heliotron J device and addressing the MHD instabilities induced by energetic particles.

A delay of the mode appearance is noted in the response of mode amplitude to the modulation of ECH. This trend is depicted in Fig. 3, showcasing the progression of mode intensity $\langle I \rangle$ against the product of line-averaged electron density $\langle n_e \rangle$ and ECE intensity, reflecting core plasma pressure. At high amplitudes of ECH modulation, the mode intensity remains low. Nevertheless, upon reduction of ECH power, the mode strength swiftly escalates, as highlighted by the red circle in Fig. 3. The intensity of the mode persists at high levels even as plasma pressure begins to rise, with eventual suppression occurring at elevated pressure levels. To decipher the primary factors governing this response, we investigated by plotting mode intensity against either $\langle n_e \rangle$ or ECE intensity. Analysis reveals that, in comparison to electron density, electron temperature exerts a more significant influence on mode strength. This finding suggests that the delay response effect is closely associated with fluctuations in electron temperature. Furthermore, disparities in the product of $\langle n_e \rangle$ and ECE intensity indicate that the suppression of mode excitation is linked not only to bulk plasma pressure but also to fast ion confinement.

The impact of ECH on EP-driven modes is

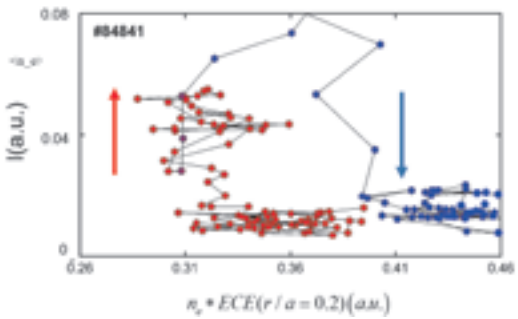

Fig.3 The evolution of the normalized mode intensity with product of $\langle n_e \rangle$ and ECE intensity.

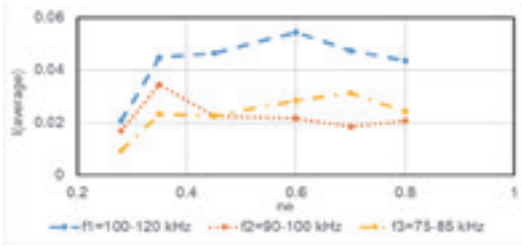

Fig.4 The evolution of the normalized intensity I with the electron density $\langle n_e \rangle$.

intricate. Nearly all factors associated with MHD stability can be influenced by ECH, encompassing both the driving and dissipative aspects. ECH has the potential to alter ion and electron Landau damping, radiation damping, and even continuous spectrum damping (via electron temperature T_e modification). Conversely, the variation in T_e also influences electron-drag collisions, thereby affecting the slowing down time.

In order to better determine the influencing factors of the mode instability, we conducted the following experiments. We initially stabilized the electron density and subsequently ramped up the ECH injection from 113 kW to 247 kW. During this phase, three instability frequency ranges emerged within the 70 kHz to 120 kHz spectrum. However, with the increase in ECH power, these instabilities were effectively suppressed. This clearly demonstrates the inhibitory effect of ECH on MHD instability as we mentioned above. Then, we kept the ECH constant and increased the electron density. When the ECH injection is held constant at 247 kW, the instabilities within the three frequency ranges are partially suppressed as the electron density increases. However, when the ECH injection is held constant at 113 kW, the instability is not suppressed; instead, it is further excited (see Fig. 4). When we increase n_e, the absorption rate of ECH and NBI also increases. NBI absorption increases which can destabilized the modes. But ECH absorption rate increases which will enhance the bulk electron pressure and the slowing-down time of energetic ions to suppress the mode. The effect of ECH depends on the electron density and the excited modes, which are linked to the equilibrium between stabilizing and destabilizing influences. ECH amplifies stabilizing effects such as continuum damping, finite Larmor radius (FLR) effects, and electron-ion Landau damping. Additionally, ECH intensifies destabilizing effects such as pressure and temperature gradients, slowing down time of EP, and EP beta through the reduction of n_e and the increase in T_e.

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Complex Plasma Systems Research Section

S. Inagaki, Professor
T. Minami, Associate Professor
S. Kado, Associate Professor
S. Ohshima, Assistant Professor
F. Kin, Assistant Professor

1. Introduction

Nuclear fusion energy has some attractive features as a future option for the base-load electrical power source and thus magnetic field confinement fusion research is thus being conducted all over the world. To realize fusion reactor, there are however several urgent issues that need to be resolved, for example (1) improvement of plasma energy confinement, (2) enhancement of fueling ability. We are tackling these issues by understanding their physical processes by experiment using a magnetic confinement device Heliotron J. In the experimental reactor stage, the development of plasma diagnostics tools is also an issue for understanding plasma physics.

Results in FY2023 featured in this report are about the improvement of confinement in the high density plasma produced by pellet injection and development of advanced diagnostics.

2. Improvement of confinement in the dense-plasma

In fusion plasma, the power output from the fusion reaction is proportional to the square of the density. In addition, the higher the density, the better the plasma confinement. Therefore, high density is required in fusion plasmas, however, as the density increases, the electromagnetic fluid nature of the plasma becomes stronger. Magneto-hydrodynamic instabilities excited in the dense-plasmas often limit the density and/or plasma pressure normalized by magnetic pressure. As experiments progress, it has been pointed out that such density limitations can be exceeded by controlling the density distribution. It is observed that high density plasma with a center-peaked profile is maintained stably. In the gas puffing method, which is a common particle refueling method, fuel gas is supplied to the periphery of the plasma, making it difficult to form a center-peaked profile. In the pellet injection method, icy solid hydrogen is injected into the plasma, so that the fuel reaches near the center as it ablates, forming a peaked density profile. Thus, the achievement of high density is closely related to the development of particle fueling methods.

We've been performing pellet injection experiments. Recently, it is confirmed that the peaked density profile is formed after pellet injection by Thomson scattering diagnostics. In this experimental campaign, it is found that the peaked density profile is sustained for a long time (about 10 ms which is of the order of the energy confinement time). Typical experimental result is shown in Fig. 1. The pellet injection at 240 ms increased to 2×10^{19} m^{-3} then the density gradually decreased. The plasma stored energy decreases after pellet injection due to decrease in the temperature due to cold electron supply, but suddenly begins to increase at 252 ms. The stored energy is an index of the plasma energy confinement and thus increase in the stored energy suggests improvement of confinement. The energy reached a maximum around 260 ms, at which time magnetic measurements indicated that the MHD had become active. Behaviors of plasma spatial structure (radial profile of density and temperature) is presumable from the spatiotemporal structure of plasma emission intensity observed with an AXUV array. Figure 1(b) indicates temporal evolution of local plasma emission estimated by using the Abel inversion technique. We can see that the emission profile changes quickly in the energy rising phase and a profile with strong emission in the peripheral is formed just before

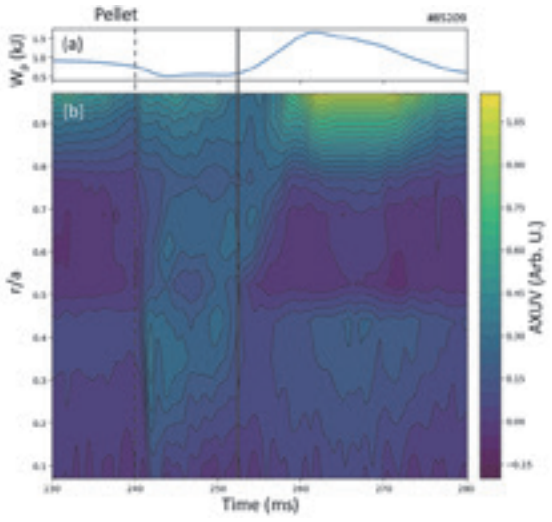

Fig. 1 Typical temporal evolution of (a) plasma stored energy and (b) radial profile of local plasma emission after pellet injection at 240 ms (indicated vertical dash line). Vertical solid line denotes when the energy rise began.

the energy reaches its maximum. Further energy increases can be expected if the mechanism that triggers such a change in radial profile is identified.

3. 2D Imaging of Emission and Density of Small Pellet Ablation Cloud

In hydrogen ice pellet injection fueling, the density of the pellet ablation cloud, consisting of the bright neutral hydrogen cloud surrounded by the high-density low-temperature plasma cloud, called *plasmoid*, is one of the key parameters to evaluate the fueling processes and efficiency. However, conventional spectroscopic methods for larger devices, such as LHD, are hard to apply to our low-density cloud in Heliotron J, which is usually categorized as a medium-sized device.

In this study, we have designed and developed a fast 2D imaging spectroscopy system and have succeeded in measuring the intensity, density, and trajectory of the ablation cloud of the small hydrogen pellet in Heliotron J.

We measured the 2D image of intensity and density from the spectral line shape of H_β at 486 nm using a high-speed (10k fps) non-unity magnification (300/180 focal ratio) grating spectrometer. The emission collected from the viewing area, 144 x 144 mm^2 square at the midplane including the pellet trajectory, is rearranged using the 2D to linear optical fiber bundle onto the entrance slit of the spectrometer.

A typical result (shot#82554 ECH+NBI heating) shows that the bright "emission cloud", indicating the pellet location, traveled along the injection trajectory at the speed of around 230 m/s, which fairly agrees with the one obtained from the arrayed Hα signal. The "density cloud" deduced from the Stark broadening, on the other hand, exhibited different features — elongated along the local magnetic field line having a density around 10^{20} –10^{21} m^{-3}.

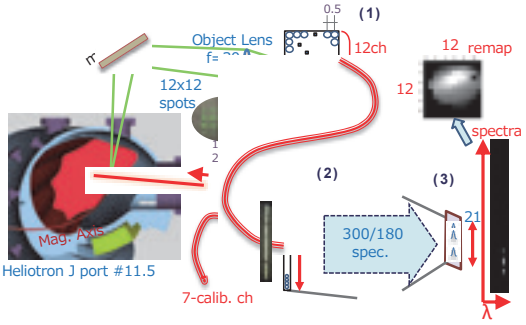

Fig. 2 Design concept of the spectrometer.
(1) 2D-1D imaging optical fiber array
(2) Non-unity magnification large aperture grating spectrometer
(3)High speed 2D detector

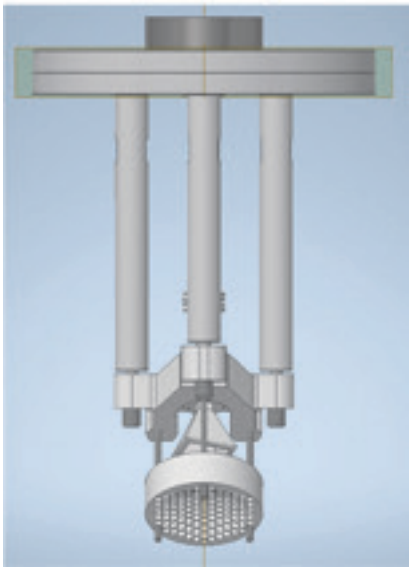

Fig. 3 Schematic illustrations of new ECE antenna.

4. Improvement of electron cyclotron emission diagnostics

The electron cyclotron emission (ECE) is one of the promising diagnostics to measure electron temperature (T_e) with high temporal resolution (0.1 μsec). The ECE measurement is sometimes disturbed by the strong emission at 70 GHz, which is injected into the H-J in order to produce plasma by electron cyclotron heating (ECH). Thus we installed new antenna far from the ECH injection port. As seen in Fig. 3, we use the metal lens for focusing the ECE. The Gaussian beam width (diameter) is approximately 5 cm. The focused beam is transmitted through horn antenna and WR-15 waveguide to the outside of the vacuum chamber. In the detection system, we have installed new front-end for down-converting RF wave in 55-70 GHz to intermediate frequency (IF) in 1-16 GHz. The new lowpass filter (54 GHz), balanced mixier, Gunn diode oscillator (54 GHz), and IF amplifier with 55 dB are used to compose the front-end. In the experiment, we have compared the new ECE diagnostic with conventional one. We have calculated the cross-coherence for signal and 70 GHz ECH noise, and we found that the coherence is dramatically reduced in the new system.

Collaboration Works

長﨑百伸, 小林進二, 南貴司, 大島慎介, Univ. Wisconsin（アメリカ）, Oak Ridge National Laboratory（アメリカ）, Max Plank Institute（ドイツ）, Stuttgart Univ（ドイツ）, CIEMAT（スペイン）, Australian National Univ.,（オーストラリア）, Kharkov Institute（ウクライナ）, Southwest Institute of Physics（中華人民共和国）, 先進ヘリカルシステムにおける周辺プラズマ・ダイバータ研究

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Advanced Energy Research Section

Rong Xiang, Foreign Visiting Researcher
(Professor in Zhejiang University,
866 Yuhang Road, Xihu District, Hangzhou, Zhejiang
Province, China)

1. Summary

The author spent three months (July. 1, 2023-Sept. 31, 2023) as a guest professor at the Uji campus of Kyoto University, hosted by the Y.Miyauchi group.

Here the author reports an investigation on (6,5) single-walled carbon nanotubes dispersion and optical characterization.

2. Introduction

Single-walled carbon nanotubes (SWCNT) possess a wide array of remarkable mechanical, chemical, and electronic properties, rendering them as ideal candidates for diverse applications, including composites, energy storage, biological and chemical sensors, flexible electronics, and transparent electrodes. In particular, the high charge-carrier mobility of semiconducting (sc-) SWCNT together with the ability for solution processing hold a great promise for high-performance low-cost transistor applications. [1] Many of these properties depend sensitively on SWCNT structure, which is characterized by the chiral index (n,m) that denotes the length and orientation of the circumferential vector in the hexagonal carbon lattice. Electronic properties are notably influenced, with subtle structural variations causing tubes to transition from metallic to semiconducting with diverse band gaps. Therefore, to fully exploit their technological potential, it is essential to have monodisperse single-chirality SWCNT with a single (n,m) index. [2]

Post-growth sorting of SWCNTs is essential due to the fact that their growth typically results in mixtures of various semiconducting and metallic nanotube species. Among the various sorting techniques available, such as gel chromatography, density gradient ultracentrifugation (DGU), and aqueous two-phase separation, selectively wrapping SWCNTs with conjugated polymers is a method that yields highly pure semiconducting and even monochiral dispersions with relatively low effort. [1] For instance, the polyfluorene copolymer poly[(9,9-dioctylfluorenyl-2,7-diyl)-alt-co-(6,60-{2,20-bipyridine})](PFO-BPy) yields almost monochiral (6,5) SWCNT dispersions. Therefore, PFO-BPy is widely used for the dispersion of single chirality SWCNT with small diameter. In general, polymer-sorted SWCNTs exhibit very low residual metallic content and little inter-tube interactions, which results in high purity dispersion. Here, we realized high purity (6,5) SWCNT dispersion by using PFO-BPy and characterized its optical properties.

3. Experimental observations

(1) (6,5) SWCNT dispersion

All (6,5) SWCNT dispersions were prepared from the same CoMoCAT® raw material (Sigma Aldrich 773735). For polymer-wrapping with tip sonication, 17.6mg PFO-BPy (American Dye Source, Lot#23G004A1) were dissolved in 30ml toluene before adding 7.6mg CoMoCAT raw material. After adding CoMoCAT and raw material, a respectively 10-minute bath sonication is required to mix the solution evenly. Subsequently, tip sonication was carried out using a BRANSON SONITIER 250 ultrasonic crusher at 40% power and 30% duty cycle for 3 hours. The solution was stirred evenly every hour, and the temperature was maintained at 20°C using a cooling bath. The dispersion step was followed by centrifugation at 19000 g (Eppendorf himac CS 100FNX) for 30 min with an intermediate supernatant extraction. Due to the high-purity (6,5) SWCNT, we can observe that the final purified solution exhibits a strong purple color in figure 1. [3] By adjusting parameters such as the power and time of tip sonication, the concentration of the solution can be adjusted, while also influencing the quality and purity of the separated carbon nanotubes.

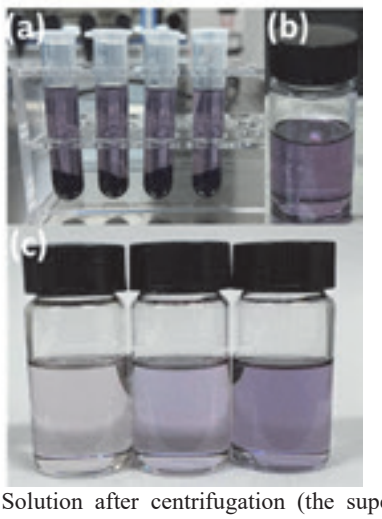

Fig. 1 (a) Solution after centrifugation (the supernatant consists of 65 tubes and the black sediment is impurities). (b) Extracted supernatant（c）Different concentrations of (6,5) solutions obtained by changing the tip sonication time

(2) Optical characterization

From absorption spectrum, each type of single-chirality species can be clearly identified. Figure 2 illustrates the absorption spectrum of the CoMoCAT

SWCNT dissolved in toluene by PFO-BPy, a typical solvent demonstrating selective extraction of semiconducting SWCNT. At 996nm, a prominent peak is evident, indicating absorption by the (6,5) SWCNT. Notably, the background absorption in the NIR region is minimal, a typical trait of PFO-dissolved SWCNT toluene solutions. This stands in stark contrast to numerous other dispersants such as surfactants, aromatic compounds, and polymers, which often exhibit significant background absorption in the NIR region. Furthermore, there is almost negligible absorption observed within the 400-550nm range, characteristic of metallic SWCNTs. This underscores a distinct advantage of PFO dispersants over many other SWCNT dispersants

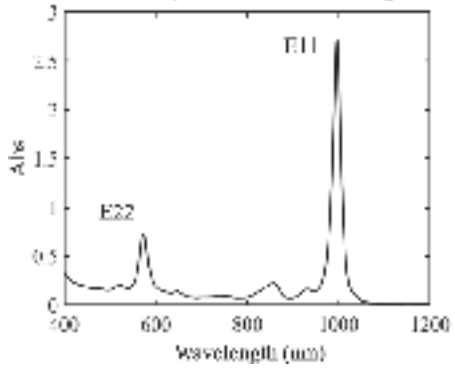

Fig. 2 Vis-NIR Absorption spectrum of dispersed (6,5) SWCNT solution

Photoluminescence (PL) spectroscopy serves as a potent tool for determining the chirality indices(n,m) of SWCNT. To identify all nanotube species within the dispersion, photoluminescence-excitation(PLE) maps are measured as shown in Fig. 3. As shown in Figure 3, we can only see the (6,5) SWCNT peak emission (996 nm) and peak excitation (575 nm) which indicates that the purity of (6,5) SWCNT in the solution is very high.

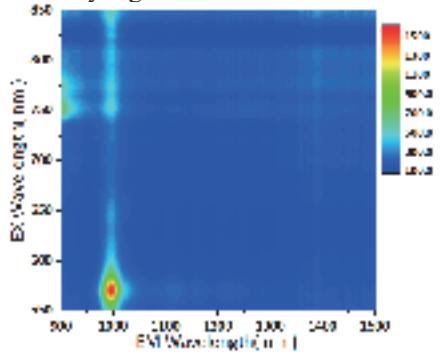

Fig. 3 PLE maps of dispersed (6,5) SWCNT solution

To further determine whether the extracted SWCNT contain other semiconducting- and/or metallic-SWCNT, the Raman spectra (532nm excitation) of the extracted tubes were measured (Figure 4). The SWCNT dispersions were drop-cast on Glass slide. The radial breathing mode (RBM) in the regions of 240-350 cm^{-1} and 150-240 cm^{-1} is attributed to the semiconducting and metallic SWCNT respectively. As depicted in the figure, for the PFO-BPy extracted SWCNT, we observe distinct peaks in the region of 240-350 cm^{-1} and almost no peaks in the 150-240 cm^{-1} region which indicates that the extracted SWCNTs are predominantly semiconducting SWCNTs, aligning well with previous reports utilizing PFOs and their derivatives. However, through normalized Raman spectroscopy, we can observe that the solution dispersed through tip sonication has a particularly high D peak, and the corresponding high GD ratio indicates that the quality of carbon nanotubes is not very high. How to improve both purity and quality is a topic that needs further research in future studies.

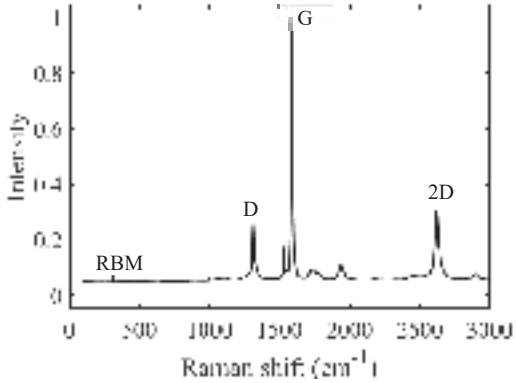

Fig. 4 Raman spectrum of dispersed (6,5) SWCNT solution

(3) (6,5) SWCNT film deposition

With high purity (6,5) SWCNT solution, we can obtain a film through filtration. Here, we use vacuum filtration to form a SWCNT film. Two viable filter papers are considered: the AAO inorganic filter paper (Whatman AnodiscTM25) and the VCWP filter paper (Merck, VCWP02500). Vacuum filtration is advantageous for achieving a uniform and complete film. Once the film is obtained, it becomes necessary to separate the film from the filter paper. The removal of VCWP filter paper is relatively simple, requiring only acetone to completely dissolve the filter paper, but the resulting film tends to be relatively impure. On the other hand, removing the AAO filter paper is relatively difficult, requiring long-term soaking to form a submonolayer[4] that facilitates the separation of the film and filter paper. However, this method results in a cleaner film.

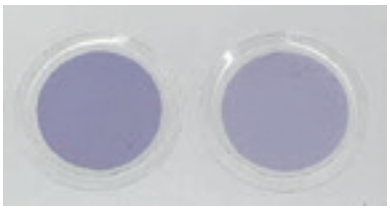

Fig. 5 (6,5) SWCNT film with different thickness

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Functional Materials Science and Engineering Research Section

Y. Miyauchi, Professor
T. Nishihara, Junior Associate Professor

1. Introduction

Our research section focuses on the physical properties, functions, and energy applications of quantum materials that exhibit significant quantum mechanical effects, such as carbon nanotubes, two-dimensional semiconductors, and recently discovered topological materials. The aim is to create new technologies for highly efficient use of solar light/thermal energy that will contribute to the realization of a sustainable energy society. To understand the unique physical properties of these materials from the fundamental principles and extract superior functions that exceed the limits of conventional materials, we are promoting interdisciplinary research that covers basic sciences, including materials synthesis and condensed matter physics, as well as thermal, mechanical, electronic, and optical engineering along with the fabrication of integrated nanomaterials. Followings are main research achievements in the year of 2023.

2. Birefringent optical responses of single-chirality carbon nanotube membranes

Membranes consisting of single-walled carbon nanotubes (SWCNTs) with a specific chirality have great potential in photonic and thermo-optic applications because of their strong and distinct light-matter interaction via excitons with high-temperature robustness. Generally, these membranes are fabricated via the vacuum filtration of single-chirality SWCNT dispersion, and SWCNTs are aligned two-dimensionally in the plane (Figure 1(a)). The electric field component normal to the membrane surface (red arrow in Figure 1(b)) is always perpendicular to the tube axis of each SWCNT. Meanwhile, the optical responses of each individual SWCNT are anisotropic with respect to the tube axis as shown in Figure 1(c). For these reasons, it is expected that the macroscopic responses of the membranes depend on the light-propagation direction. However, their anisotropic optical features and complete complex refractive index spectra remain to be unveiled, hindering the design of devices to deal with light propagating in arbitrary directions using SWCNT membranes as opto-functional materials.

In this study, we revealed the birefringent optical response of a single-chirality SWCNT membrane, as examined using polarization- and angle-resolved reflection spectroscopy [1]. We determined the ordinary (in-plane) and extraordinary (out-of-plane) complex refractive index spectra for it. The membrane was fabricated via the vacuum filtration of a (6,5) SWCNT dispersion prepared using gel chromatography, and the spectra were obtained in the near-infrared-to-visible region using homemade optical setups. All spectral features were consistent with a uniaxial birefringent membrane, reflecting the random in-plane orientations of SWCNTs. Figure 1(d) shows the obtained complex refractive index spectra. The ordinary one presented a series of sharp resonances of parallel-polarized excitons while the extraordinary one is ~1.9 with the small contribution from the cross-polarized exciton resonance (S_{cross}). We found that this resonance is small but indispensable for properly predicting angle-dependent optical responses of the membrane. The complete knowledge of the birefringence and complex refractive index spectra of the single-chirality SWCNT membrane facilitates the precise and diverse design of photonic and thermo-optic devices based on SWCNTs.

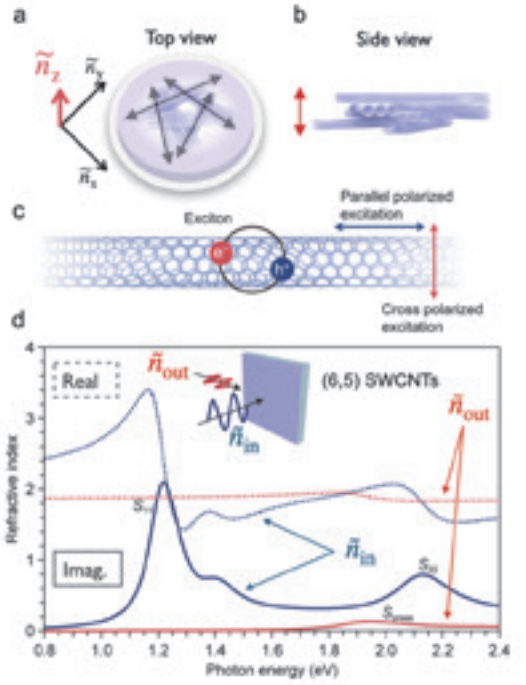

Fig. 1 Schematic of the (a) top and (b) side views of a single-chirality SWCNT membrane fabricated via vacuum filtration. (c) Anisotropy in the exciton optical response in an individual SWCNT. (d) Ordinary (in-plane, $\tilde{n}_{\mathrm{in}}$, blue) and extraordinary (out-of-plane, $\tilde{n}_{\mathrm{out}}$, red) complex refractive index spectra of the membrane.

3. Fabrication of pure carbon nanotube membrane without mid- and far-infrared optical absorption

In this study, high purity single-chirality SWCNT thin films were fabricated using a polymer dispersion method, and their complex refractive index spectra were determined [2]. It was found that the Drude-type mid- and far-infrared absorption, which normally increases at lower photon energies (long wavelengths), hardly appears in the absorption spectra of high-purity semiconducting SWCNT thin films. This may be attributed to extremely suppressed thermal free carrier generation because thermally excited electrons and holes attract each other by Coulomb force to form strongly bound excitons. This study confirmed that it is possible to fabricate SWCNT thin films with almost no mid- and far-infrared absorption which causes unwanted radiative energy leak in photon-energy selective solar absorber and/or thermal emitters for efficient solar and thermal energy harvesting technologies.

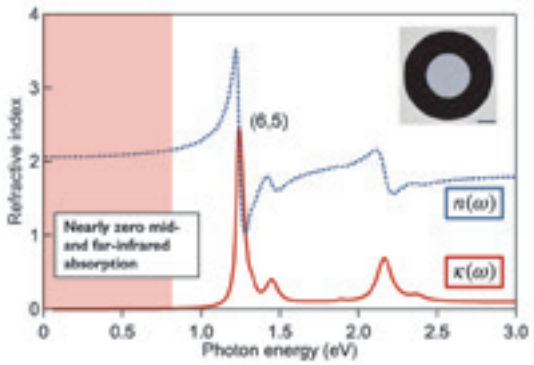

Fig. 2 Real $n(\omega)$ and imaginary $\kappa(\omega)$ parts of complex refractive index spectra of the polymer-dispersed (6,5) SWCNT film shown as the inset.

4. Exciton energy transfer under low temperature in a lateral heteromonolayer of WSe_2–$MoSe_2$

Controlling exciton motion in monolayer transition metal dichalcogenides (TMDCs) has been attracting much attention, because it enables new-type optoelectronic devices such as exciton transistors and exciton routers which exhibit an extremely reduced energy consumption and fast operating speed. In our previous study, the unidirectional exciton energy transport has been demonstrated in a lateral TMDC heteromonolayer at room temperature [3]. However, physical parameters related to exciton motion such as mobility and lifetime strongly depend on temperature, and it is still elusive that how temperature affects exciton kinetic property, energy transfer process.

In this study, we examined the exciton energy transfer process in a lateral heteromonolayer of WSe_2–$MoSe_2$ at low temperature [4]. Position-dependent photoluminescence excitation (PLE) spectroscopy measurements revealed the occurrence of exciton

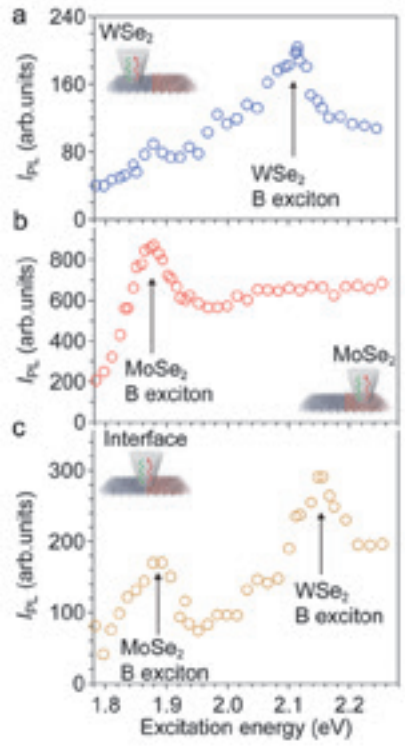

Fig. 3 Photoluminescence excitation (PLE) spectra at at 15 K recorded at (a) the WSe_2, (b) the $MoSe_2$ and (c) the interface. The inset figures display the excitation and detection positions.

energy transport from WSe_2 to $MoSe_2$ both at room temperature and 15 K. The effective energy transport distance in WSe_2 was longer at 15 K than at room temperature, suggesting that the dark excitons with longer diffusion length than bright excitons preferentially contributed to the exciton energy transport across the heterojunction interface at 15 K. This study provides useful insights for the development of excitonic devices based on exciton transport in transition metal dichalcogenides.

Acknowledgement

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Advanced Laser Science Research Section

T. Nakajima, Associate Professor

1. Introduction

We use lasers to fabricate the functional materials and also to probe the dynamics without perturbing the various processes. This year we have developed three different techniques. The first one is to probe the bubble dynamics of hydrogen evolution reaction through alkaline water electrolysis, and the second one is to fabricate the optical elements. The third one is to obtain the high quality holes and lines, which are the most elementary unit structures for laser micromachining with unprecedented quality.

2. Role of the surface morphology of the electrodes to form hydrogen and oxygen bubbles during water electrolysis

Hydrogen evolution via water electrolysis is one of the promising candidates for renewable energy production. Toward efficient hydrogen evolution, not only the catalysis development but also the morphological design of the electrode surface to attain the high surface-area-to-volume ratio is important. However, bubbles sitting on the electrode surface reduce the active surface area and increase the ohmic resistance between electrolyte and electrode interface, and it is important to find the optimal morphology of the electrode surface so that the bubble detachments occur soon after their formations with a minimal duration on the electrode surface. Our previous study has revealed that the hydrogen bubbles are preferentially formed at the sites with pits or crevices on the electrode surface. A natural question is whether those sites also serve as the forming sites of oxygen bubbles when the polarity of the electrode is reversed.

In this study, we carry out the comparative study on the forming sites of hydrogen and oxygen bubbles using the identical Ni electrode with a single laser-induced microstructure by reversing the polarity of the electrode, and we take the movie of the bubbles on the electrode surface during the electrolysis (Fig. 1(a)). The bubbles in the vicinity of the electrode surface are illustrated in Fig. 1(b). Representative optical images of hydrogen and oxygen bubbles during hydrogen as well as oxygen evolution reaction (HER and OER) are shown on the left side of Fig. 1(c), where the hydrogen and oxygen bubble forming sites are marked by thick-white and thin-blue circles, respectively. It is very interesting to point out that all the forming sites of

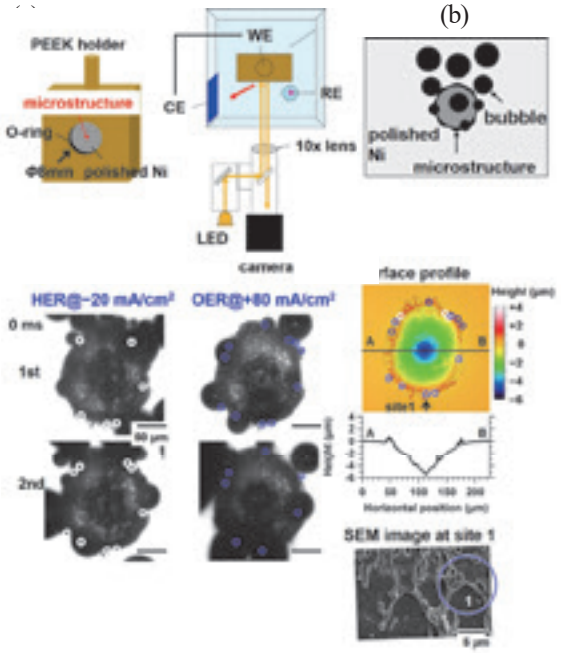

Fig. 1 (a) Setup for the water electrolysis and bubble measurements. (b) Schematic of bubbles on the microstructured Ni electrode. (c) Representative optical images of hydrogen and oxygen bubbles forming at the microstructure, false-colored surface profile, and the SEM image at site 1 indicated in the surface profile.

hydrogen bubbles are found only at the periphery of the microstructure, while those of oxygen bubbles are found not only at the periphery of the microstructure but also on the flat area around the microstructure. This suggests that, although the shallow surface structure is preferred to form bubbles and the local surface morphology plays a crucial role for hydrogen bubbles, it plays a lesser role for oxygen bubbles and some other factors such as local convection play some roles. Those findings are very important to design the electrode surface structure toward efficient HER.

3. Facile fabrication of optical diffusers by ablation-assisted nanosecond laser micromachining

Optical diffusers are essential elements to alter the spatial distribution of incident light, and frequently used as essential components in optoelectronic

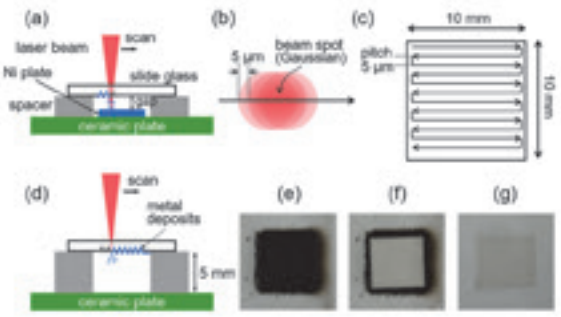

Fig. 2 Change of the diameter of fabricated holes on the Ni substrates with and without Ni films as a function of laser fluence.

devices. It is known that there are two approaches to fabricate the optical diffusers. The first one is to produce micro/nanostructures on the surface of a transparent glass substrate by direct laser writing, and the second one is to produce appropriate patterns through the introduction of fillers or lithography to a transparent polymer film through the wet chemical processes.

For the direct laser writing of micro/nanostructures at the surface of a transparent glass substrate an ultrashort laser is usually employed. It is practically impossible to structure the transparent glass with nanosecond laser in the visible or near-infrared wavelength range. One way out of this is to use energetic fragments to etch glass, and we undertake ablation-assisted laser micromachining of glass substrate by nanosecond laser pulses in the near-infrared range. The fabrication procedures of optical diffusers are shown in Fig. 2. Briefly, we ablate the Ni plate which is placed behind the slide glass with a small (<~1 mm) gap with nanosecond laser pulses (40 ns at 50 kHz) with various laser powers at the scanning speeds of 250 to 2000 mm/s (Fig. 2(a)-(c)). Then, we remove the Ni plate and perform laser cleaning to remove debris from the slide glass (Fig. 2(d)-(g)). Tis way, we do not have to introduce any wet chemical cleaning process to fabricate the optical diffuser. A representative surface morphology of the diffuser and beam profile through it is shown in Fig. 3. The advantage of the developed technique is that it is very quick and efficient without any wet process. This demonstrates that cost-effective nanosecond laser can be a convenient tool for laser micromachining of transparent materials.

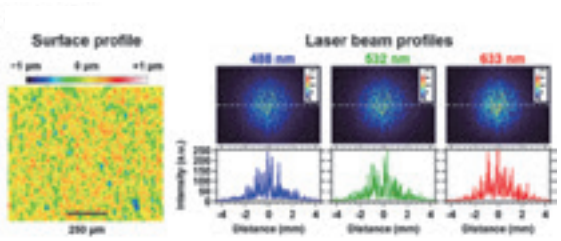

Fig. 3 Representative surface morphology of the fabricated diffuser and beam profile through it.

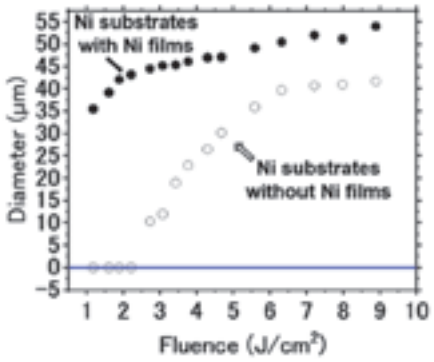

Fig. 4 Change of the diameter of fabricated holes on the Ni substrates with and without Ni films as a function of laser fluence.

4. Fabrication of depth-controlled high quality holes and lines on a metal substrate by nanosecond laser pulses

It is widely believed that an expensive femtosecond laser is necessary to fabricate high quality holes with very little ablation rims, while the use of inexpensive nanosecond laser suffers from the formation of pronounced ablation rims. It is not always so only if we can somehow suppress the heat problems. Our idea to realize such situation is to introduce a thin metal film on a metal substrate, and selectively blown out the film with laser pulses of modest fluence. This is possible, as we show in Fig. 4 for a Ni substrate with a Ni film of 80 nm thickness, because the ablation threshold of a metal film on a metal substrate is much lower than that of the bare metal substrate.

After ensuring that we can selectively blow out the Ni film while the Ni substrate is intact, we perform nanosecond laser micromachining of Ni substrate with a Ni film of 80 nm thickness to fabricate the high quality hole and line (Fig. 5), which exhibit the very flat bottoms without notorious rims. This demonstrates that the metal substrate with a metal film is a nice workpiece to fabricate high quality holes and lines by nanosecond laser micromachining.

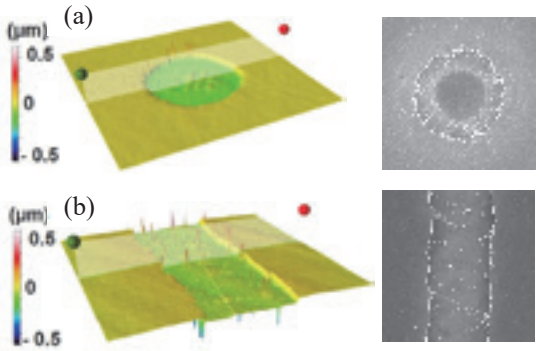

Fig. 5 Morphologies and SEM images of the fabricated (a) hole and (b) line on the Ni substrates with a Ni film.

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Advanced Energy Structural Materials Research Section

K. Morishita, Associate Professor
K. Yabuuchi, Assistant Professor

1. Introduction

The development of robust materials and the establishment of reliable system management are essential for the safe and efficient operation of advanced nuclear energy systems. This section addresses the mission of establishing maintenance management methodologies as well as materials R & D for advanced nuclear energy systems such as fusion and fission reactors. Our research interests include:

(1) Theory, modeling, numerical simulation, and data-driven science & technology of irradiated materials: Radiation damage processes of materials during irradiation occur at various time and length scales. To understand these processes, so-called multiscale viewpoint and statistical arguments are required. In this section, efforts are made to model material behavior during irradiation complementarily using several computational techniques such as MD, ab-initio calculations, kinetic Monte-Carlo, rate-equation analysis, FEM and CFD. Recently, additional efforts have also been devoted to this research using machine learning, AI, and data-driven techniques.

(2) Plant integrity analysis: Structural integrity of a reactor pressure vessel (RPV) during pressurized thermal shock (PTS) events is of critical importance in the quantitative assessment of reactor safety. We evaluate this using 3D CFD and FEM. The risk of the RPV function loss is quantified and then is proposed as an indicator available for optimizing maintenance strategy.

(3) Effects of irradiation on the microstructure and mechanical property changes of materials: High energy particle irradiation leads to the formation of oversaturated interstitials and vacancies. The behavior of those defects is responsible for the evolution of the microstructure, which may cause degradation of the mechanical properties of the material. The elucidation of the behavior of point defects is essential for understanding the mechanisms responsible for the changes in mechanical properties. In our study, the microstructure evolution under high energy particle irradiation has been investigated experimentally and computationally.

2. Size distribution of defect cluster production in irradiated materials

In materials of fusion reactor components, high energy neutrons entering the material collide with many target atoms, initiating displacement cascade processes. This process produces locally dense athermal point defects within the material, some of the point defects aggregate to form defect clusters. This has a profound effect on the material's microscopic composition and structure thus altering its mechanical properties. Therefore, it is important to investigate the impact of these processes in the design and selection of component materials. However, the displacement cascade process occurs on an extremely short timescale of several tens of picoseconds, it is very difficult to observe it experimentally. As such, computer simulation techniques are often employed instead. Among them, molecular dynamics (MD) is one of the most powerful tools. In this study, the factors influencing the generation of clusters were investigated through the MD simulation of the collision cascade in Fe.

Fig.1 shows a snapshot of the displacement cascade in Fe at 0.2 ps, which is initiated from a PKA with a kinetic energy of 50 keV. It can be seen from this figure that the nucleation of an SIA loop (marked by green line) is formed at a relatively early stages. The formation of such cascade clusters is thought to have a major impact on the subsequent microstructural developlement, making it difficult to develop fusion reactor materials with excellent radition resistance.

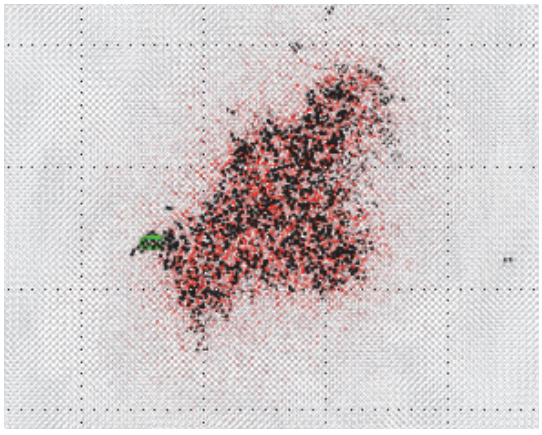

Fig. 1: Evolution of displacement cascades in Fe

3. Effect of irradiation environments on microstructural evolution in Fe during irradiation

Many studies have been done so far using numerical simulations to develop tools to predict material degradation under irradiation. However,

many conventional predictions mainly evaluate the "average" behavior of the changes due to irradiation without taking into account the effects of fluctuations. The fracture behavior of a material does not depend on the average behavior of the material, but rather is dominated by the material's property at its weakest point. Therefore, it is important to focus on fluctuations in defect microstructural evolutions.

In this study, the fluctuations in defect generation and associated microstructural changes caused by irradiation are focused. The probability distribution function (PDF) of the number of point defects and that of the number of cascade clusters are obtained as a function of recoil energy using our molecular dynamics simulations (MD). The recoil energy spectrum for a specific neutron irradiation facility, e.g., high flux isotope reactor (HFIR) in ORNL, is then obtained using the nuclear library JENDL constructed by JAEA. Using these data evaluated here, the average and fluctuations of point defect generation rate and those of cascade cluster generation rate are evaluated individually for the specific irradiation facility. These generation rates are furthermore employed as a source term in the rate theory equations to evaluate the microstructural changes of materials during irradiation. Our calculation results showed that the fluctuation in microstructural changes is highly dependent on irradiation conditions; for example, the coefficient of variation in concentrations of defect clusters accumulated varies by up to 40 % in HFIR.

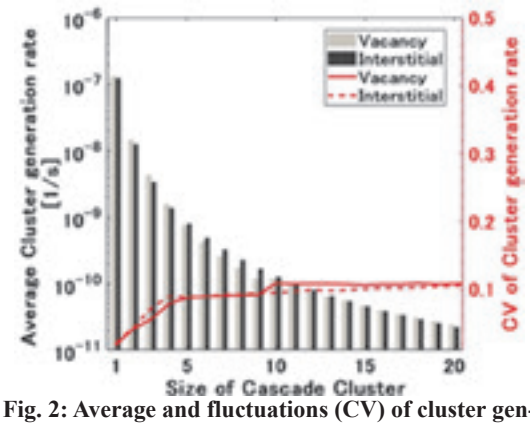

Fig. 2: Average and fluctuations (CV) of cluster generation rate

4. Modeling of SiC materials for application in nuclear energy system: first principles calculations

Since its excellent properties such as high strength and low induced radioactivity, SiC materials are being developed and validated as nuclear materials. However, before practical application in nuclear reactors, it is necessary to study the effects of high temperature and irradiation environment of nuclear systems on the properties of SiC materials.

To simulate the radiation damage behavior of materials using molecular dynamics methods, a reliable potential function is required. However, it is known that the Tersoff, MEAM, and GW potential functions widely used in molecular dynamics simulations of SiC materials are inconsistent with highly accurate first principles calculations. Therefore, it is necessary to develop new potential functions that can accurately describe the interactions between atoms.

On the other hand, with the development of artificial intelligence technology, neural networks have been proven to be able to construct high-precision potential functions and apply them to material modeling research. Therefore, in order to conduct reliable molecular dynamics simulations of irradiation behavior, this study used a high-precision first principles calculation method to calculate the total potential energy of SiC materials and provided teaching data for constructing neural network potential energy functions.

First principles calculation was carried out by supercomputer system using SIESTA code. We constructed 3C-SiC model with 216 atoms composed of $3 \times 3 \times 3$ supercells and approximated the exchange interaction of electrons using generalized gradient approximation. To obtain a good generalization ability for the neural network potential function to be developed, not only the calculation of the perfect crystal SiC but also the cases for different lattice constants, vacancies and interstitial atoms were calculated. A total of 149 calculations were conducted. As input parameters for the neural network potential function, atomic coordinates, energy and force have been calculated and extracted.

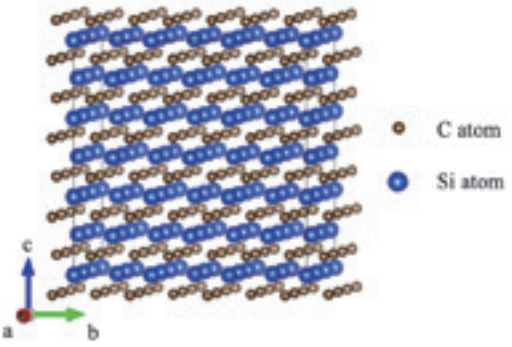

Fig. 3: 3C-SiC perfect crystals.

5. Application of AI technology to the image analysis for nuclear materials development

TEM image analysis of post-irradiation metals has often been conducted in the field of nuclear material development research, where an interpretation of imges is different unfortunately from person to person. To avoid this gap, a new attempt is being made to apply the state-of-the art AI technology to the image analysis. If this attempt progresses successfully, it should be possible to bridge the gap between the skill levels of skilled and novice users.

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Optical Nano-science Research Section

K. Matsuda, Professor
K. Shinokita, Assistant Professor

1. Introduction

We are engaged in fundamental and applied research of nano-materials from a viewpoint of optics and material science. Our research aims to explore new physical and chemical phenomena leading to the applications of novel nano-materials including carbon nanotubes, layered transition metal dichalcogenides, perovskites for the efficient utilization of light energy and the development of future optoelectronic devices with ultra-low energy consumption. The followings are main the research achievements in the year of 2023.

1. Quantum Phenomena of Moiré Excitons in a $WSe_2/MoSe_2$ Heterobilayer

A quantum two-level system has garnered considerable attention in recent years due to its numerous potential applications in the fields of physics, such as quantum simulation, quantum computing, and quantum information processing. The development of these systems facilitates the construction and utilization of quantum bits (qubits), which serve as fundamental units for quantum computing and quantum information. Resonant light–matter interactions, such as Rabi oscillation, Ramsey interference, and Hahn echoes enable the manipulation of quantum two-level systems by generating superposition states. However, the superposition states of qubits suffer from the interaction and fluctuation from the environment, resulting in an accelerated decoherence process. This decoherence process imposes a temporal limitation on the precise manipulation of quantum systems, hindering their potential applications.

Recent progress in artificial van der Waals (vdW) structures, achieved by stacking atomically thin two-dimensional (2D) materials, has opened up opportunities for designing novel quantum platform. vdW heterobilayer assembled from monolayers of semiconducting transition metal dichalcogenides exhibited various intriguing physical phenomena, including strongly correlated insulator phases, superconductivity, and novel ferromagnetism. Moiré superlattices with varying atomic registries in vdW heterobilayers can be constructed using monolayer semiconducting transition metal dichalcogenides with a small lattice mismatch or twist angle. The resulting moiré superlattice leads to the formation of periodic, ordered potential traps, confining and spatially organizing optically generated bound electron–hole pairs (excitons) into periodic arrays of quantum two-level systems. The trapped excitons in moiré potentials are expected to exhibit long quantum coherence due to their limited degree of freedom as 0D quantum systems; furthermore, coupling interactions can be formed between spatially separated moiré potentials, leading to quantum interference of emitted photons. These results establish moiré exciton quantum systems as not only a promising platform for achieving extended coherence but also an effective tool for exploring interactions within or between quantum systems. However, experimentally, important information on the quantum coherence and interference of moiré excitons in vdW heterobilayers remains unexplored. This is due to the overlapping of multiple emission peaks from moiré excitons in their inhomogeneously broadened spectra, hindering these intrinsic insights within the diffraction limit of light. The experimental approaches of strain-

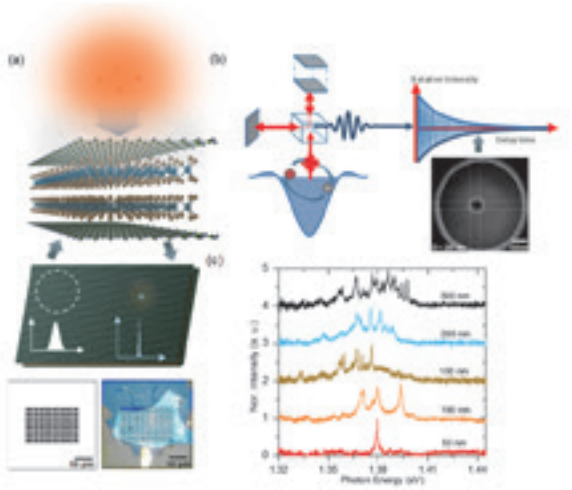

Figure 1 (a) (b) Schematic of the concept in this study. Nanoscale fabrication using reactive-ion etching enables to obtain emissions from a single moiré exciton and the observation of its quantum coherence with Michelson interferometer in $MoSe_2/WSe_2$ heterobilayer. Designed pattern for RIE (left) and the optical image of $MoSe_2/WSe_2$ heterobilayer with an array of nanofabricated structures (right) are presented in (a). A SEM image of typical pillar is presented in (b). The inner dotted circle shows a pillar with a diameter of 240 nm corresponding to the optical excitation and observation area of moiré potential. Optical spectra from the pillars are Fourier-transformed to temporal interferograms using the Michelson interferometer. (c) PL spectra of $MoSe_2/WSe_2$ heterobilayers with various pillar sizes at 4 K. (d) Integrated PL intensity and calibrated intensity of heterobilayer as a function of pillar size.

induced exciton traps introduced by metallic nanopillars in heterobilayers have been previously reported, to observe spectra with discrete emission lines; however, the intrinsic properties of the moiré exciton system might be inadvertently concealed due to the additional strain-induced effects.

Figures 1a and 1b illustrate schematics of the concept using a nanostructure fabrication process, and experimental setup employed in this study. Nanoscale fabrication using reactive-ion etching (RIE) enables emissions from a single moiré exciton and the observation of its quantum coherence in the $MoSe_2/WSe_2$ heterobilayer. During usual optical measurements, obtaining clear spectrum from moiré excitonic states is difficult due to the inhomogeneity of the moiré potential, leading to ensemble-averaged and broadened emissions comprising multiple peaks. This issue arises because the focused laser light with a spot size of approximately 1.5 μm is determined by the diffraction limit of light, which excites a large number of moiré potentials due to the much smaller spatial period of moiré potentials. To address this, in the microfabrication process, we applied a nanoscale fabrication technique to reduce the optical excitation and detection area of the $MoSe_2/WSe_2$ heterobilayer with a nano-pillar structure. The nanofabricated heterobilayer, with a pillar size smaller than the wavelength of light, will result in a reduced number of spectral peaks beyond the diffraction limit of light. Thus, this approach allows for the anticipated observation of emission from a single moiré potential, enabling the revelation of the quantum coherence of moiré excitons.

Figure 1c displays the photoluminescence (PL) spectra of the nanostructure-fabricated $MoSe_2/WSe_2$ heterobilayer, measured at 4 K with varying pillar sizes. In the heterobilayer with a pillar size of 500 nm, the PL spectrum reveals an inhomogeneously broadened ensemble average of multiple peaks from large number of moiré excitons. This finding agrees with previously reported results. The broadened spectrum, characterized by a Gaussian distribution, arises from the inhomogeneity of moiré potentials in the heterobilayer. As the pillar size decreases, the number of peaks in the spectra significantly decreases. Consequently, the PL spectrum of the heterobilayer with a 50-nm pillar size reveals a singular emission peak from a moiré exciton, attributed to the reduced number of moiré potentials within the optical excitation and detection area determined by the pillar size.

To obtain the information on the quantum coherence, the first-order correlation function of emission signals from a moiré exciton is measured using a Michelson interferometer. Figure 2a presents the counter map of interferometry of the PL spectra as a function of delay time at 4 K for an excitation power density of 14 W/cm^2. The amplitude of the oscillation fringe between the maximum and minimum intensities gradually decreases with increasing delay time, indicating

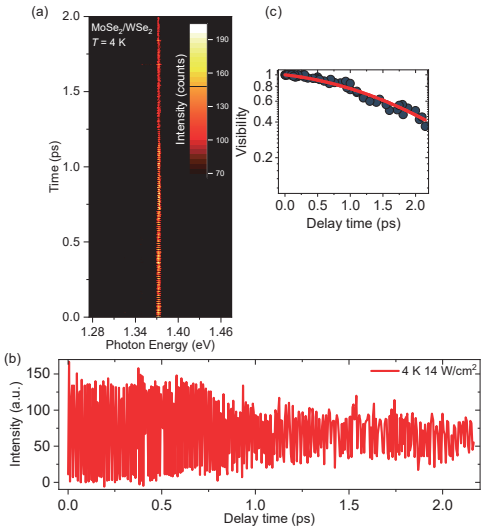

Fig. 2 (a) Counter plot of the first-order correlation function of PL signals as a function of delay time, measured using the Michelson interferometer. (b) Interferogram of the moiré exciton peak in the time domain at 4 K in the excitation power condition of 14 W/cm^2. (c) Decay profile of visibility in the interferogram, with solid curve representing the fitted result of the product of an exponential and a Gaussian func-

the process of decoherence, as presented by the temporal interferogram in Fig. 2b. Figure 2c shows the visibility as a function of delay time from Fig. 2b.

The visibility as a function of delay time, corresponds to the Fourier transform of the emission spectrum, with the convolution result of extrinsic inhomogeneous and intrinsic inhomogeneous linewidth, in form of Lorentz and Gaussian functions, respectively. Consequently, the delay time-dependent visibility in Fig. 2c can be modeled by the product of exponential and Gaussian functions. The fitted result by the model function of Lorentz and Gaussian functions well reproduce the experimental results of visibility as a function of delay time. With consideration of the energy relaxation lifetime, the population relaxation process hardly contributes to the dephasing process. As a result, pure dephasing time of this position is evaluated to be 7.1 ps, corresponding to a homogeneous linewidth of 184 μeV. The long coherence of moiré exciton revealed in this study offer potential applications of moiré quantum systems in quantum technologies.

Collaboration Works

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Clean Energy Conversion Research Section

Yasuhiro Suzuki, Visiting Professor
(Hiroshima University)

1. Introduction

The heat transport on the magnetic island and stochastic magnetic field are essential in magnetic confinement fusion research because the magnetic island and stochastic magnetic field sometimes simultaneously appear in the fusion plasma. For example, in tokamaks, the magnetic island is generated by the MHD instability of the tearing mode. If two magnetic islands simultaneously appear and overlap in the reversed magnetic shear, the magnetic field may be stochastic. On the other hand, for stellarators, due to the lack of toroidal symmetry, the magnetic field can become naturally stochastic.

For a long time, it has been believed that the temperature gradient cannot be kept if the magnetic field structure is strongly stochastic. Rechester and Rosenbluth theoretically discussed the electron heat transport on the strongly stochastic magnetic field[1]. On the strongly stochastic magnetic field, the diffusion of the magnetic field lines enhances the diffusion process, and then the electron temperature flattens. That is, there is no temperature gradient on the stochastic field. However, in many tokamak and stellarator experiments, although the stochastic magnetic field is expected, a finite temperature gradient is observed from the measurement. Thus, some believe that the finite temperature gradient is evidence where the magnetic field does '*not*' become stochastic. However, this is not true.

Dewer and Hudson studied the chaos in the perturbed magnetic field and successfully constructed the nearby integrable field, the so-called quadratic-flux-minimizing (QFM) surface or ghost surface[2]. Then, they proved that a near-integrable surface is a KAM surface. The heat transport is studied on the analytical and realistic stochastic magnetic field. If some KAM surfaces exist on the stochastic magnetic field, those KAM surfaces can be worked as a transport barrier. In addition, depending on the ratio of the parallel and perpendicular heat conductivity, $\chi_{\parallel}/\chi_{\perp}$, the finite temperature gradient can be kept on the stochastic magnetic field.

In this study, we numerically study the heat transport on the stochastic magnetic field of a stellarator. In particular, the heat transport depending on the different diffusions is considered.

2. Model and Numerical Implementation of anisotropic heat diffusion

In this study, we study the anisotropic heat diffusion on the stochastic magnetic field following numerical studies in tokamaks. At first, it assumes that heat transport is dominated by heat conduction. Then, the heat transport equation is considered as follows:

$$\frac{3}{2}n\frac{\partial}{\partial t}T = -\nabla\cdot\mathbf{q} + Q$$

where n and T are electron density and temperature, q is the electron heat flux, and Q is the heat source. Here, the convection term is neglected. For simplicity, the constant density is assumed. So, the heat transport equation is rewritten as

$$\frac{\partial T}{\partial t} = -\nabla\cdot\mathbf{q} + Q$$

This is a starting equation.

In this study, the equation is numerically solved. Here, the strong anisotropy is given by the heat flux,

$$\mathbf{q} = -(\chi_{\parallel}\nabla_{\parallel}T + \chi_{\perp}\nabla_{\perp}T)$$

Gradients of the T along the parallel and perpendicular directions can be defined by,

$$\nabla_{\parallel}T = \mathbf{bb}\cdot\nabla T$$

and

$$\nabla_{\perp}T = \nabla T - \nabla_{\parallel}T = (\mathbf{I} - \mathbf{bb})\cdot\nabla T$$

where, b is the unit vector of the magnetic field, B/B, and I is the unit tensor.

This study approximates these gradients by the finite difference scheme on the cylindrical coordinate (R,ϕ,Z). In previous studies, the parallel and perpendicular gradients are approximated by metrics of the magnetic field. However, guaranteeing enough accuracy, particularly along the parallel direction, is challenging. Therefore, this study uses the field line tracing method to improve the numerical accuracy of calculating the parallel gradient. At first, the anisotropic heat diffusion equation is simplified in the given magnetic field as

$$\frac{\partial T}{\partial t} = \left(\chi_{\parallel}\nabla_{\parallel}^{2}T + \chi_{\perp}\nabla_{\perp}^{2}T\right)$$

Next, two magnetic field lines are traced from a computational grid on (R,ϕ,Z) to b and $-b$

directions, respectively. Here, the equation of the magnetic field lines is defined by

$$\frac{dR}{dl} = B_R/B$$
$$\frac{d\phi}{dl} = B_\phi/RB$$
$$\frac{dZ}{dl} = B_Z/B$$

where the integral variable is l.

If the length L of the field line tracing from the computational grid can be defined, the parallel gradient at $L/2$ can be defined as

$$\frac{\partial T}{\partial l}\Big|_{l=+\frac{L}{2}} = \frac{T|_{l=+L} - T|_{l=0}}{\Delta l}$$

where l is the arch length of the field line from the grid and $T|_{l=+L}$ is the temperature at $L = +l$. Here, the $l = 0$ is the grid. Thus, the parallel diffusion on the grid can be defined as

$$\frac{\partial^2 T}{\partial l^2}\Big|_{l=0} = \frac{\frac{\partial T}{\partial l}\Big|_{l=+\frac{L}{2}} - \frac{\partial T}{\partial l}\Big|_{l=-\frac{L}{2}}}{\Delta l}$$

The magnetic field line is traced by the 4th-order Runge-Kutta method, and the 4th-order scheme interpolates the temperature. At the beginning of the simulation, the field line is traced, and two end points of the field line at $l = +L$ and $-L$ starting from $l = 0$ are stored in the memory. On the other hand, the perpendicular diffusion on the cylindrical coordinate may be simplified as

$$\nabla_\perp^2 T \sim \frac{\partial^2 T}{\partial R^2} + \frac{\partial^2 T}{\partial Z^2}$$

where the metric along the R direction is ignored. The second-order finite difference scheme approximates the second derivate, and the derivative along the R direction is defined as

$$\frac{\partial^2 T}{\partial R^2} = \frac{T_{i-1,j,k} - 2T_{i,j,k} + T_{i+1,j,k}}{\Delta R^2}$$

The time evolution of the anisotropic heat diffusion is integrated by the 4th-order Runge-Kutta method.

In this study, the heat source is given by the Gaussian profile on the magnetic axis. The plasma response effect is not included, and the magnetic field is fixed in time.

3. Results

We applied a new code that implemented the above ideas to a stellarator, $L/M = 2/10$ Heliotron configuration.

The $\chi_\parallel/\chi_\perp$ is scanned from 10^6 to 10^{10} in figure 1. A top panel shows enlarged T/T_0 profiles on Z =*const.* plane, and a bottom panel shows a Poincare plot at the horizontally elongated cross section for the vacuum standard configuration. Two purple circles indicate the stochastic magnetic field region. Due to the increased $\chi_\parallel/\chi_\perp$, the T/T_0 profile is changed, and the small flattening of the temperature appears from $\chi_\parallel/\chi_\perp = 10^7$. However, for the cases of $\chi_\parallel/\chi_\perp = 10^8$ - 10^{10}, the change of the profile is not large. According to Fitzpatrick's theory[3], the flattening width of the temperature on the magnetic island is proportional to the following equation,

$$W_d \sim \left(\frac{r_s}{nq'}\right)^{\frac{1}{2}} \left(\frac{\chi_\perp}{\chi_\parallel}\right)^{\frac{1}{2}} \sim \left(\frac{\chi_\perp}{s\chi_\parallel}\right)^{\frac{1}{2}}$$

If the$\chi_\parallel/\chi_\perp$ is 10^8, the W_d/r_s is roughly 10^{-2}. The flattening size in this study is consistent with the theoretical prediction.

5. Summary

We numerically study the anisotropic heat diffusion on the stochastic magnetic field in the Heliotron configuration. The smooth temperature profile appears if the perpendicular diffusion is significant, although the magnetic field becomes stochastic. However, if the ratio of $\chi_\parallel/\chi_\perp$ increases to 10^8, the small flattening of the temperature profile appears on the stochastic magnetic field. In that region, the connection length of the magnetic field line is sufficiently long. Therefore, the finite temperature gradient can be kept.

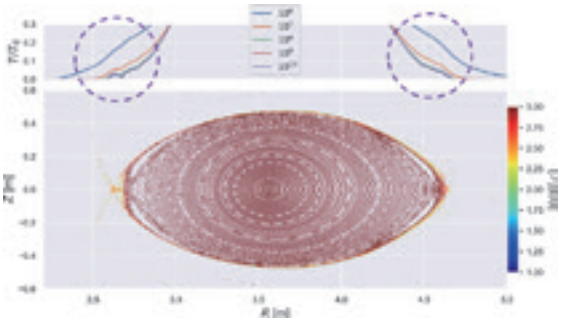

Fig. 1: A comparison of the anisotropic heat diffusion with the different $\chi_\parallel/\chi_\perp$ is shown. The $\chi_\parallel/\chi_\perp$ is scanned from 10^6 to 10^{10}. A top panel shows enlarged T/T_0 profiles on Z = *const.* plane, and a bottom panel shows a Poincaré plot at the horizontally elongated cross section for the vacuum standard configuration. Two purple circles indicate the stochastic magnetic field region. Due to the increased $\chi_\parallel/\chi_\perp$, the T/T_0 profile is changed.

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Chemical Reaction Complex Processes Research Section

T. Nohira, Professor (concurrent)
K. Kawaguchi, Program-Specific Associate Professor
T. Yamamoto, Assistant Professor
Y. Norikawa, Assistant Professor

1. Introduction

In this research section, we study electrochemistry and materials science. We also apply them to the development of new water electrolysis, new metal plating processes, and new rechargeable batteries.

In this fiscal year, we have researched a highly efficient water electrolysis using hydrate melt, a tungsten film plating process using molten salts, and dual carbon batteries using ionic liquids.

2. Development of Highly Efficient Water Electrolysis Using Hydrate Melt

Hydrogen production by water electrolysis using electricity from renewable energy sources is attracting attention. However, one of the challenges in conventional water electrolysis, including alkaline water electrolysis (AWE), is the improvement of energy efficiency. Recently, we reported that water electrolysis using an 85 wt% KOH hydrate melt (KOH:H_2O = 65:35 mol%) at 150°C significantly reduced the overpotential for the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) compared to a conventional 30 wt% KOH aqueous solution (KOH:H_2O = 12:88 mol%) at 80°C [1].

In this fiscal year, we focused on a NaOH–KOH hydrate melt (NaOH:KOH:H_2O = 9:61:30 mol%), which has a lower melting point (88°C) than the KOH hydrate melt (101°C), and investigated HER and OER behavior at a Ni electrode.

Fig. 1 shows a comprehensive summary of the overpotentials for HER and OER at 200°C in the NaOH–KOH hydrate melt. This summary includes data for each current density, highlighting the total overpotential and the corresponding reduction in comparison with the KOH aqueous solution at 500 mA cm^{-2} and 80°C (total overpotential: 1133 mV). At a current density of 500 mA cm^{-2}, the total overpotential of 545 mV is 588 mV (52%) lower than that of the KOH aqueous solution at 80 °C. At an increased current density of 1000 mA cm^{-2}, the total overpotential of 619 mV is 514 mV (45%) lower. Even at 2000 mA cm^{-2}, the total overpotential of 714 mV is 419 mV (37%) lower. Water electrolysis utilizing the NaOH–KOH hydrate melt shows promising potential for significantly enhancing the energy efficiency, even at higher current densities relative to conventional AWE.

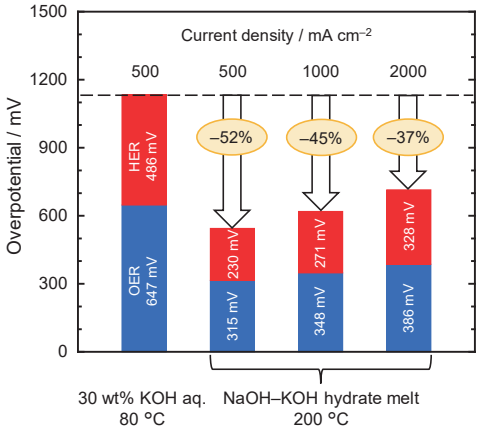

Fig. 1. Comparison of overpotential on a Ni electrode in 30 wt% KOH aqueous solution at 80°C and the NaOH–KOH hydrate melt at 200°C.

3. Development of W film Plating Process Using Molten Salt Electrolyte: Effect of O^{2-} Ion Concentration on the Crystal Structure of W Films

Tungsten (W) is a metal with superior properties, such as heat resistance, high strength, and low thermal expansion. However, its hardness and brittleness make it difficult to process into complex shapes and conventional tungsten processing methods are costly. Thus, the electrodeposition in molten salts was explored as an alternative processing method [2]. Typically, α-W was electrodeposited from molten salts. However, we have electrodeposited β-W, metastable phase of W, from CsF-CsCl-WO_3 melt at 773 K [3,4]. We predicted that oxygen content in W films, which is affected by O^{2-} ion concentration in molten salt, has an influence on the crystal structure. To investigate the effect of O^{2-} ion concentration, W electrodeposition was performed in molten CsF–CsCl at 773 K with different W sources and Li_2O concentration.

W was electrodeposited in molten CsF–CsCl–WCl_6 at −200 mA cm^{-2} for 360 C cm^{-2} and in molten CsF–CsCl–WO_3 with various added amounts of Li_2O at −4 mA cm^{-2} for 90 C cm^{-2}. Phase identification of the samples was conducted by X-ray diffraction (XRD). As shown in Fig. 2, the pre-dominant α-W formation was observed in molten CsF–CsCl–WCl_6, while only β-W formation was confirmed in molten CsF–CsCl–WO_3. Furthermore, the addition of Li_2O increased the orientation of β-W crystal

to the 111 plane. The structure of W(IV) complex ions might depend on O^{2-} ion concentration, resulting in different crystal structures of electrodeposited W and crystal orientation.

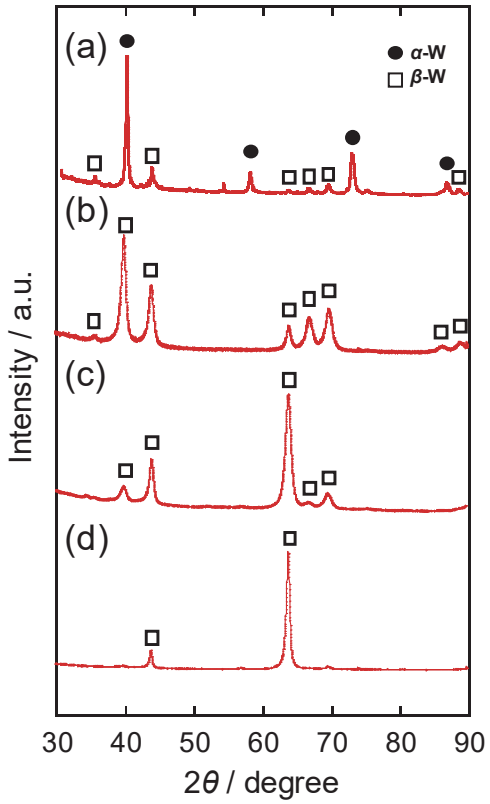

Fig. 2. XRD patterns of W films electrodeposited in molten CsF–CsCl with (a) WCl_6 (1.0 mol%), (b) WO_3 (2.0 mol%), (c) WO_3 (2.0 mol%)–Li_2O (1.0 mol%), and (d) WO_3 (2.0 mol%)–Li_2O (2.0mol%) at 773 K.

4. Development of Dual-Carbon Batteries Using Ionic Liquid Electrolytes

The large-scale electrochemical energy storage (EES) devices are indispensable for the establishment of energy supply system with intermittent renewable energy resources such as solar photovoltaic and wind power. Current lithium-ion batteries (LIBs), which are being used for portable electronic devices, have been the candidates of the EES system. However, the geological scarcity and uneven distribution of lithium and cobalt resources cannot fulfill the increasing demands of large-scale EES devices, evoking the necessity of other viable options. To address these issues, we have developed LIB alternatives such as sodium and potassium secondary batteries because sodium and potassium resources are abundant in the Earth's crust and seawater [5].

Furthermore, we recently investigated the feasibility of dual-carbon batteries (DCBs) [6,7]. Since carbon-based materials are used for both positive and negative electrodes in DCBs, the conventional metal oxide-based positive electrodes containing scarce metals like cobalt and nickel are no longer necessary. Also, we adopted ionic liquids (ILs) as promising electrolytes because DCBs are categorized in reserve-type batteries that require a large amount of charge carriers in electrolytes at the initial state. Fig. 3 shows the discharge capacities of graphite/graphite full cell with K[FTA]–[C_4C_1pyrr][FTA] IL electrolyte (FTA = (fluorosulfonyl)(trifluoromethylsulfonyl)amide, C_4C_1pyrr = *N*-butyl-*N*-methylpyrroridinium) at 298 K. In the initial 10 cycles, the discharge capacity gradually decreases from 84.0 (1st) to 69.5 (10th) mAh g^{-1}. Thereafter, the full cell shows the stable cycling performance and retains the reversible capacity of 62.5 mAh g^{-1} at 100th cycle, which indicates the feasibility of DCBs utilizing IL electrolytes.

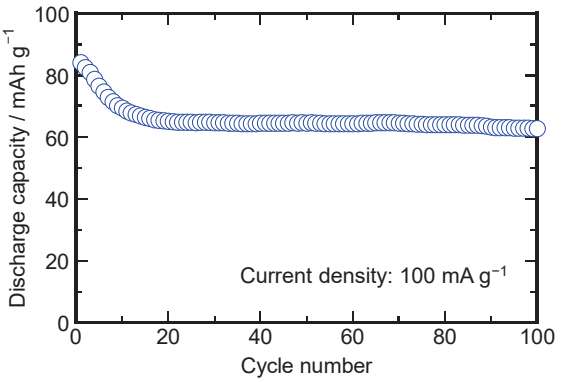

Fig. 3. Discharge capacities of graphite/graphite full cell at 298 K. Electrolyte: K[FTA]–[C_4C_1pyrr][FTA] (molar fraction: x(K[FTA]) = 0.20). Capacity and current density are expressed per the active material weight in the positive electrode.

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Molecular Nanotechnology Research Section

H. Sakaguchi, Professor
T. Kojima, Assistant Professor
S. Nobusue, Assistant Professor

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.

Main research achievements in Molecular Nanotechnology Research Section in 2023 are described below.

2. Bottom-Up On-Surface Synthesis of Edge-functionalized Graphene Nanoribbon

Graphene nanoribbons (GNRs) 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 is required for desired properties. Bottom-up synthesis of GNRs is one of the suitable methods to satisfy these requirements because of the definition of their edge structures and widths by the shape of precursors. Atomically precise synthesis of armchair-edged GNRs has 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 of 1 Torr from halogenated polycyclic aromatic hydrocarbon (PAH) precursors. This technique successfully produced a series of armchair-edged GNRs in high yield. The attractive features of this method originate from an independent temperature control of the 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.[1] Additionally, we demonstrate a new concept of 'conformation-controlled surface catalysis'; the 2Z-CVD 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 an Au(111) surface, results in the efficient formation of acene-type GNRs with a width of 1.45 nm through optimized cascade reactions. These cascade reactions on the 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 concept analogous to the biological catalyst, enzyme, is useful for the fabrication of new nanocarbon materials.[2]

Recently, GNRs having an asymmetrically functional substitution at each edge have attracted much attention due to the realization of ferroelectric or ferromagnetic properties predicted by theory. However, it has been difficult to produce them because of the decomposition of functional substitution at high-temperature process during the dehydrogenation reaction. To overcome these drawbacks, we have developed a brand new method, molecular-vapor-assisted low-temperature growth (MVLTG), based on a massive dose of gaseous hydrogen-accepting molecules to the prepolymer on the metal surface at a low temperature.

After producing precursor polymers using the 2Z-CVD method with Z-bar-linkage having a different substitution at each edge as a precursor, hydrogen acceptor was fed into the reactor (evacuated quartz tube), which promote dehydrogenation reaction resulting in giving asymmetrical GNRs without decomposition of functional substitution at a lower temperature. Then, we succeeded in the direct observation of asymmetric GNRs produced on Au(111) with a low-temperature scanning tunneling microscope. The low-voltage STM measurement and dI/dV mapping suggest that

MVLTG successfully enhanced the dehydrogenation reaction without the decomposition of the functionalized group of the GNRs' edges.[3-5]

3. Solution Synthesis of Asymmetrically Functionalized Graphene Nanoribbon toward the Application for Functional Materials

Solution-phase synthesis is one of the most promising strategies to obtain well-defined graphene nanoribbons (GNRs) with tunable electronic and optical properties. Asymmetrically edge-functionalized GNRs have attracted a great deal of interest in view of the relationship between their unique structure and properties. Several theoretical predictions have been made to change the properties of these systems through edge modifications. The introduction of different functional groups to the edges of GNRs backbone would offer a promising strategy to exhibit new properties. Although the solution-phase syntheses of GNRs having symmetric substitutions have already been reported, our approach, however, has remained unexplored.

We previously reported the on-surface synthesis of acene-type GNR from the Z-shaped precursor which consists of two terphenyl units. Inspired by this work, we envisioned that the asymmetrically substituted GNRs would be obtained from asymmetrically Z-shaped precursor in the solution synthesis. However, the desired product was not obtained probably due to the skeletal rearrangement in the oxidative dehydrogenation reaction. To develop the synthetic method for asymmetrically edge-functionalized GNR, we have synthesized nanographenes as a model compound and GNRs from Z-shaped precursor by Pd-catalyzed cyclization followed by oxidative dehydrogenation reactions.

Based on this method, we investigated the synthesis of GNR having symmetric substitutions. As a result, we have developed the synthetic method via head-totale polymerization followed by cyclization with Pd-catalyzed bond formations and oxidative dehydrogenation reactions. This method is applicable to the preparation of asymmetric GNR having different functional groups at opposite sides of the edges. We developed this method for the asymmetric GNR. The relationship between the functionalization of edge structures and their properties was identified by absorption spectra.

As an additional step, we designed asymmetric functional GNR. Asymmetrically functionalized and sterically hindered GNRs adopt twisted conformation and have dipolar moments along the long and short axis by asymmetrically modifying both edges. We hypothesized that polarity of the twisted GNR would be controlled by applying an electric field. We succeeded in the preparation of helically twisted GNR through modified synthetic methods and tested voltage-current characteristics in the solid state with sandwitch-type cell. As a result, when the positive and negative voltage were swept up to 30 V, clear peaks probably due to ferroelectric properties were observed. These results indicated that conformational changes of twisting molecules took place even in the solid state by applying voltages.

4. Deceptive orbital confinement at edges and pores of carbon-based 1D and 2D nanoarchitectures

The properties of graphene-based nanomaterials are defined by their electronic structure. However, when conducting experiments using scanning tunneling microscopy/spectroscopy (STM/STS) on graphene nanoribbons (GNRs), nanographenes, and nanoporous graphene (NPG), researchers have often observed an apparent confinement of electronic orbitals into the edges and nanopores. This has led to dubious interpretations such as image potential states or super-atom molecular orbitals. Our research shows that these measurements are subject to a wave function decay into the vacuum, which masks the undisturbed electronic orbital shape. To explore this, we used Au(111)-supported semiconducting gulf-type GNRs and NPGs as model systems fostering frontier orbitals that appear confined along the edges and nanopores in STS measurements. DFT calculations confirm that these states originate from valence and conduction bands. The misleading electronic orbital confinement observed is caused by a loss of Fourier components, corresponding to states of high momentum. This effect can be generalized to other 1D and 2D carbon-based nanoarchitectures and is important for their use in catalysis and sensing applications.[6]

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坂口浩司, 挑戦的研究（萌芽）, 分子スケール極細幅を持つ黒リン・ナノリボンのボトムアップ合成技術の開発
小島崇寛, 基盤研究(C), 巨大強誘電性を志向した非対称エッジ型 GNR の低温表面合成

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Biofunctional Chemistry Research Section

T. Morii, Professor
E. Nakata, Associate Professor
P. Lin, Assistant Professor

1. Introduction

A transition to renewable energy technologies requires new chemistry to learn from nature. For almost 3 billion years, nature has developed fantastic solutions to convert solar energy into chemical energy and to use it in exceptionally efficient way. Our challenge is to understand nature's efficient bioenergetic processes and to design bio-inspired energy utilization systems. The research interests of 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 biological molecular recognition and chemical reactions. Proteins and protein/nucleic acid assemblies are explored to realize the biomimetic function of biological systems, such as visualization of cellular signals by fluorescent biosensors, directed self-assembly of peptides and proteins to build up nano-bio materials, tailoring of 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 nanoar-chitectures. The following are the major research achievements in the fiscal year 2023.

2. An Artificial Liposome Compartment with Size Exclusion Molecular Transport

The cellular compartment plays an essential role in organizing the complex and diverse biochemical reactions within the cell. By mimicking the function of such cellular compartments, the challenge of constructing artificial compartments has been taken up to develop new biochemical tools for efficient material production and diagnostics. The important features required for the artificial compartment are that it isolates the interior from the external environment and is further functionalized to control the transport of target chemicals to regulate the interior concentration of both substrate and reaction products. In this study, an artificial compartment (lipo-WS) with size-selective molecular transport function was constructed by using a DNA origami-guided liposome prepared by modifying the method reported by Perrault *et al.* (*ACS Nano* 2014, **8**, 5132). This completely isolates the liposome interior (lipo), including the DNA origami skeleton (WS), from the external environment and allows the assembly of a defined number of molecules of interest inside and/or outside the compartment. By incorporating a bacterial membrane protein, OmpF, into the liposome, the resulting artificial compartment (lipo-OmpF-WS) was shown to transport only the molecule of interest with a molecular weight below 600 Da from the external environment into the interior of the compartment.

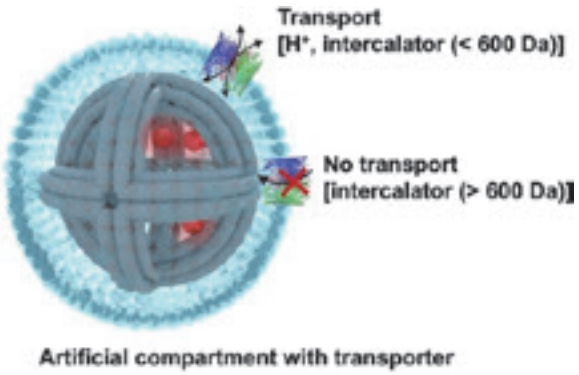

Fig. 1 Illustration of the insertion of OmpF into the membrane of lipo-WS (lipo-OmpF-WS) to construct an artificial compartment with a transporter.

3. Near Quantitative Ligation Results in Resistance of DNA Origami Against Nuclease and Cell Lysate

There have been limited efforts to ligate the staple nicks in DNA origami which is crucial for its stability against thermal and mechanical treatments, and chemical and biological environments. Here, two near-quantitative ligation methods for the native backbone linkage at the nicks in origami are demonstrated: i) a cosolvent dimethyl sulfoxide (DMSO)-assisted enzymatic ligation and ii) enzyme-free chemical ligation using CNBr. Both methods achieved over 90% ligation in 2D origami, only the CNBr method resulted in ≈80% ligation in 3D origami, while the enzyme alone yielded 31–55% (2D) or 22–36% (3D) ligation. Only the CNBr method was efficient for 3D origami. The CNBr-mediated reaction was completed within 5 min, while DMSO method took overnight. Ligation by these methods improved the structural stability up to

30 °C, stability during the electrophoresis and subsequent extraction, and stability against nuclease and cell lysate. These methods are simple, non tedious, and superior in terms of cost, reaction time, and efficiency.

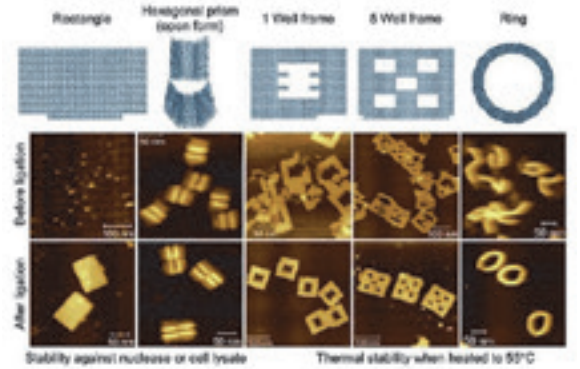

Fig. 2 Various DNA Origami shapes and atomic force microscopy images before and after ligation.

4. A Ratiometric Fluorescent Probe for pH Measurement over a Wide Range Composed of Three Types of Fluorophores Assembled on a DNA Scaffold

The desirable characteristics of the sophisticated fluorescent pH probe are ratiometric detection characteristics and a wide detection range. In this study, three types of fluorophores with different fluorescence properties were assembled on a DNA origami nanostructure. The DNA nanostructure has the advantage of being a scaffold that can assemble different types of fluorophores with control over their number and position. The defined number of three different fluorophores, i.e., pH-sensitive fluorescein (CF) and Oregon Green (OG), and pH-insensitive tetramethylrhodamine (CR), assembled on the DNA scaffold provided a ratiometric fluorescent pH probe with a wide pH detection range that could cover the variation of intracellular pH.

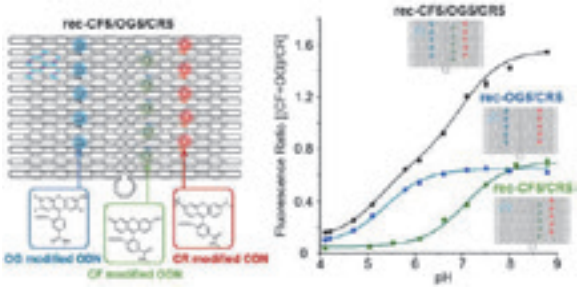

Fig. 3 An illustration of a DNA origami scaffold assembled with three types of fluorophores and their response.

5. Macropinoscope: Real-Time Simultaneous Tracking of pH and Cathepsin B Activity in Individual Macropinosomes

A fluorescent sensor that allows simultaneous analysis of environmental factors in a confined cellular space is useful for understanding precise molecular interactions in living cells and their biological responses. Macropinocytosis is a ubiquitous endocytic pathway for massive uptake of extracellular fluids, resulting in the formation of macropinosomes. Although macropinocytosis can affect intracellular delivery and cancer proliferation, information on the intracellular behavior of macropinosomes is limited. Here, we aimed to develop a macropinoscope, a sensor that simultaneously detects pH and cathepsin B activity in individual macropinosomes. A macropinosome-specific marker, dextran (70 kDa), was used as a platform, onto which fluorescein (CF), Oregon Green (OG), and tetramethylrhodamine (CR) were loaded for ratiometric pH sensing and imaging. A cathepsin B-cleavable peptide sequence carrying sulfo-Cy5 and the quencher BHQ-3 was also loaded; cleavage of the sequence was detected as an increase in sulfo-Cy5 fluorescence. A steep decrease in pH was observed 5–10 min after macropinosome formation, which was accompanied by an immediate increase in cathepsin B activity. Our design concept will lead to the development of other macropinoscopes for the simultaneous detection of other parameters in individual macropinosomes.

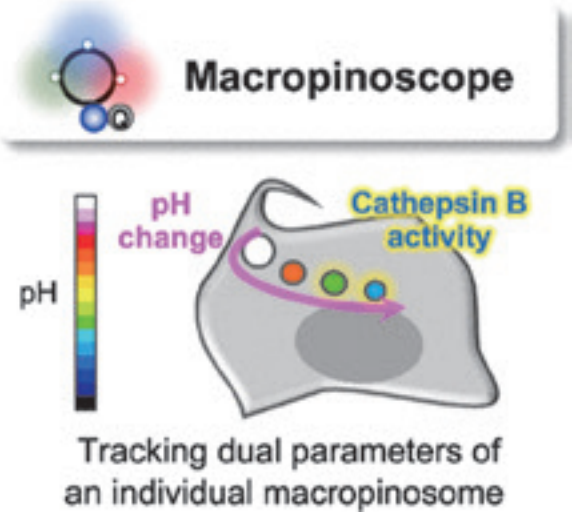

Fig. 4 Illustration of the analysis of simultaneous sensing of pH and cathepsin B activity using CF/OG/CR/CTSBsub-Dex in live cells.

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Structural Energy Bioscience Research Section

M. Katahira, Professor
T. Nagata, Associate Professor
Y. Yamaoki, 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 2023.

2. Structural insights and mutagenesis of *Acremonium alcalophilum*'s feruloyl esterase unveil superior catalytic activity

This research provides groundbreaking insights into the enzymatic mechanisms and potential biotechnological applications of feruloyl esterases (FAEs) in the subfamily 5 (SF5), derived from *Acremonium alcalophilum* (*Aa*FaeD). By elucidating the crystal structure of *Aa*FaeD's catalytic domain (CD) for the first time, both in its free form and when complexed with ferulic acid (FA), the study illuminates the critical role of a hydrophobic cleft in substrate binding and catalysis. This structural analysis revealed that FA binds within a distinct hydrophobic cleft, leading to targeted mutagenesis experiments which demonstrated the significance of key hydrophobic residues for enzymatic activity. Remarkably, a specific mutant, F120Y, displayed a 1.5-fold increase in activity towards methyl ferulate compared to the wild type. The study's comparison of SF5 FAEs with those in subfamilies 2 and 3 highlighted a broader substrate specificity for SF5 FAEs, capable of processing both monomeric and dimeric phenolic substrates. This capability contrasts with the preference of SF2 and SF3 FAEs for monomeric substrates, showcasing the unique potential of SF5 FAEs in biotechnological applications for sustainable biomass degradation. These findings significantly advance our understanding of SF5 FAEs' structure-function relationships and pave the way for exploiting these enzymes in developing more efficient methods for biomass conversion, contributing to sustainable biofuel production and biorefining processes.

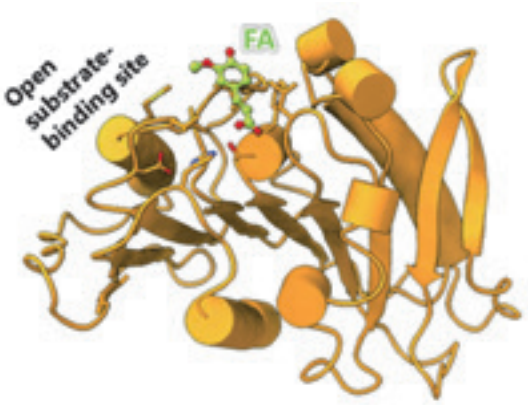

Figure 1. The determined crystal structure of *Aa*FaeD.

3. Synergistic effects of co-displayed xylanase and feruloyl esterase on *Pichia pastoris*

This study explores an innovative approach to enhancing lignocellulosic biomass degradation using yeast surface display (YSD) technology to co-display xylanase (XYN) and feruloyl esterase (FAE) on the surface of *Pichia pastoris* (*Komagataella phaffii*). By engineering three *P. pastoris* strains—X-Pichia with XYN, F-Pichia with FAE, and X/F-Pichia with both enzymes—the research examines the synergistic action and the impact of enzyme proximity on the decomposition of acid-pretreated sugarcane trash. The findings reveal a clear synergistic effect when XYN and FAE are co-displayed, with X/F-Pichia showing a 1.5-fold increase in reducing sugar yield compared to X-Pichia alone, and a 1.1-fold increase in ferulic acid production over F-Pichia or a mixture of X-Pichia and F-Pichia. These results highlight the potential of enzyme co-display on *P. pastoris* for significantly improving biomass degradation efficiency. The study demonstrates the enhanced bioconversion process made possible through the strategic co-localization of XYN and FAE on the yeast cell surface, facilitating effective substrate turnover and increased product

yields. This synergistic and proximity effect of co-displayed enzymes offers a promising avenue for efficient and sustainable utilization of lignocellulosic biomass, contributing to advancements in bioprocessing technologies for biofuel production and biorefining, thereby supporting more sustainable and environmentally friendly biotechnological applications.

4. *Cs*MnP-catalyzed polymerization and condensation for high-value material synthesis

This study delves into the catalytic potential of manganese peroxidase (MnP) derived from *Ceriporiopsis subvermispora* (*Cs*MnP) for lignin modification and its application in Kraft lignin (KL) condensation to create high-value lignin-based materials. Using guaiacylglycerol-β-guaiacyl ether (GGE) as a model compound, *Cs*MnP's ability to polymerize the phenolic β-O-4′ lignin substructure was explored, revealing the formation of compounds with higher molecular weights indicative of polymerization. Specifically, NMR analysis of the products highlighted the formation of dimeric structures through 5-5′ linkages. Further experiments with KL demonstrated *Cs*MnP's efficacy in increasing the molecular weight of KL by 360% within 24 hours, with NMR spectroscopy suggesting condensation through α-5′, 5-5′, and 4-O-5′ linkages and a notable decrease in phenolic content by 37%. These findings underscore the capability of *Cs*MnP to not only degrade lignin but also to engineer its structure, offering a biotechnological route to valorize lignin into more complex and functional materials. The successful demonstration of *Cs*MnP-mediated condensation reactions provides a promising approach for the synthesis of novel lignin-based polymers, paving the way for their application in various industries, including materials science and sustainable chemistry. This research highlights the versatility of MnP enzymes as tools for lignin valorization, contributing to the development of environmentally friendly and resource-efficient bioprocesses.

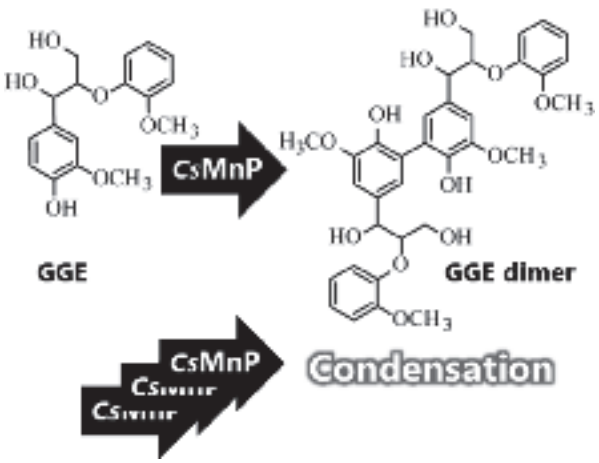

Figure 2. The conversion of GGE catalyzed by *Cs*MnP.

5. The structure and interaction with ligands of an RNA aptamer targeting HIV-1 Tat in living human cells analyzed by in-cell NMR

An RNA aptamer, which exhibits strong binding to the trans-activator of transcription (Tat) protein of HIV-1 within living human cells, holds potential as a therapeutic drug for HIV. To explore the structure and interactions of this RNA aptamer in living cells, in-cell NMR serves as a potent method. In this study, we investigated the interaction between the RNA aptamer and a peptide derived from Tat, which is crucial for the aptamer's binding, in living human cells using in-cell NMR experiments. The aptamer and the peptide were introduced into living HeLa cells, and we obtained in-cell NMR spectra of the aptamer-peptide complex. Through comparison of *in vitro* and in-cell NMR spectra, we discovered that the aptamer forms two U-A-U base triples upon binding to the peptide, even within the cellular environment. These base triples expand the originally narrow major groove of the aptamer, creating a space to accommodate two critical arginine residues of Tat during the binding process. Our research rationally explains the high binding affinity of the aptamer for the peptide in the cellular environment, leveraging both *in vitro* and in-cell NMR analyses.

6. Direct inhibition of human APOBEC3 deaminases by HIV-1 Vif

HIV-1 Vif is known to counteract the antiviral activity of human APOBEC3 (A3), a cytidine deaminase. Vif forms a complex called VβBCC, comprising CBFβ and the components of E3 ubiquitin ligase, Elongin B, Elongin C, and Cullin5. Together with the ubiquitin-conjugating enzyme, VβBCC induces ubiquitination-mediated proteasomal degradation of A3. Here, we elucidated that VβBCC inhibits deamination by A3G, A3F, and A3B, independently of proteasomal degradation. Surprisingly, we discovered that this inhibition for A3G is directly attributed to the interaction between VβBCC and the C-terminal domain of A3G which was not supposed to interact with Vif. Our findings suggest that inhibiting the interaction between VβBCC and the C-terminal domain, as well as the N-terminal domain known to be targeted for ubiquitination, of A3G may be needed to prevent counteraction by Vif.

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Self-Assembly Science Research Section

A. Rajendran, Junior Associate Professor

1. Introduction

Structural DNA nanotechnology[1] has attracted much attention during the past one and a half decades due to the addition of the scaffolded DNA origami method[2] to the field. This method has enabled the synthesis of DNA nanomaterials with a dimension of ~100 nm in diameter, whereas the initially prepared non-scaffolded structures were ~10 to 20 nm in size. Since the invention of scaffolded origami, various two- (2D) and three-dimensional (3D) DNA materials have been synthesized and self-assembled further to create even larger materials in the dimension of micrometers. Due to their self-assembly nature and addressability, these materials have been used as novel scaffolds for nanopatterning of various nanoparticles and quantum dots, attachment of carbon nanotubes, immobilization of biomolecules such as proteins[3] and viral capsids, carriers of drugs, a platform for the analysis of single molecular reactions and processes,[4] and so on. The specific interest to us is the application of these materials as scaffolds for organizing enzyme cascades related to biomass energy conversion.[3]

Besides the application of origami materials, one major issue with these nano-biomaterials is their unsatisfactory thermal stability, which prevents them from being used in various conditions to withstand thermal, mechanical, and chemical modifications.[5] For instance, the DNA origami structures that use most of the staples of length 32 bases melt below 50 °C. Similar to the non-scaffolded DNA tube,[6] the 3D DNA origami structures such as cuboid may also break open when deposited on mica or scanned by force-based methods such as atomic force microscopy (AFM), and disintegrate in deionized water. The biomass product contains several carboxylic acids with a pH of 2 to 2.5. However, origami materials are stable only between pH 4.5-10 but denature at a lower pH.[7] The reason for the stability issues of the origami materials is the presence of breaks in the phosphate backbone, the so-called nicks, in the staple strands. Increasing the staple length would improve the thermal stability, but at the same time would lead to practical difficulties such as increased cost of synthesis, decreased product yield and purity, and limitations on the maximum length of synthetic oligo DNAs.

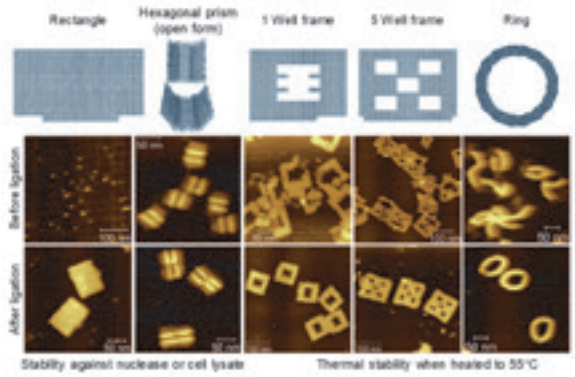
2. Currently available methods

There have been few reports on stabilizing DNA origami structures, including photo-cross-linking using 8-methoxypsoralen. Another method is the UV light-induced cyclobutane pyrimidine dimer formation by placing thymidines nearby within DNA origami.[9] However, these methods are unsuitable where native-like DNA is anticipated, as they introduce chemical cross-links to the DNA strands. Also, the irradiation of UV light for 1 to 2 h often leads to DNA damage. The alternative method is the enzymatic ligation of the nicks,[10] which is routinely used in molecular biology. Enzymatic ligation was also applied for the tiny DNA nanostructures such as the DNA nanotubes with the size of ~10 nm in diameter that contain only five nicks or only two sticky ends, DNA triangles containing double crossover molecules, four-arm DNA junctions, and the DNA triple crossover complexes. Among these structures, the short DNA nanotube was ligated with an average efficiency of 68 to 77%, while no ligation yield was reported for other structures. Also, enzymatic ligation is not widely applied to scaffolded DNA origami. DNA origami structure is a bundle of tightly packed anti-parallel duplexes. Thus, the enzymatic ligation on that is expected to differ from that of a simple duplex DNA or non-scaffolded DNA nanostructures consisting of relatively few ssDNAs. Crystal structures of ligases suggest that the enzymes completely encircle the nicked DNA to ligate the nick. The tightly packed DNA origami may restrict access to the ligase; thus, optimization of the conditions and well characterization of the ligation is necessary. Further, it is essential to develop methods to stabilize DNA origami nanomaterials for diverse applications, especially when dealing with enzymes involved in biomass energy conversion.

3. Cosolvent-assisted enhanced enzymatic ligation

The previous investigations of the effect of organic solvents, such as DMSO, on the ligation indicated that it increased the extent of the ligation reaction, or showed no effect, or increased the specificity while decreasing the efficiency. This motivated us to test the effect of DMSO and other solvents on the

Figure 1. Top panel: DNA origami nanomaterials used in this study. Middle panel: AFM images indicating the



unsatisfactory stability of the origami materials. Bottom panel: AFM images of the ligated origami materials indicate improved stability against thermal treatment, nuclease digestion, and cell lysate.

ligation of DNA origami. The initial ligation experiments were carried out with four different 2D DNA origami structures, namely rectangle (Rec)[2] and frame-shaped origami containing 1 (1WF),[11] 3 (3WF),[12] and 5 wells (5WF, Figure 1, top panel).[13] Several organic solvents were screened to determine the best-performing cosolvent on the enzymatic ligation of origami using 1WF. All the staple stands were purified to eliminate the kinase inhibitors such as ammonium and phosphate ions, 5′-phosphorylated with ~100% yield, and utilized to fold M13mp18. After folding, the excess staples were removed by spin column filtration, and the origami was ligated by T4 DNA ligase in the absence or presence of cosolvent. To our surprise, the ligation proceeded much better and resulted in near-quantitative ligation in the presence of DMSO when compared to ligase alone. Additionally, we confirmed that only DMSO successfully enhanced the enzymatic ligation of origami, and other organic solvents failed to do so. As we anticipated, the ligated origami resulted in much better stability of the origami materials against various treatments (Figure 1, middle and bottom panels).

4. Chemical method to stability the DNA origami

CNBr was used to ligate the origami staples chemically. Agarose gel electrophoresis (AGE) was used to characterize the ligation reaction. The chemically ligated origami migrated faster than the native and enzymatically ligated origami. This indicated that the chemical ligation method is more efficient than other methods. Moreover, the chemical ligation reaction was completed within 5 min, highlighting the advantage over enzymatic ligation, which typically requires overnight reaction time for saturation. Reaction conditions were carefully adjusted to optimize the ligation yield. As a result, the highest possible ligation efficiency, exceeding 90%, was achieved under the optimized conditions. This ligation method improves the structural stability up to 30ºC, enhances stability during electrophoresis and subsequent extraction, and provides resistance against nuclease and cell lysate. In addition to its superior efficiency, this method is straightforward and non-tedious, with a cost advantage over other methods, making it an attractive option.[14]

5. Conclusions

Our study demonstrates the use of organic solvent on enzymatic ligation and chemical ligation as efficient methods for nick ligation in DNA origami nanomaterials. We could ligate staple nicks in origami with near-quantitative yields by optimizing the reaction conditions. These methods were successfully tested on four different 2D DNA origami structures. The advantages of using CNBr-mediated ligation include a faster reaction time of just 5 min, along with quantitative reaction yields and native phosphate ligation. Additionally, the ligation of origami using these methods enhances their stability against thermal treatments, during electrophoresis and purification, and provides resistance against nuclease and cell lysate. Overall, our findings suggest two highly effective methods for achieving efficient and stable nick ligation in DNA origami, with potential applications in biomass-related enzymes in particular and in nanotechnology, biophysics, and synthetic biology in general.

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Broad Band Energy Science Research Section

T. Kii, Associate Professor
F. Kin, Assistant Professor

1. Introduction

We are engaged in research aimed at new applications of energy over a wide range of spatiotemporal scales. For magnetic field energy and plasma energy, we are working on establishing powerful and precise magnetic field control methods, pioneering new local high field and strong gradient applications, optimizing fusion plasma confinement by magnetic fields, and clarifying plasma transport phenomena.

2. Generation of strong periodic magnetic field

Synchrotron radiation is produced when charged particles are accelerated. If the acceleration is periodically applied by a device that generates a periodic magnetic field, so called an undulator, intense synchrotron radiation can be obtained via interference. Therefore, generation of strong and precise periodic magnetic field is quite attractive to develop high performance future synchrotron light sources. The resonant wavelength of the emitted radiation from planer undulator λ_R can be expressed using period length of the undulator λ_U, energy of the electron beam E, and the maximum transverse magnetic field strength of the undulator B_0 as following equations (1) and (2).

$$\lambda_R[\text{Å}] = \frac{\lambda_U}{2\gamma^2}\left(1+\frac{K^2}{2}\right) \approx 13.056\frac{\lambda_U[\text{cm}]}{(E[\text{GeV}])^2}\left(1+\frac{K^2}{2}\right) \quad (1),$$

$$K = \frac{e\cdot B_0\cdot\lambda_U}{2\pi\cdot m_0 c} \approx 93.36 B_0[T]\cdot\lambda_U[m] \quad (2).$$

Here, γ is the Lorentz factor, K is the undulator parameter which determines property of radiation, e is the charge of the electron, m_0 is the mass of electron, and c is the speed of light. The unit of wavelength is Å, undulator period length is cm, electron energy is GeV, and magnetic field is Tesla respectively. According to Eq. (1), use of high energy electron beam is essential to generate short wavelength synchrotron lights. Thus, high brightness hard X-ray higher than 10 keV, which play an important role in material science, has been provided mainly at 6-8 GeV-class large synchrotron radiation facilities such as SPring-8 or high-energy linac facilities such as SACLA. In order to increase usability of the hard X-ray, new innovative technology for generation of hard X-rays in a compact and energy-saving 3 GeV-class accelerator facilities is desired. Therefore, we focused on bulk superconductors, which can handle ultra-high currents, and have been working on an innovative undulator that enable to generate hard X-ray even at the 3 GeV-class accelerator facility.

The new undulator consists of stacked bulk high critical temperature superconductor array and a 6 T superconducting solenoid magnet. In this year, we have developed a hybrid array structure consisting bulk GdBaCuO superconductor and vanadium permendur. Photograph of the new undulator prototype and the hybrid array is shown in fig. 1. Magnetic field performances were widely surveyed for different period length, structure, and operating temperature (fig. 2)

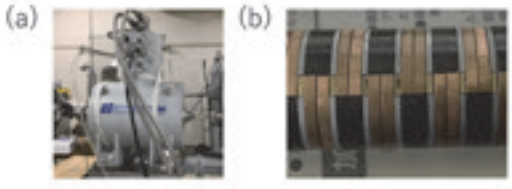

Fig. 1 (a) Photograph of the new unduloator prototype and (b) the new hybrid stacked array.

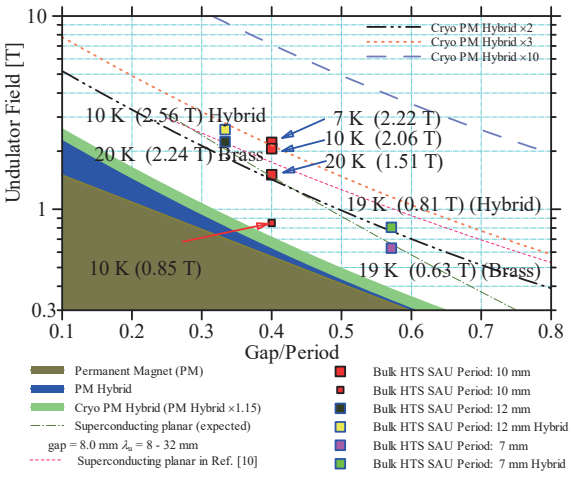

Fig. 2 Performance comparison

Compared to conventional permanent magnet

undulators, the performance of this type of undulator is about twice as high at 20 K and about three times as high at 10 K over a wide range of gap/period ratios.

3. Introduction

The transport barrier formation in magnetic confinement plasmas has been the central topic for achieving fusion reactor. Especially, the internal transport barrier (ITB) is essential for steady-state operation in tokamaks, because the ITB drives plasma current to keep the plasma confinement stable. Conventionally, the ITB is formed due to local turbulence suppressions, however, several experiments suggest the global dynamics of ITBs that extend beyond the range of turbulence reduction regions. Based on these backgrounds, we have investigated the global transport effect on the ITB formation observed in JT-60U tokamak plasmas [1].

4. Impact of avalanching transport on the internal transport barrier (ITB) formation

We have investigated the avalanche type of transport, which is a domino-like event that propagates sequentially to neighbors via local critical excitations. Since avalanches can propagate with a long-radial distance, the study of avalanches could provide new insights into the formation mechanism of the ITB.

In this experiment, the power of the neutral beam (NB) injection was scanned to investigate the ITB transition in JT-60U plasmas, with NB powers of 8, 10, 11 and 12 MW. We have detected the avalanche events from density fluctuations measured by reflectometer. As shown in Fig. 1, density fluctuation level is increased when the NB power reaches 10 MW. In addition, the density fluctuation intermittently increases in time, showing a bursty feature. The bursty increases of density fluctuations, called as bursty fluctuation (BF), are synchronized to the large avalanche events in electron temperature fluctuations measured by electron cyclotron emission (ECE) diagnostics. At the avalanche events, the electron temperature fluctuation indicates void (δ Te < 0) and bump (δ Te > 0), propagating in opposite direction to relax the electron temperature gradient.

When q_{min} (minimum value of the safety factor) crosses the rational surfaces, a transient increase of temperature is phenomenologically observed in tokamaks. Similar to the previous studies, electron temperature is increased when q_{min} reaches 5 (Fig. 3). The T_e increases were transient in the 8, 10, and 11 MW discharges, whereas the T_e increase was continuous in the 12 MW discharge and finally reached the stationary ITB. The BFs continuously and partially appeared in the 10 and 11 MW discharges, whereas they were completely decreased in the 12 MW discharge. Especially in the 11 MW discharge, the short-time decay of the electron temperature is synchronized to the BFs. From these results, we found that the formation of ITB is disturbed by the occurrence of avalanches.

Acknowledgement

These researches were partly supported by grants from JSPS KAKENHI (JP22H03870).

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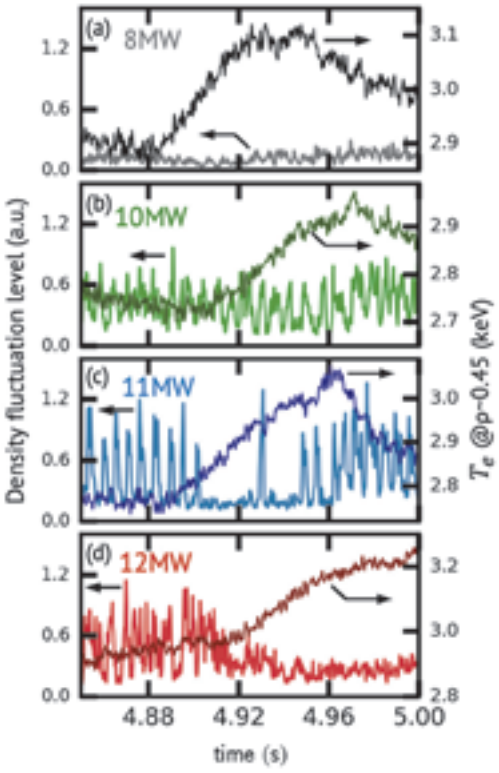

Fig. 3 Temporal evolution of BFs and electron temperature for NB-power of (a) 8MW, (b) 10MW, (c) 11MW and (d) 12MW.

Financial Support

Grant-in-Aid for Scientific Research
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Environmental Microbiology Research Section

T. Hara, Program-Specific Professor
Y. Takatsuka, Program-Specific Associate Professor

1. Introduction

The relationship between energy resource consumption and environmental protection is crucial to developing a sustainable society. Despite our heavy reliance on fossil energy, there is concern that greenhouse gas emissions are disrupting the harmony of the global environment. Additionally, environmental pollution continues to be the shadow of civilization's progress due to the energy consumption of fossil fuels. One of the solutions is to develop a practical method that uses 'enzymes' derived from environmental microorganisms with high energy utilization efficiency in catabolism. Meanwhile, we are also working on sustainable agricultural techniques, which are the source of life energy. We are collaborating with academics, biotechs, and university start-ups globally to network research towards the social implementation of our technologies.

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

We have developed a composite microbial catalyst that can efficiently degrade polychlorinated biphenyls (PCBs), well-known pollutants found widely in the environment. Biphenyl dioxygenase (BDO) plays a crucial role in the degradation of PCBs. It incorporates two oxygen atoms into the PCB's aromatic ring, which then induces aromatic ring cleavage. In more technological detail, our laboratory has designed a composite catalytic enzyme consisting of two BDOs with different substrate specificities. We have also forged a bioreactor that generates oxygen microbubbles to enhance the enzymatic activities of BDOs. With these innovations, we have constructed a practical system that degrades 99.3% of 40 mg L^{-1} of domestic major commercial PCBs (Kanechrol KC-300 and KC-400 of KANEKA CORP.) in 24 hours. This result meets the waste disposal measure defined by the Ministry of the Environment Government of Japan (Figure 2).

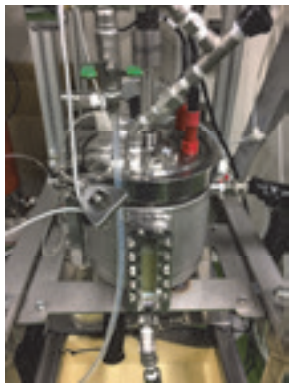

Figure 1: The composite BDOs-microbial catalyst was tested in a dedicated experimental bioreactor with an oxygen microbubble generation device.

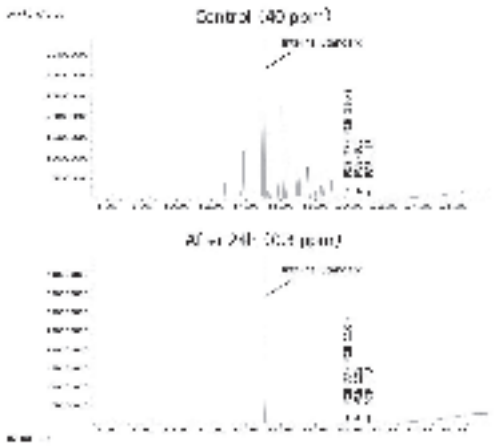

Figure 2: Gas chromatography-quadrupole mass spectrometer data show the degradation of PCBs by the composite BDOs-microbial catalyst.

2-2. Several bacterial species associated with PCB dechlorination were genetically identified at PCB-contaminated sites.

We have been developing an artificial enzyme that can dechlorinate PCBs by two-electron reduction. To do this, we collected sediments from freshwater pit pools contaminated with PCBs in the Yodogawa riverside in the Osaka area and investigated whether bacteria associated with PCB dechlorination exist.

According to 16S rRNA gene phylogenetic analysis, it has been observed that *Dehalobacter* sp. and *Desulfitobacterium* sp. are present in that specific location. Wang and He (Environ Sci Technol, 2013) have reported that "*Deharobacter*" can dechlorinate penta- and hexa-chlorinated biphenyls while "*Desulfitobacterium*" can dechlorinate tetra-chlorinated

biphenyls that are hydroxylated at the para position.

We successfully prepared the medium for growing two specific bacterial species and developed a suitable cultivation method. In addition, we observed that these bacterial species can reduce PCBs in an artificial model of a polluted environment. Even today, after a decade of starting this investigation, we continue to observe their long-term effects to confirm the accuracy of our results.

3-1. A new protein secreted by *Rhizoctonia solani* suppresses filamentous fungi growth.

Rhizoctonia solani is a filamentous fungus belonging to the phylum Basidiomycota. This fungus is well-known for its ability to infect and cause severe diseases in many crops, such as rice sheath blight, which significantly impacts paddy-rice production. The exact mechanism by which this phytopathogenic fungus infects plants has yet to be fully understood. However, studies have shown that when wheat bran is added to the growth medium, this fungus secretes glycosidases that digest plants and fungi cell walls. Our team has discovered a new protein secreted from *R. solani* when cultured with wheat bran as a solid medium. This protein has a molecular weight of approximately 10 kDa and exhibits anti-fungal properties against filamentous fungi. We reported this finding for the first time at the 2023 Annual Meeting of the Japan Society for Bioscience, Biotechnology, and Agrochemistry[1]. This protein inhibited the growth of *Fusarium fujikuroi*, another phytopathogenic filamentous fungus belonging to the phylum Ascomycota. It was suggested that this protein also inhibited conidium formation and germination of *F. fujikuroi*.

After conducting an amino acid sequence analysis, it was found that the partial amino acid sequence of this protein suggests that it has an unknown function. Additionally, the full-length amino acid sequence of the protein was deduced after investigating the whole genome sequence of the *R. solani* strain that produces it. The BLAST search results on this sequence also suggested that the protein has an unknown function.

According to the process and sequence analysis of the cDNA that encodes this protein, the complete amino acid sequence of the protein was found to be 122 residues. The mature protein's amino acid sequence, which excludes the assumed signal peptide sequence, was 88 residues in length. Based on this information, the estimated molecular weight of this protein was 9648.24. Furthermore, this particular antifungal protein has made us aware of unique structural features in its primary amino acid sequence that have never been reported. The protein consists of 88 residues and has a double-repeat structure of 41 residues, with a high homology of 92% across the central 6 amino acid residues. The functional role of such repetitive sequences still needs to be better understood. We have named this antifungal protein "**Double-Repeating Homologous Sequence Anti-Fungal Polypeptide (DRHS-AFP)**."

3-2. The completion of the genetic recombination of DRHS-AFP and investigation of its antifungal spectrum.

We have designed a system for expressing DRHS-AFP as genetically recombinant proteins. The DRHS-AFP gene was amplified by PCR and encoded the mature protein's 88 residues with an additional initiation of methionine. Then, we inserted this DRHS-AFP gene into the pET-15b, *E. coli* expression vector, to create the DRHS-AFP expression plasmid, pEp10. Finally, we transformed the *E. coli* host strain BL21(DE3) with pEp10 for the protein expression.

The efficacy of recombinant DRHS-AFP in confronting filamentous fungi that typically infect paddy rice was tested. The pathogens tested included *Fusarium fujikuroi* (Figure 3), *Trichoderma viride*, *Pyricularia oryzae*, *Pythium* sp., *Rhizoctonia solani*, and *Rhizopus microsporus*. The results indicated that the genetically modified DRHS-AFP had a growth-suppressive effect on *F. fujikuroi* and *T. viride*. Likewise, it was suggested that the anti-filamentous fungal activity of the genetically modified DRHS-AFP was equivalent to that of the native DRHS-AFP.

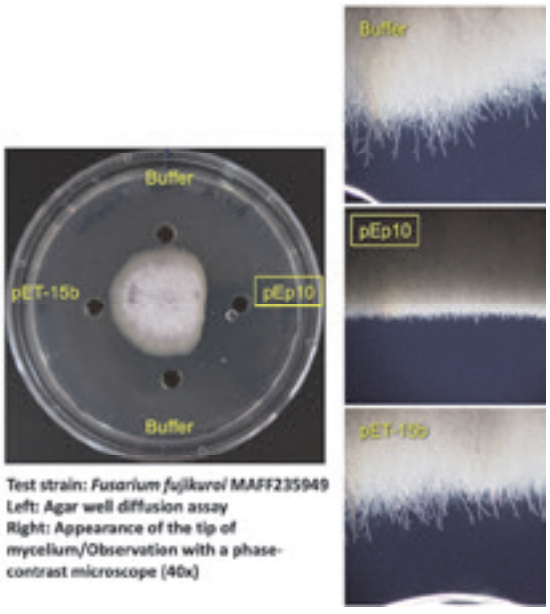

Figure 3. The anti-filamentous fungal activity of genetically recombinant DRHS-AFP.

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Financial Support

1. Grant-in-Aid for Scientific Research
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髙塚由美子, 基盤研究(C), 高塩素置換型ポリ塩化ビフェニル類の還元的脱塩素化を大気下で実現させる

2. Others
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Integrated Research Center for Carbon Negative Science

T. Nohira, Professor
K. Kondo, Program-Specific Associate Professor
S. Chuaychob, Program-Specific Assitant Professor
A. Yadav, Program-Specific Assistant Professor

1. Introduction

In order to achieve carbon neutrality by 2050, we need to develop new energy systems that include active carbon dioxide fixation processes in addition to "zero-emission" technologies. Our research center is conducting research on such carbon negative technologies. To be specific, we are working on the conversion of carbon dioxide into useful materials by using renewable energy and biomass, etc.

In this fiscal year, we have investigated the conversion of CO_2 into carbon material by molten salt electrochemical process. We have also studied CO_2 fixation reaction which is facilitated by an enzyme called ribulose 1,5-bisphosphate carboxylase/oxygenase (RuBisCO).

2. Conversion of CO_2 into Carbon Material by Molten Salt Electrochemical Process

As one of the Carbon dioxide Capture and Utilization (CCU) technologies, the electrochemical synthesis of carbon in molten salts is attracting much attention [1]. By using molten salts containing O^{2-} ions, CO_2 can be captured as CO_3^{2-} ions.

$$CO_2 + O^{2-} \rightarrow CO_3^{2-}$$

Then, CO_3^{2-} can be reduced to carbon as follows.

$$CO_3^{2-} + 4e^- \rightarrow C + 3O^{2-}$$

Many allotropes of carbon, for example, diamond [2], amorphous carbon, graphite, carbon nanotubes, and carbon nanofibers have been electrodeposited in molten salt. In this fiscal year, the electrodeposition of carbon from molten LiCl–KCl–K_2CO_3 was conducted at various potentials (0.6–1.0 V vs. Li^+/Li) and temperatures(773–973 K) to investigate the effect of electrolysis conditions on carbon deposition.

Fig. 1 shows the transitions of current density during electrolysis. The current density increased as the potential became negative. The photograph of a typical sample on a Ni substrate is shown in Fig. 2. The black deposits were attached to the substrate and the black powders were obtained after washing. Fig. 3 shows the Raman spectrum of the sample obtained at 0.80 V. Broad bands attributed to the D-band (around 1350 cm^{-1}) and G-band (around 1570 cm^{-1}) are observed. These spectra are specific to amorphous carbon, which has both sp^2 and sp^3 hybrid orbital. There is no significant difference in the electrodeposited carbon at the different potentials and temperatures.

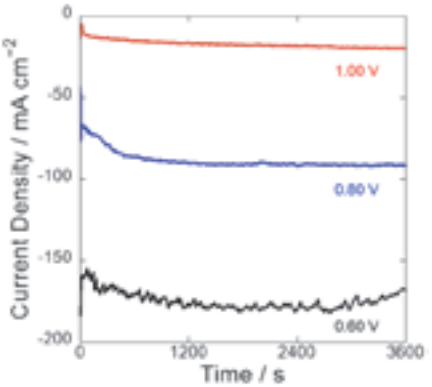

Fig. 1. Transitions of current density during the electrolysis at 0.60 V, 0.80 V, and 1.00 V in molten LiCl–KCl–K_2CO_3 at 973 K.

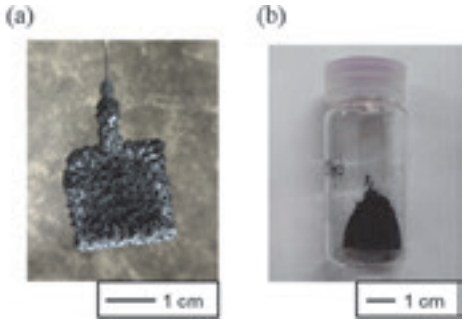

Fig. 2. Photographs of the sample electrodeposited by potentiostatic electrolysis at 0.6 V for 30 min at 873 K in molten LiCl–KCl–K_2CO_3. (a) As electrodeposited, (b) after washed.

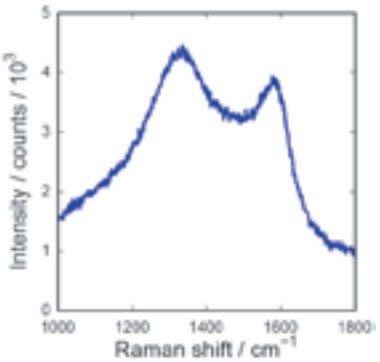

Fig. 3. Raman spectra of carbon electrodeposited at 0.80 V in molten LiCl–KCl–K_2CO_3 at 973 K.

Table 1 Current efficiencies in the electrodeposition of carbon in molten LiCl–KCl–K_2CO_3 at various electrolysis conditions.

	0.4 V	0.6 V	0.8 V
773 K	97%	94%	98%
873 K	89%	93%	91%
973 K	61%	71%	72%

Table 1 summarizes the current efficiencies of carbon deposition under various potentials and temperatures. High current efficiencies of 89–98% were achieved at 773 and 873 K. On the other hand, the current efficiencies tended to decrease at 973 K. This may be because, at 973 K, the current used for carbon monoxide generation instead of carbon deposition increased.

3. Novel Process for Carbon Fixation Reaction

RuBisCO enzyme, the most abundant enzyme on earth, catalyzes the primary CO_2 fixation reaction in plants, algae, and bacteria via the Calvin–Benson–Bassham (CBB) pathway. This enzyme catalyzes two competing reactions: (1) carboxylase reaction producing 3-phosphoglycerate (3-PGA) from ribulose 1,5-bisphosphate (RuBP), CO_2, and H_2O, and (2) oxygenase reaction adding O_2 to RuBP, resulting in 3-PGA and 2-phosphoglycolate. The oxygenase reaction reduces photosynthesis efficiency. Furthermore, RuBisCO is an enzyme that has low turnover efficiency.

As one of RuBisCOs, *T. kodakaraensis* KOD1, or *Tk*-RuBisCO enzyme shows extreme thermostability, high carboxylase activity, and specificity at a high-temperature range. This suggests that the enzyme's stable protein scaffold can tolerate higher degrees of mutations at ambient temperatures compared to other types. These outstanding properties make *Tk*-RuBisCO an attractive target for structure-function studies and protein engineering to improve CO_2 fixation activity.

By using the recombinant *Tk*-RuBisCO, an initial examination as to whether a *Tk*-RuBisCO could extend the substrate rather than RuBP. A *Tk*-RuBisCO was expressed in *E. coli* and used for CO_2 fixation activity after purification (Fig. 4). Activity was investigated and confirmed with two different substrates such as RuBP and ribulose 5-phosphate (Ru5P) via the NADH-linked spectrophotometric assays using GAPDH coupling enzymes for measuring RuBisCO activity.

Fig. 5 shows the enzymatic activities of *Tk*-RuBisCO that 3-PGA was produced. Along with the native RuBP substrate, significant levels of CO_2 fixation activity were observed as a result of the increase in 3-PGA production (Fig. 5a). On the other hand, the 3-PGA production detected from an alternative Ru5P substrate (Fig. 5b) was lower than that of the native substrate one. That could be a lack of affinity for Ru5P compared to RuBP. Thus, the activity could be observed only at a high concentration of Ru5P.

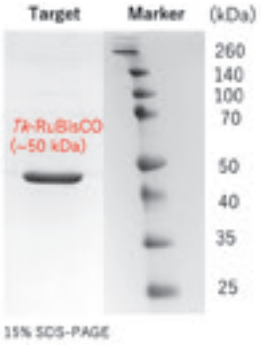

Fig. 4. SDS-PAGE analysis of *Tk*-RuBisCO.

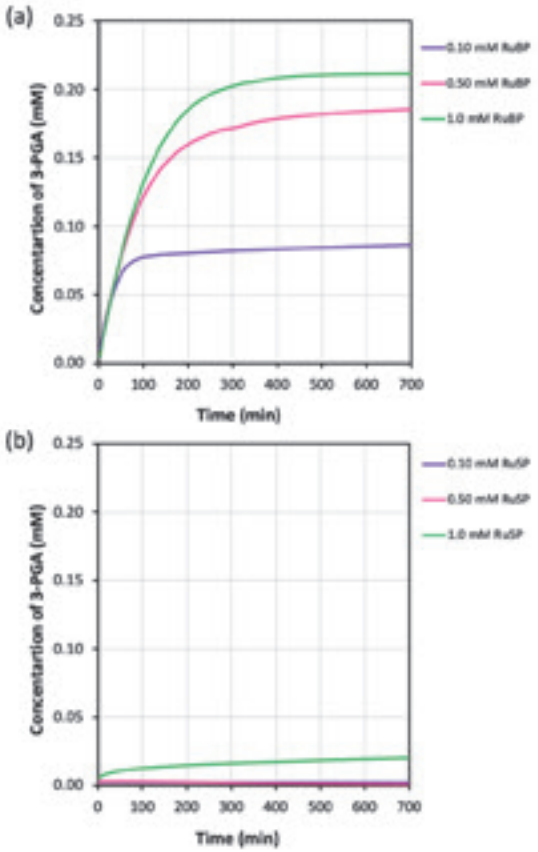

Fig. 5. The production of 3-PGA from CO_2 fixation reaction is catalysed by *Tk*-RuBisCO using native RuBP (a) and alternative Ru5P (b) substrates.

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野平俊之, コスモ石油-京都大学, 「溶融塩電解による CO_2 の炭素固定化技術」に関する研究

Financial Support

1. Grant-in-Aid for Scientific Research

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近藤敬子, 基盤研究(C), 木質の多糖分解およびリグニン分解に関わる酸化還元酵素間の協奏効果の解析

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3-2. AWARD

Incentive Award in the 19th AESJ Kansai meeting

Advanced Atomic Energy Research Section
Toshiro Sakabe (D3)

The 19th Atomic Energy Society of Japan (AESJ) Kansai meeting, sponsored by the Kansai Branch of AESJ, was held on 4th March 2024 at the Osaka Science and Technology Center. This event provides young researchers and students in nuclear fission and fusion science and engineering and the surrounding area an opportunity to present their works.

Mr. Toshiro Sakabe (D3) attended and made an oral presentation titled "Effect of the water-cooling feedthrough system for the cathode on the neutron production rate in the discharge type of fusion neutron source". He presented the effect of the cathode cooling system on the neutron production rate in the glow discharge type of DD fusion neutron source. In this meeting, he received the Incentive Award from the Kansai Branch of AESJ.


表彰状

Best Presentation Award in the 17th JEMEA Symposium

Advanced Atomic Energy Research Section
Hiroyuki Tamiya (D2)

Hiroyuki Tamiya was awarded Best Presentation from the Japan Society of Electromagnetic Energy Applications (JEMEA) on January 27th, 2024. Best Presentation is annually given to a researcher who has achieved outstanding academic results in the field of electromagnetic energy applications. He was awarded this prize for the achievements of “Novel Reactions in Microwave Heating of Cellulose with Magnetite and Their Applications”.

In his award lecture, which was held on October 26th, 2023 at Kitakyushu International Conference Center, he presented the effects of microwave heating of cellulose with magnetite and steam feeding. A series of descriptions of needs, equipment assembly, and product analysis were highly evaluated for a presentation award.


ベストプレゼンテーション賞

Student Poster Award in the 14th International Symposium of Advanced Energy Science

Functional Materials Science and Engineering Research Section
Kaichi Teranishi (M2)

The 14th International Symposium of Advanced Energy Science was held on August 30- September 1st, 2023, jointly by the Institute of Advanced Energy, Kyoto University and Joint Usage/Research Center for Zero-Emission Energy Research. This event provides young researchers and students an opportunity to present their works on energy science related to zero-emission energy.

Kaichi Teranishi (M2) made a poster presentation at the symposium with the topic of "Exciton effects at high temperatures in the transmittance spectra of single-walled carbon nanotube membranes". His presentation was highly evaluated, and he received the Student Poster Award. His research provides the basis for exploiting exciton effects in carbon nanotubes for highly efficient solar and thermal energy harvesting technologies.

Student Poster Award in the 14th International Symposium of Advanced Energy Science

Functional Materials Science and Engineering Research Section
Zhirui Liu (M2)

The 14th International Symposium of Advanced Energy Science was held on August 30- September 1st, 2023, jointly by the Institute of Advanced Energy, Kyoto University and Joint Usage/Research Center for Zero-Emission Energy Research. This event provides young researchers and students an opportunity to present their works on energy science related to zero-emission energy.

Zhirui Liu (M2) made a poster presentation at the symposium with the topic of "Fabrication and optical properties of high-purity carbon nanotube membrane without far-infrared absorption". His presentation was highly evaluated, and he received the Student Poster Award. His research provides the basis for exploiting high purity carbon nanotubes for efficient solar and thermal energy harvesting technologies.

Student Poster Award in the 14th International Symposium of Advanced Energy Science

Functional Materials Science and Engineering Research Section
Hengkai Wu (D1)

The 14th International Symposium of Advanced Energy Science was held on August 30- September 1st, 2023, jointly by the Institute of Advanced Energy, Kyoto University and Joint Usage/Research Center for Zero-Emission Energy Research. This event provides young researchers and students an opportunity to present their works on energy science related to zero-emission energy.

Hengkai Wu (D1) made a poster presentation at the symposium with the topic of "Determination of the complex refractive index spectra of single-structure-enriched carbon nanotube membrane toward solar energy harvesting and utilization". His presentation was highly evaluated, and he received the Student Poster Award. His research provides important information necessary for the practical utilization of carbon nanotubes in various thermal and optical applications including solar thermal energy harvesting.

Young Scientist Poster Award in the 65th Fullerenes-Nanotubes-Graphene General Symposium

Functional Materials Science and Engineering Research Section
Hayato Nakamura (M2)

The 65th Fullerenes-Nanotubes-Graphene General Symposium was held on September 4th–6th, 2023. This conference provides researchers and students an opportunity to present their recent studies on nanomaterials science.

Hayato Nakamura (M2) made a poster presentation at the symposium with the topic of "Photoluminescence excitation spectroscopy on carbon nanotubes synthesized by fullerene coalescence in boron nitride nanotubes". His presentation was highly evaluated, and he received the Young Scientist Poster Award. His work revealed that the exciton properties of carbon nanotubes with a protective shell layer of boron nitride can be maintained in their aggregates, providing a basis for exploiting the quantum effects of carbon nanotubes in bulk materials at high temperatures.

Student Session Outstanding Achievement Award in the Japan Society of Maintenology (*Prize for Outstanding Achievements*)

Advanced Energy Structural Materials Research Section
Sakura Nishikawa (M2)

The Japan Society of Maintenology was founded in 2003 to establish “Maintenology” of nuclear power plants, other complex artifacts, and the natural environments, emerged by collecting a wide variety of information and knowledge of engineering, technology, natural science, sociology.

At the 2023 annual meeting of this society held at Tohoku University on August 27, 2023, Sakura Nishikawa provided an oral and poster presentation on "Validation of the Advanced prediction method for Irradiation Embrittlement using Deep Learning Technique". This is an effort to explore a new method for predicting irradiation embrittlement, and although the data is small, it is highly innovative research that applies the latest machine learning techniques to material irradiation embrittlement data. Her talk attracted a lot of attention at the meeting, and her presentation eventually won the Student Session Award, “Prize for Outstanding Achievements”.

(Nishikawa is in the middle)

Student Session Outstanding Achievement Award in the Japan Society of Maintenology (*Prize for originality*)

Advanced Energy Structural Materials Research Section
Yu Shi (M2)

The Japan Society of Maintenology was founded in 2003 to establish “Maintenology” of nuclear power plants, other complex artifacts, and the natural environments, emerged by collecting a wide variety of information and knowledge of engineering, technology, natural science, sociology.

At 2023 annual meeting of this society held at Tohoku University on August 27, 2023, Yu Shi provided the oral and poster presentations on "Molecular dynamics evaluation of microscopic crack growth conditions”. His and his co-workers’ effort is to explore the conditions for the propagation of small cracks in metallic materials under external stress from the microscopic point of view. Their effort received high attention from the many reviewers, and his presentation eventually won the Student Session Award, “Prize for Originality”.

(Shi is on the far right.)

Student Poster Session Encouragement Award in the Atomic Energy Society of Japan Student Network

Advanced Energy Structural Materials Research Section
Sakura Nishikawa (M2)

The Atomic Energy Society of Japan was founded in 1959 as the only organization in Japan that aims to contribute towards progress in the development of atomic energy by seeking academic and technological advances pertaining to the peaceful use of atomic energy.

In the 2023 Annual Fall Meeting held at Nagoya University, Sakura Nishikawa made a poster presentation on her and her coworkers' effort on "Validation of Advanced Prediction Methods for Irradiation Embrittlement using Machine Learning Techniques". Her presentation was highly praised by the reviewers and finally received the Student Session Encouragement Achievement Award for their creative research using Machine Learning and Material multi-scale modelling techniques. Their research will be the beginning of a fundamental change in the methodology for predicting irradiation embrittlement soon.

Atomic Energy Society of Japan 2023 Fall Meeting Atomic Energy Society of Japan Student Network Excellent Prize

Advanced Energy Structural Materials Research Section
Chen Yuting (D3)

The Atomic Energy Society of Japan 2023 Fall Meeting Organized by the Atomic Energy Society of Japan was held at Nagoya University on September 6, 2023. The student poster section aims to provide more opportunities for students in the nuclear field to display and communicate.

Chen Yuting attended and made a poster presentation on the topic of " Mechanisms for the Generation of Large-Size Clusters in Cascade Collisions: Insights from Molecular Dynamics Simulations". This poster mainly discusses the generation process and mechanisms of defect clusters generated in nuclear power plant structural materials during the irradiation process.

Her presentation was highly focused and eventually received Atomic Energy Society of Japan Student Network Excellent Prize.


日本原子力学会
学生ポスターセッション
優秀賞
京都大学
陳　昱婷殿
あなたは「日本原子力学会2023年秋の大会」学生ポスターセッションにおいて優秀な成果を収められましたので、ここに表彰します
2023年9月6日
一般社団法人日本原子力学会
会長　新堀　雄一

Outstanding Poster Award, The 3rd Student Research Presentation Meeting in Institute of Advanced Energy, Kyoto University

Advanced Energy Structural Materials Research Section
Sakura Nishikawa (M2)

The 3rd IAE Student Research Presentation competition, which was sponsored by the Institute of Advanced Energy (Kyoto University), was held on December 8 (Fri.), 2023.

Sakura Nishikawa provided the poster presentation on “Advanced Methods for Predicting Irradiation Embrittlement using Machine Learning”. Her and her coworkers’ efforts are to explore the new methodology to predict irradiation embrittlement by using machine learning and material multi-scale modelling techniques. Her presentation was highly focused, and eventually won the Poster Award from Institute of Advanced Energy, Kyoto University.


優秀ポスター発表賞

西川さくら 殿

P-20
機械学習を用いた照射脆化予測法の高度化

第３回京都大学エネルギー理工学研究所学生研究発表会において発表されました上記研究に対し優秀な成果を認め、ここに優秀ポスター発表賞を贈り表彰いたします

令和５年１２月８日

京都大学エネルギー理工学研究所

所長 森井 孝

2023Best Figure Prize, Materials Scienece and Technology Division, Atomic Energy Society of Japan

Advanced Energy Structural Materials Research Section
Kazunori Morishita (Associate Professor)

Kazunori Morishita, along with Dr. Yoshiyuki Watanabe of National Institute for Quantum Science and Technology (QST), was awarded for the 2023 Best Figure Prize from Materials Science and Technology Division, Atomic Energy Society of Japan. This award is annually given to those who have left behind academic drawings that are recognized to have had a significant impact on the progress of research on nuclear materials. This year, Watanabe and Morishita drew a thoughtful illustration, clearly showing the quantitative difference in cavity formation in materials irradiated at various irradiation fields, which were obtained their kinetic rate theory analysis. The title of their work is “the irradiation field-dependence of void swelling behavior in ferritic steel: kinetic rate theory analysis incorporating cavity nucleation behavior”. Their work was highly acclaimed by the division reviewers, and they eventually received this prize. The award ceremony was held on March 28, 2024, at the annual division meeting held at Kindai University, Osaka.

(Morishita is on the left, and Watanabe is on the right.)

Young Researcher's Award in the 5th Conference of 2.5 D Materials

Optical Nano-science Research Section
Shuichi Asada (D1)

The 5th Conference of 2.5 D Materials was held on July 2nd and 3rd, 2023 at Osaka University, organized by the Grant-in-Aid for Transformative Research Areas (A) "Science of 2.5 Dimensional Materials: Paradigm Shift of Materials Science Toward Future Social Innovation". The conference provides young researchers and students in the field of related research fields to present their works.
Shuichi Asada (D1) attended and made a poster presentation on the topic of "Study of nonlinear photovoltaic effect and magnetic correlation at $MoS_2/CrPS_4$ heterointerface". In this presentation, he was awarded the Young Researcher's Award from the Grant-in-Aid for Transformative Research Areas (A) "Science of 2.5 Dimensional Materials: Paradigm Shift of Materials Science Toward Future Social Innovation".

賞　状

若手奨励賞

朝田 秀一 殿

あなたは第５回領域会議ポスター発表において 優秀な研究発表をされましたので ここにその栄誉を称え これを賞します

令和５年７月３日

学術変革領域研究(A)
２.５次元物質科学：
社会変革に向けた物質科学のパラダイムシフト
領域代表　　第５回領域会議実行委員長

Award for encouragement of research at The 64th Fullerenes-Nanotubes-Graphene General Symposium

Optical Nano-science Research Section
Wang Haonan (D3)

The 64th Fullerenes-Nanotubes-Graphene General Symposium was held by the Fullerenes, Nanotubes and Graphene Research Society on March 1-3, 2023 at Nagoya University. Wang Haonan (D3) attended and made a poster presentation on the topic of "Observation of a single moiré exciton in nano-fabricated twisted $MoSe_2/WSe_2$ heterobilayers".

He received the award for encouragement of research from the Fullerenes, Nanotubes and Graphene Research Society.

Young Scientist Poster Award

This is to certify that

Wang Haonan

has been awarded Young Scientist Poster Award for paper entitled

"Observation of a single moiré exciton in nano-fabricated twisted MoSe2/WSe2 heterobilayers"

at The 64th Fullerenes-Nanotubes-Graphene General Symposium
Nagoya University
March 1 – 3, 2023

Yutaka Ohno

President,
The Fullerenes, Nanotubes and Graphene Research Society

Oral Presentation Award (Green Chemistry Award) at The 13th ionic liquid symposium

Chemical Reaction Complex Processes Research Section
Takayuki Yamamoto (Assistant Professor)

The 13th ionic liquid symposium was held on 21st–22nd November, 2023 at Niigata, Japan, which was organized by Ionic Liquid Research Association. In this annual symposium, researchers present their recent studies on ionic liquids and the presentation awards are conferred on young scientists and students.

Assistant Professor Takayuki Yamamoto attended the symposium and made an oral presentation on the topic "Charge–discharge behavior of graphite positive electrode in amide-based ionic liquid electrolytes". He received the Oral Presentation Award (Green Chemistry Award), which was given by Royal Society of Chemistry.


ROYAL SOCIETY OF CHEMISTRY

Presentation Prize

This is to certify that

Takayuki Yamamoto

Institute of Advanced Energy,
Kyoto University

has been awarded an oral presentation prize from
Green Chemistry
The 13th Symposium on Ionic Liquids in Japan
21-22 November 2023
Niigata, Japan

Student Poster Award at The 2023 Joint Symposium on Molten Salts (MS12)

Chemical Reaction Complex Processes Research Section
Yoshifumi Ishio (M2)

The 2023 Joint Symposium on Molten Salts (MS12) was held on 12th–16th November, 2023, at Kyoto, Japan, which was organized by Molten Salt Committee of The Electrochemical Society of Japan. This symposium provides many researchers in the field of molten salts and its surrounding area an opportunity to present their works.

In this symposium, Mr. Yoshifumi Ishio (M2) attended the symposium and made a poster presentation on the topic "*In-situ* Raman spectroscopic analysis of the electrode/electrolyte interface in the sodium secondary battery utilizing FSA-based ionic liquids", and received the Student Poster Award.

Research Encouragement Award at The 95th Workshop of Materials Tailoring Society

Chemical Reaction Complex Processes Research Section
Keita Goto (M2)

The 95th workshop of Materials Tailoring Society was held on 3rd–5th August, 2023, at Karuizawa, Japan, which was organized by Materials Tailoring Society. The purpose of this workshop is to systemize the basic study of nanostructured interface creation that induces high-performance physical properties by non-equilibrium processing such as plasma and electrolytic processes and to also apply them to energy conversion and strage.

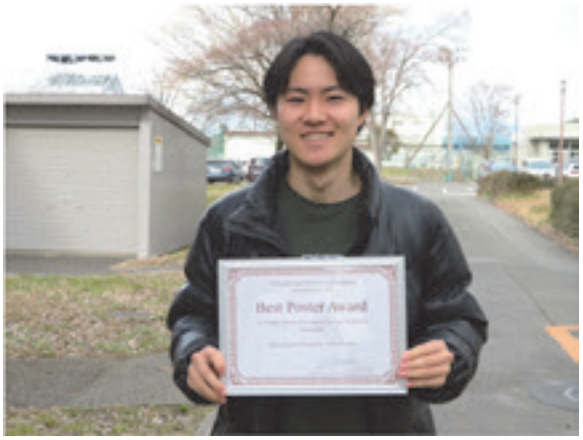
Mr. Keita Goto (M2) attended this workshop and made a poster presentation on the topic "Novel High-Temperature Alkaline Water Electrolysis Using Molten KOH–H_2O System". He received the Research Encouragement Award.

Best Poster Award at The 3rd Nucleation and Growth Research Conference

Chemical Reaction Complex Processes Research Section
Keita Goto (M2)

The 3rd Nucleation and Growth Research Conference was held on 9th–11th November, 2023, at Kyoto, Japan, which was organized by Materials Tailoring Society. The prime purpose of this conference is to discuss in-situ measurements as well as mathematical models of the relevant non-equilibrium reaction and deposition processes, in which electrons, ions, radicals, and clusters interact at the substrate surface.

Mr. Keita Goto (M2) attended this conference and made a poster presentation on the topic "Novel Highly Efficient Water Electrolysis Using NaOH–KOH Hydrate Melt". He received the Best Poster Award.

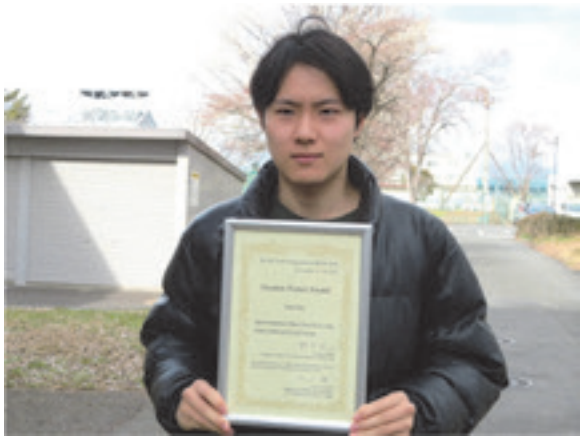


Student Poster Award at The 2023 Joint Symposium on Molten Salts (MS12)

Chemical Reaction Complex Processes Research Section
Keita Goto (M2)

The 2023 Joint Symposium on Molten Salts (MS12) was held on 12th–16th November, 2023, at Kyoto, Japan, which was organized by Molten Salt Committee of The Electrochemical Society of Japan. This symposium provides many researchers in the field of molten salts and its surrounding area an opportunity to present their works.

Mr. Keita Goto (M2) attended this symposium and made a poster presentation on the topic "High-Temperature Water Electrolysis Using Molten NaOH–KOH–H_2O System". He received the Student Poster Award.



Kansai Electrochemistry Encouragement Award at The 3rd Kansai Electrochemistry Seminar

Chemical Reaction Complex Processes Research Section
Haochen Wang (M2)

The 3rd Kansai Electrochemistry Seminar was held on 9th December 2023 at Kobe University, which was held by the Kansai Branch of the Electrochemical Society of Japan. This event provides young researchers and students in the field of electrochemistry and its surrounding area an opportunity to present their works.

Mr. Haochen Wang (M2) attended this meeting and made a poster presentation with the topic of "Effect of O^{2-} Ion on W Electrodeposition in Molten CsF–CsCl". In view of his performance, he was prized the Kansai Electrochemistry Encouragement Award.

Best Poster Award at The 11th Kyoto International Forum for Environment and Energy (KIFEE-11)

Chemical Reaction Complex Processes Research Section
Wataru Moteki (D2)

The 11th Kyoto International Forum for Environment and Energy was held on March 3–5th, 2024 at Tendo, Japan. This event provides many researchers and students in the field of environment and energy an opportunity to present their works.

Wataru Moteki (D2) attended and made a poster presentation on the topic of "Formation of Crystalline Si Using Liquid Zn Electrode in Molten KF–KCl–K_2SiF_6". He received the Best Poster Award.

Student Poster Award at The 2023 Joint Symposium on Molten Salts

Chemical Reaction Complex Processes Research Section
Wataru Moteki (D2)

The 2023 Joint Symposium on Molten Salts (MS12) was held on 12th–16th November, 2023, at Kyoto, Japan, which was organized by Molten Salt Committee of The Electrochemical Society of Japan. This symposium provides many researchers in the field of molten salts and its surrounding area an opportunity to present their works.

Wataru Moteki (D2) attended and made a poster presentation on the topic of "Electrodeposition of Crystalline Si film Using Liquid Zn Electrode in Molten KF–KCl–K_2SiF_6". He received the Student Poster Award.

Student Poster Award in The 14th International Symposium of Advanced Energy Science

Chemical Reaction Complex Processes Research Section
Wataru Moteki (D2)

The 14th International Symposium of Advanced Energy Science was held on August 30–September 1, 2023. This event provides young researchers and students in the field related with energy an opportunity to present their works.

In the meeting, Mr. Wataru Moteki (D2) attended and made a poster presentation on the topic of "Electrodeposition of Crystalline Si Film in Molten KF–KCl–K_2SiF_6 Using Thin Liquid Zn". He received the Student Poster Award.

The Award of Japan Society of Nucleic Acids Chemistry (Ikehara Award 2023)

Biofunctional Chemistry Research Section
Takashi Morii (Professor)

Professor Takashi Morii was awarded the Ikehara Award 2023 by the Japan Society of Nucleic Acids Chemistry on November 2nd, 2023. The Ikehara Prize is awarded annually to researchers who have played a leading role in deepening and developing new research in nucleic acid chemistry through their outstanding research achievements, and who have made original and outstanding contributions to the field. He received the award for his work on "Molecular recognition and functionalization of nucleic acid and protein assemblies".

In his award lecture at the 50th International Symposium of Nucleic Acids Chemistry held in Miyazaki on November 2nd, 2023, he presented on his leading role in establishing the basic science for realizing biopolymers that can function as desired through his original ideas on molecular recognition involving the cooperative nature of nucleic acid-protein complexes and molecular design using chemical synthesis.

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 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 and the third phase in FY2022. 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 FY2023, there were 94 Joint Usage/Research collaboration subjects (including 2 workshops) on Zero Emission Energy, with more than 300 visiting participants, including graduate and undergraduate students, from 40 universities and institutions all over Japan. Researchers from 3 foreign universities also participated in the program. The results of these collaborations are summarized in the report "IAE Joint Usage/Research Program on Zero Emission Energy 2023". On March 28, 2024, a meeting was held online to present some of the outstanding results obtained in FY2023. If you are interested in this collection, please contact the office of Zero Emission Energy Research.

In addition to the Joint Usage/Research collaborations, we organized "The 14th International Symposium of Advanced Energy Science - Research Activities on Zero-Emission Energy Network" on August 30 to September 1, 2023. This symposium was the first full-scale in-person event since the onset of the COVID-19 pandemic and was able to accommodate participants from distant locations. This symposium consisted of oral session, ZE poster session, student poster session, and parallel seminars. The oral session was also simultaneously streamed on YouTube. The oral session was attended by 252 participants and the parallel seminars by 61 researchers, attracting a large number of participants. In total, 324 scientists and students, including 5 foreign and 5 domestic invited speakers, participated in the symposium. At the student poster session, awards were given for outstanding presentations.

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 FY2022, the Integrated Research Center for Carbon Negative Science was established at the Institute under the new concept of energy science and engineering, which sprouted from zero-emission energy research. We will continue to promote high-quality research and high-quality collaborations in multidisciplinary academic fields and work closely with domestic and international research institutions to contribute to the related communities and to the enhancement of Japan's research capabilities.

Poster of the 14th International Symposium

List of Zero Emission Energy Joint Usage/Research Subjects in FY 2023

(Subject, Principal Researcher, IAE Key Person)

Ionics of super-locally-concentrated electrolytes, Atsushi Kitada, Masato Katahira

Development and evaluation of Fe_2M type bulk Laves compounds, Ryuta Kasada, Keisuke Mukai

Structural analysis of lignocellulosic biomass by NMR spectroscopy toward decarbonized society, Hiroshi Nishimura, Masato Katahira

Fermentation of a useful polysaccharide using hydrogen sulfide as energy source, Minoru Takeda, Masato Katahira

Influence of Alloying Elements on Radiation Damage Formation and Hydrogen Isotope Trapping in Tungsten, Yuji Hatano, Kiyohiro Yabuuchi

Visualization of mitochondrial temperature fluctuation towards the development of energy production system mimicking mitochondria, Reiko Sakaguchi, Takashi Morii

Determining the conditions of heat treatments for extending the lifetime of nuclear reactors (2), Yoshitaka Matsukawa, Kiyohiro Yabuuchi

Development of anode/electrolyte interface for advanced Na-ion battery, Hiroki Sakaguchi, Toshiyuki Nohira

Formation of buffer layer on lithium-ion conductive electrolyte diaphragm for electrodialysis, Kazuya Sasaki, Keisuke Mukai

Photoinduced electron-transfer reactions of photosensitizers bound to the active site of enzyme, Hiroshi Takashima, Eiji Nakata

Constructing fluorescent biosensor for visualizing nuclear localization signal of transcription factor Sp1 involved in regulating metabolic pathway, Shunsuke Tajima, Eiji Nakata

Isolation of phase-separation regulatory long noncoding RNA and NMR analysis of its molecular mechanism, Riki Kurokawa, Masato Katahira

Novel pulsed terahertz source by super-radiance free electron laser oscillator, Kazuyuki Sakaue, Heishun Zen

Structural basis of DNA recognition by the replication initiator ORC, Shou Waga, Yudai Yamaoki

Application of mode-selective phonon-excitation method in semiconductors of energy functionality with mid-infrared free-electron laser, Kan Hachiya, Hideaki Ohgaki

Generation of High intensity THz pulse by superposition of undulator superradiant, Shigeru Kashiwagi, Heishun Zen

Research for control of cell growth mechanism using viral protein-derived peptides, Hideki Kusunoki, Takashi Nagata

Change in hardness by hydrogen charging in tungsten irradiated with Fe and He ions, Koichi Sato, Kiyohiro Yabuuchi

Observation of a distribution of mode-selectively excited phonon on SiC, Kyohei Yoshida, Hideaki Ohgaki

Wavelength-dependent degradation of polyurethane with molecular vibrational excitation, Takayasu Kawasaki, Heishun Zen

Study on development of compound-based anode for K-ion battery and on compatibility with ionic liquid electrolyte, Yasuhiro Domi, Takayuki Yamamoto

Ionaization energy of Ce3+ ion in multicomponent garnets determined by photoinduced free carier plasma absorption spectroscopy using a MIR free-electron laser, Mamoru Kitaura, Heishun Zen

Analysis of transition from axisymmetric torus to helical axis toroidal plasma, Akio Sanpei, Kazunobu Nagasaki

Experimental verification of hydrogen adsorption and desorption behavior for advanced neutron multipliers, Jae-Hwan Kim, Keisuke Mukai

Development of Solid-State Emitters Applicable to Luminescent Solar Concentrators, Masaki Shimizu, Hiroshi Sakaguchi

Study of Hydrogen Isotope Separation Technology by Molten Salt, Hisayoshi Matsushima, Toshiyuki Nohira

Evaluation of Irradiation Effects on High-Entropy Compound Superconductors, Naoko Oono, Kiyohiro Yabuuchi

Irradiation and Material Variables Dependence of Bubbles/Voids Formation in Fusion Reactor Structural Materials, Takuya Yamamoto, Kiyohiro Yabuuchi

Irradiation Effects on Ceramics Coatings, Sosuke Kondo, Kiyohiro Yabuuchi

Study and experiment of an interaction process between a low-density stacked CNT and a high-power, Ryutaro Matsui, Kazunari Matsuda

NMR analysis of biomolecules for development of novel biomaterials, Taiichi Sakamoto, Takashi Nagata

Irradiation damage effect on plasma driven hydrogen isotope permeation for plasma facing materials, Yasuhisa Oya, Kiyohiro Yabuuchi

Investigation on interaction structure and dynamics of room-temperature ionic liquid solvation using pulse-selected MIR free-electron laser, Sakhorn Rimjaem, Hideaki Ohgaki

Structural Analysis of Cell Wall Lignin for Advanced Biomass Utilization: Precise analysis of differences in lignin structure in each cell wall layer, Yasuyuki Matsushita, Masato Katahira

Chemical approach to surface reaction of ablation on organic material, Jun Fujioka, Heishun Zen

Development of strong superconducting bulk magnets with high shape-flexibility, Takanori Motoki, Toshiteru Kii

Development of negative ion source using microwave and its application to nano processing, Haruhiko Himura, Shigeru Inagaki

Identification of quadruplexes that can regulate gene expression, Yoichiro Tanaka, Takashi Nagata

Analysis and Design of Electrode/Electrolyte Interface for All Solid State Battery, Ikuma Takahashi, Keisuke Mukai

Development of the crystalline cellulose degradation system consisting of the psychrophilic fungus-type hybrid enzymes., Masataka Horiuchi, Takashi Nagata

Physical properties of heterostructures of atomic layer materials, Susumu Okada, Kazunari Matsuda

Development of highly efficient fabrication technique of two-dimensional heterostructures., Ryo Kitaura, Yuhei Miyauchi

Surface processing of semiconductors using graphene nanoribbons, Kazuhiro Fukami, Hiroshi Sakaguchi

Development of reduced activation high entropy materials for high energy reactor, Naoyuki Hashimoto, Kiyohiro Yabuuchi

Fabrication and characterization of two-dimensional heterostructures for energy conversion applications, Wenjin Zhang, Yuhei Miyauchi

A small-molecule-based technology for live-cell imaging of energy metabolism, Shin-ichi Sato, Takashi Morii

High performance nanocarbon material development based on molecularly functionalized carbon nanotubes for zero emission energy society, Tomohiro Shiraki, Yuhei Miyauchi

Highly efficient photochemical reactions induced by optimal laser pulses, Yukiyoshi Ohtsuki, Takashi Nakajima

Study of temporal evolution of coherent edge radiation during free-electron laser oscillations, Norihiro Sei, Hideaki Ohgaki

Development of hydrogen-oxidizing bacteria strains with high prolifiration capability in low hydrogen concentration condition, Yasunori Aizawa, Takashi Morii

Rooftop PV Hosting Capacity in AC Low Voltage Distribution Systems: Future Perspective in Cambodia, Vannak Vai, Hideaki Ohgaki

Structural studies on hierarchical molecular architectures created in microfluidic device, Munenori Numata, Eiji Nakata

Oxidation behavior of mechanically alloyed oxide dispersion strengthened alloy powders, Noriyuki Iwata, Kiyohiro Yabuuchi

AFM/EM imaging of intracellular metals with nanostructures constructed via signal amplification systems, Ippei Takashima, Eiji Nakata

Elucidation of the novel competitive function between microorganisms of genus Rhizoctonia by genomic approach, Yuh Shiwa, Tomijiro Hara

Development of an RNA eiding oligonucleotide to regulate the biological energy system in the cell, Masatora Fukuda, Takashi Morii

Development of novel guanine-tethered antisense oligonucleotides, Masaki Hagihara, Takashi Morii

Bactericidal effect of the infrared free electron laser, Toshizo Toyama, Heishun Zen

Study of minor element addition (Ni, Si) on irradiation hardening of pressure vessel model steels, Ken-ichi Fukumoto, Kiyohiro Yabuuchi

Gas Ionization with Ultrafast Intense Long-Wavelength Infrared Pulses, Ryoichi Hajima, Heishun Zen

High intensity broadband THz pulse generation using external optical cavity, Yosuke Honda, Heishun Zen

Ultra Sensitive Electrochemical Nucleic Acid Sensor, Kazushige Yamana, Takashi Morii

Enzyme-free selective structural control of glycan by means of molecular vibrational excitation, Takashi Honda, Heishun Zen

Application of infrared free electron laser to insulin ball seen in diabetes patients, Kazuhiro Nakamura, Heishun Zen

In-situ measurement of periodic nanostructures on semiconductor surface induced by mid-infrared free electron lasers, Masaki Hashida, Heishun Zen

Development of 3 dimensional radiative distribution measurement system using incoherent digital holography in Heliotron J., Hayato Kawazome, Shinichiro Kado

Development of dispersion strengthened high entropy alloys for high burn-up core materials, Hiroshi Oka, Kiyohiro Yabuuchi

Optimization of reactive oxygen radical production process by atmospheric pressure plasma irradiation, Hiroto Matsuura, Shinichiro Kado

Experimental study on the advanced methods of fault diagnosis and reliability evaluation to be applied for complex energy systems, Hidekazu Yoshikawa, Kazunori Morishita

Raman Spectroscopy of Molten Salts Containing Boron Ions, Yumi Katasho, Yutaro Norikawa

Synthesis of apatite-coated surface-modified organic polymer microspheres at ambient temperature and pressure, Takeshi Yabutsuka, Kiyohiro Yabuuchi

Study of nanomaterials toward efficient and high-performance energy conversion, Satoru Konabe, Yuhei Miyauchi

Development of a New Method for Controlling Thermal Radiation by Quantum Metamaterials, Atsushi Sakurai, Yuhei Miyauchi

Development of automated algorithms for high-speed camera image analysis, Nobuhiro Nishino, Shinichiro Kado

Study on reaction mechanism of visible-light-inducedliving radical polymerization for high energy efficiency, Yusuke Miyake, Hiroshi Sakaguchi

NMR analysis of the three-dimensional solution structure of the sequence-specific RNA-binding protein Musashi1 involved in translation control of the downstream target RNA, Takao Imai, Takashi Nagata

High beta plasma formation in advanced heliotron configuration using stochastic acceleration, Masayuki Yoshikawa, Shinji Kobayashi

Analysis of reaction mechanism of haloacid dehalogenase, Takashi Nakamura, Takashi Morii
Kinetic study on the Paraquat Dichloride removal in the water., Pannipha Dokmaingam, Hideaki Ohgaki

High-efficient plasma current drive by electron cyclotron waves in fusion reactor, Kenji Tobita, Kazunobu Nagasaki

Development of New Semiconductor Power Control Devices Aiming for Carbon Neutrality, Kensho Okamoto, Kazunori Morishita

Laser decontamination using a high repetition-rate nanosecond fiber laser, Atsushi Kosuge, Takashi Nakajima

Thermal properties of photoluminescence in single-walled carbon nanotubes for optical thermometry, Shun Aota, Yuhei Miyauchi

Hydrogen and Oxygen evolution on the micro/nano-structured electrode, Kota Ando, Takashi Nakajima

Study on emission process and evaluation of light outputs for novel scintillation materials using the one electron beam II, Shunsuke Kurosawa, Hideaki Ohgaki

Development of a method for compsiting Li_2TiO_3 and nanocarbon by microwave irradiation, Sadatsugu Takayama, Keisuke Mukai

Radial Correlation Analysis on Edge Plasma Turbulence in a Toroidal Plasma and its Dependence on Plasma Configuration, Yoshihiko Nagashima, Shinsuke Ohshima

Deuterium desorption from heavy ion irradiated tungsten using isothermal desorption method, Naoko Ashikawa, Kiyohiro Yabuuchi

Role of irradiation defects in the formation of plasma induced surface structures on tungsten, Mingzhong Zhao, Kiyohiro Yabuuchi

Study of ion irradiation effects on oxide dispersion strengthened ferritic steel, Jingjie Shen, Kiyohiro Yabuuchi

Lithium Migration Phenomena in Graphite - SiO Composite during Relaxation, Shigeomi Takai, Takashi Morii

Intracellular calcification of Corynebacterium matruchotti by FEL irradiation, Tetsuro Kono, Hideaki Ohgaki

Distributed Workshop on "Physics and control of non-linear and non-equlibrium plasma based on the concept of broad-band energy science", Yasuaki Kishimoto, Kazunari Matsuda

Active Learning for Public Outreach in Energy Science, Takeshi Yao, Kazunori Morishita

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 of Advanced Energy to promote joint activity of 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". For this purpose, 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 the fiscal year of 2023, strong advancement of the collaboration was achieved.

Close connection between related research fields in the institute have yielded unique and interesting outcomes from the collaboration. The laboratory takes charge of organizing and promoting the cooperative research project as a center of research activity in the Institute. The research teams were formed by mostly young generation staffs and students in the institute lead by associate professor or assistant professor, and participated in specific projects to carry out their subjects. The cooperative research activities will be published in a publication edited in the laboratory at the end of the fiscal 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. Following the reduction of the threat of COVID-19, meetings or exchanges were begun to restart.

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 groups, 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 the institute.

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, NMRs including 800 MHz LC-MS/NMR, Solar Simulator, KU-FEL and various laser systems.

2. The cooperative research program

In the fiscal year of 2023, two categories were set up: (1) “Cooperative Research” for cross sectional research and (2) “Sprouting Research” for challenging research proposal by Assistant Professor. The submitted proposals were evaluated by the selection committee organized by a center director, a program chair and three division chairs. One “Cooperative Research” proposal and four “Sprouting Research” proposals were approved. The number of research subjects is listed in Table 1 according to the division. A brief summary of the cooperative research subjects carried out in FY2023 is shown in the next page.

Table 1 Number of the accepted research subjects according to the division

Category			Total
A1	A2	A3	
4	2	2	8

The individual research subjects are as follows.

Supporting Activities on International and Industrial Collaborative Research

A1

"Organization of the sixth research seminar on RNA research, and presentation and exchange of information in the seminar"

- M. Katahira, T. Nagata (IAE, Kyoto University)
- R. Kurokawa, R. Yoneda (Saitama Medical University)
- T. Yamashita (University of Tokyo)
- N. Ueno (NIBB)
- N. Shiina, S. Hirano (NIBB)
- N. Fukuda (Niigata University)
- S. Ishigaki (Nagoya University)
- K. Hitachi (Fujita Health University)
- T. Oyoshi (Shizuoka University)
- T. Manen (Ritsumeikan University)
- R. Yoneda (Saitama Med. University)
- A. Takeuchi (Ehime University)
- Y. Oishi (Nippon Medical School)
- H. Tani (Yokohama University of Pharmacy)
- T. Nobeyama (Tsukuba University)

"Support for collaborative research with Laos on biological control of coffee plant diseases and promotion of its technology popularization."

- T. Hara, H. Ohgaki, Y. Takatsuka (IAE, Kyoto University)
- A. Nonaka (Pentalink Inc.)
- M. Yoneda (Farmer)

"7th International Symposium of the Kyoto Biomolecular Mass Spectrometry Society"

- T. Nagata (IAE, Kyoto University)
- H. Nishimura, T. Imai, S. Kuwashima, A. Sugiyama, K. Takahashi, S. Tazuru, Y. Tobimatsu (Research Institute for Sustainable Humanosphere, Kyoto University)
- M. Uesugi, M. Nakamura, S. Futaki, K. Masuguchi, S, Yamaguchi, S. Yamago, A. Fujihashi (Institute for Chemical Research, Kyoto University)
- J. Matsuo, K. Nishimura (Faculty of Engineering, Kyoto University)
- T. Ara (National Institute of Genetics)
- N. Kakuda (Doshisha University)
- T. Nirasawa (Bruker Japan)
- J. Watanabe (Shimadzu Corporation)

"India, Thailand, Korea, Japan ISFT network activity and attendant, presentation, and exchange of information in STBP 2024."

- E. Nakata, H. Ohgaki, T. Morii (IAE, Kyoto University.)
- N. Kumar (Delhi Technological University, India)
- M.S. Kim (Seoul National University, South Korea)
- Y.T. Kang (Korea University, South Korea)
- N. Watjanatepin (Rajamangala University of Technology Suvarnabhumi, Thailand)
- R.C. Singh, R. Chaudhary, R.M. Singari (Delhi Technological University, India)
- R. Dubey (University of South Florida, USA)
- S. Jonnalagadda (University of Kwazulu-Natal, South Africa)
- S. Chakraborty (University of Calabria, Italy)

Cooperative Research

A2

"Nitride/Oxide double coating using dielectric barrier discharge"

- J. Yagi, S. Inagaki, S. Kobayashi (IAE, Kyoto University)
- D. Fujii (Graduate School of Energy Science, Kyoto University)

"Reproducing Aurora Green Emission in Laboratory Plasma"

- S. Kado (IAE, Kyoto University.)

Sprouting Research

A3

"Construction of artificial carboxysomes for the efficient carbon fixation"

- L. Peng, T. Morii, E. Nakata (IAE, Kyoto University.)
- F. Komatsubara, Y. Hui (Graduate School of Energy Science, Kyoto University)

"Development of the in-cell NMR methods to investigate the dynamics and structure of biomacromolecules at various time-scales"

- T. Nagata, Y. Yamaoki, T. Sakamoto, Eladl Mohamed Mahmoud Omar Sobhi, M. Katahira (IAE, Kyoto University)

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. In the fiscal year of 2023 the aims and progress reports of five cooperative researches were presented and discussed, as summarized below. The Laboratory also planned a symposium on April 5, 2024 for presentation of the cooperative research results in FY2023.

(1) August 2, 2023
J. Yagi
"Usage of liquid lithium for fusion blanket"
IAE, Kyoto University

(2) September 13, 2023
P. Lin
"Design of artificial carboxysomes for efficient carbon dioxide fixation"
IAE, Kyoto University

(3) October 4, 2023
S. Kado
"Can the aurora green spectrum be reproduced in laboratory plasma?"
IAE, Kyoto University

(4) November 29, 2023
T. Nagata
"Development of the in-cell NMR methods to investigate the dynamics and structure of biomacromolecules at various time-scales"
IAE, Kyoto University

6. INTEGRATED RESEARCH CENTER FOR CARBON NEGATIVE SCIENCE

2023 Activities

Introduction

The Integrated Research Center for Carbon Negative Science (ICaNS) was established in August 2022 to promote carbon negative science research toward the realization of a carbon neutral society in 2050. Currently, the balance between carbon dioxide emissions and absorption has been disrupted, resulting in an excess of carbon dioxide emissions and a serious impact on the earth in the form of climate change. Restoring the balance is difficult with "zero emission" technologies alone and requires the development and implementation of more active carbon dioxide fixation processes, so-called "carbon negative" technologies. The Center will work to develop such new carbon dioxide fixation technologies in collaboration with the Graduate School of Engineering and Graduate School of Energy Science at Kyoto University. It will also work to develop human resources for "carbon negative science," which has not been done before.

Last fiscal year (FY2022), three major research projects were launched: 1) Solar Energy Utilization for CO_2 Capture and Conversion, 2) Conversion of CO_2 into Useful Substances, 3) Biological Utilization of CO_2. This fiscal year (FY2023), continuing from the previous year, we promoted these priority research projects and established an educational system for "carbon negative science". In addition, an international seminar on carbon negative energy science was held, and the center's laboratories were upgraded and experimental equipment was installed.

1. Solar Energy Utilization for CO_2 Capture and Conversion

The objective of this group is to establish novel science and technology for efficient solar energy utilization required for capturing CO_2 and/or converting CO_2 into valuable materials. In FY2023, the following studies were primarily conducted in this group: Studies on high-purity carbon nanotube membranes toward solar energy harvesting and utilization, optical science and applications of quantum materials for carbon negative energy science, low-temperature growth of functionalized graphene nanoribbons with electrochemical on-surface synthesis, efficient hydrogen evolution with laser-textured electrodes, research on the effective use of long wavelength light using mid-infrared free electron laser. Based on these results, we will continue our efforts to realize new solar energy utilization technologies.

2. Conversion of CO_2 into Useful Substances

This project group aims to convert CO_2 into useful substances. We are particularly interested in electrochemical methods of conversion. By using high-temperature molten salts as electrolytes, for example, CO_2 could be converted into a wide variety of valuable carbon materials, such as diamonds, carbon nanotubes, and graphite. If aqueous solutions, organic solvents, or ionic liquids are used as electrolytes at relatively low temperatures, CO_2 can be converted into methane, ethylene, and other materials. In FY2023, various types of carbon were electrodeposited using chloride molten salts at 600-900°C. They were analyzed by Raman spectroscopy, and mainly amorphous carbons were obtained. A small amount of diamond was obtained under certain appropriate electrolytic conditions. It was also suggested that other carbon allotropes could be obtained.

3. Biological Utilization of CO_2

Research in this project focuses on bio-related methods, materials and enzymes with the goal to contribute to Carbon Negative Science. In FY2023, studies that were carried out include the following: the development of tools to better understand the biological cell and its energy conservation, and technology to enhance and/or prolong the activity of enzymes, particularly those related to CO_2-fixation. Development of membranes, reactors and processes to enhance biomass utilization and establish efficient biorefineries have been performed. New microbial enzymes or metabolic pathways that can utilize CO_2 or prevent its release have been identified. Although the individual groups may specialize in diverse areas, we will continue our collaborative research to achieve our common goals and contribute towards developing a bio-based society.

4. Education Activity

The content of "Carbon Negative Energy" was incorporated into the existing undergraduate course "Advanced Energy Science" and started in the second semester of FY2023. As for graduate-level lectures, "Carbon Negative Energy" was incorporated into "Socio-Environmental Energy Science I and II" in the Graduate School of Energy Sciences, as in the previous fiscal year. The concept of "Carbon Negative Energy" was also promoted to visitors to the institute.

5. Other Activities

We further upgraded Laboratory 1-5, Waiting Room 1-2, Program-Specific Associate Professor's Room and Program Specific Assistant Professor's

Room in the main building of the Uji Campus. As for experimental equipment, an ultrasonic homogenizer, electric furnaces for molten salt electrolysis, a vacuum oven and box-type dryers were installed, as shown in Figs 1-1, 1-2, and 1-3.

Fig. 1-1 An ultrasonic homogenizer.

Fig. 1-2 Electric furnaces for molten salt electrolysis.

Fig. 1-3 A vacuum oven and box-type dryers.

ICaNS Events

April 5: The 1st Steering Committee meeting was held.
May 1: Program-Specific Assistant Professor was appointed.
June 12: The 2nd Steering Committee meeting was held.
July 25: ICaNS website was launched.
September 1: Symposium on Exploring Carbon Negative Energy Science 2023 was held as a parallel seminar of the 14th International Symposium of Advanced Energy.
September 8: The 3rd Steering Committee meeting was held.
October 1: Program-Specific Assistant Professor was appointed.
October 27: The 4th Steering Committee meeting was held.
February 15, 2024: The 5th Steering Committee meeting was held

7. PROJECTS WITH OTHER UNIVERSITIES AND ORGANIZATIONS

NIFS Bilateral Collaboration Research Program on Heliotron J

The Heliotron J group at IAE, Kyoto University has joined the Bilateral Collaboration Research Program managed by National Institute for Fusion Science (NIFS) since FY2004. This unique collaboration program promotes joint research bilaterally between NIFS and research institutes or research centers of universities that have 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 the advanced helical magnetic field and to improve the plasma performance through advanced helical-field control in Heliotron J. Picked up in FY2022 are the following seven key-topics; (1) magnetic configuration control for energy confinement, (2) production and confinement of high-density NBI plasmas and high-beta plasmas with novel fuelling methods, (3) electron thermal turbulent transport with self-criticality, (4) control of MHD and its physical mechanism, (5) edge plasmas in advanced helical systems, (6) production of energetic (MeV) electrons by non-resonant microwaves, and (7) development of new plasma diagnostics and analysis methods.

Two results from this collaboration research in FY2023 are shortly reported below. The annual report for all the collaboration subjects in this program will be published by NIFS.

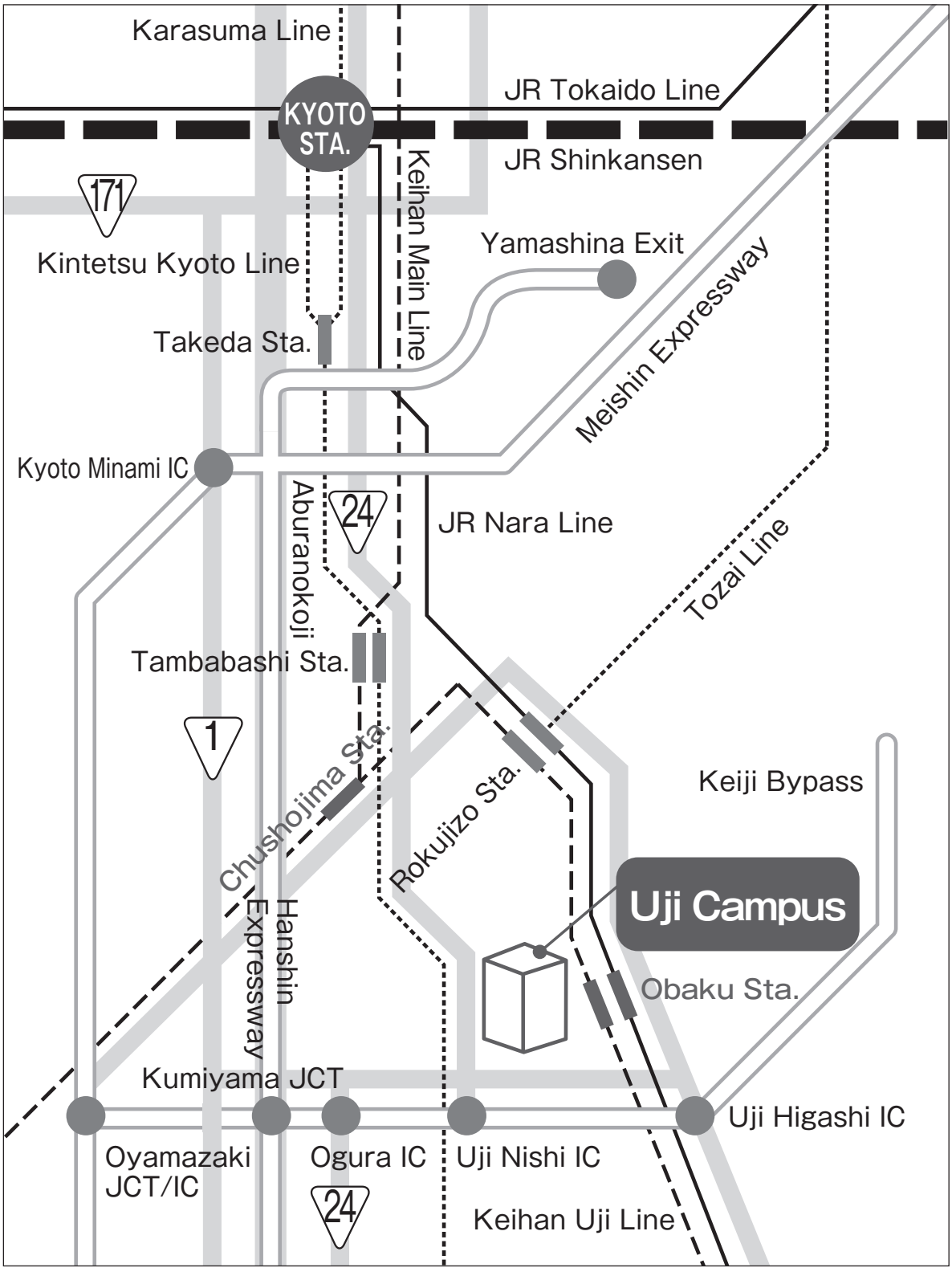
Role of rational surface on energy confinement: In rotational transform control experiments, no clear dependence of energy confinement on the helical ripple has been observed, therefore the contribution of turbulence transport is anticipated. Generally, no profile stiffness is observed in temperature profiles in helical systems, and the transport may be driven under a critical gradient compared to tokamaks. Since the avalanche transport is generated at the gradient around the critical gradient, comparison between helical systems and tokamaks provides understanding of profile formation. We have analyzed the electron thermal avalanche transport in Heliotron J and JT-60U, comparing their properties.

Electron thermal fluctuations in the low-frequency component ($f < 3$ kHz) observed by an ECE radiometer have been analyzed in the heating power scan experiments in Heliotron J and JT-60U. The temperature profiles show little variation with heating input for both devices. This indicates the confinement degradability with respect to heating power common to both devices. Since the transfer entropy is a quantity that quantifies the causal relationship between two signals as a quantity of information, the spatio-temporal evolution of the transfer entropy shows the spatial propagation of thermal fluctuations. The electron thermal fluctuation propagates from the center (ECH heating position) to the periphery in about 0.2 ms (about the diamagnetic drift velocity) in Heliotron J and from the vicinity of the maximum temperature gradient to the center and periphery in about 1 ms (about 1/10 of the antimagnetic drift velocity) in JT-60U. In both cases, the time and spatial scales of propagation are non-diffusive, which is characteristic of avalanche transport, but there are differences in the direction and speed of propagation. The Hurst index, a measure of avalanche transport, is also compared. In Heliotron J, it increases with increasing ECH power and is close to unity over the entire radial range, while in JT-60U, no such dependence on heating power is observed and the Hurst exponent tends to depend on the magnitude of the temperature gradient.

Statistical acceleration using non-resonant wave heating: In Heliotron J, energetic electrons exceeding 2 MeV have been observed when non-resonant 2.45 GHz O-mode microwaves are injected at the magnetic field of about 1 T. Relativistic electron production requires multiple accelerations by an electric field. Statistical acceleration is a possible acceleration mechanism. Simulation studies on the diffusion process of the electron energy distribution show that the diffusion coefficient is proportional to the electron energy to the power of 3.6, and that this strong energy dependence is the essence of the power-law spectrum formation.

A model equation shows that the change in kinetic energy due to an electric field is proportional to the product of the electron's initial speed relative to the speed of light and its Lorentz factor, i.e., the larger the initial energy of the electron, the larger the change in kinetic energy. We have performed electron acceleration simulations by changing the initial electron energy in the range of 10 keV to 1 MeV and investigated the amount of change in the kinetic energy of electrons that are accelerated or decelerated in an electric field. The results obtained from the simulations agreed with the experimental ones. On the other hand, to model the diffusion coefficient, it is necessary to evaluate the incremental energy determined by both the initial phase and the final phase when exiting from the electric field region, and the issue is how to incorporate the randomness of the phase considering the electron orbit in the confining magnetic field.

8. HOW TO GET TO THE IAE



京都大学エネルギー理工学研究所 ANNUAL REPORT
Institute of Advanced Energy, Kyoto University

Gokasho, Uji, Kyoto 611-0011 Japan
Phone. +81-774-38-3400　Fax. +81-774-38-3411
E-mail: office@iae.kyoto-u.ac.jp
https: //www.iae.kyoto-u.ac.jp

〒611-0011　京都府宇治市五ケ庄
TEL 0774-38-3400　FAX 0774-38-3411