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Institute of Advanced Energy
Kyoto University

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

ANNUAL REPORT

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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 Institute has established the Laboratory for Complex Energy Processes, which supports and stimulates collaborative research to address issues related to complex energy processes. The Integrated Research Center for Carbon Negative Science (ICaNS) was establishedIn 2022. The Center will create new concepts, academic foundations, and science and technology for the effective use of carbon dioxide to realize a carbon neutral society through extensive collaboration with researchers from the Graduate Schools of Energy Science and Engineering.

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 use and conversion based on the principles of materials science and energy use 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 will continue 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 novel scientific research.

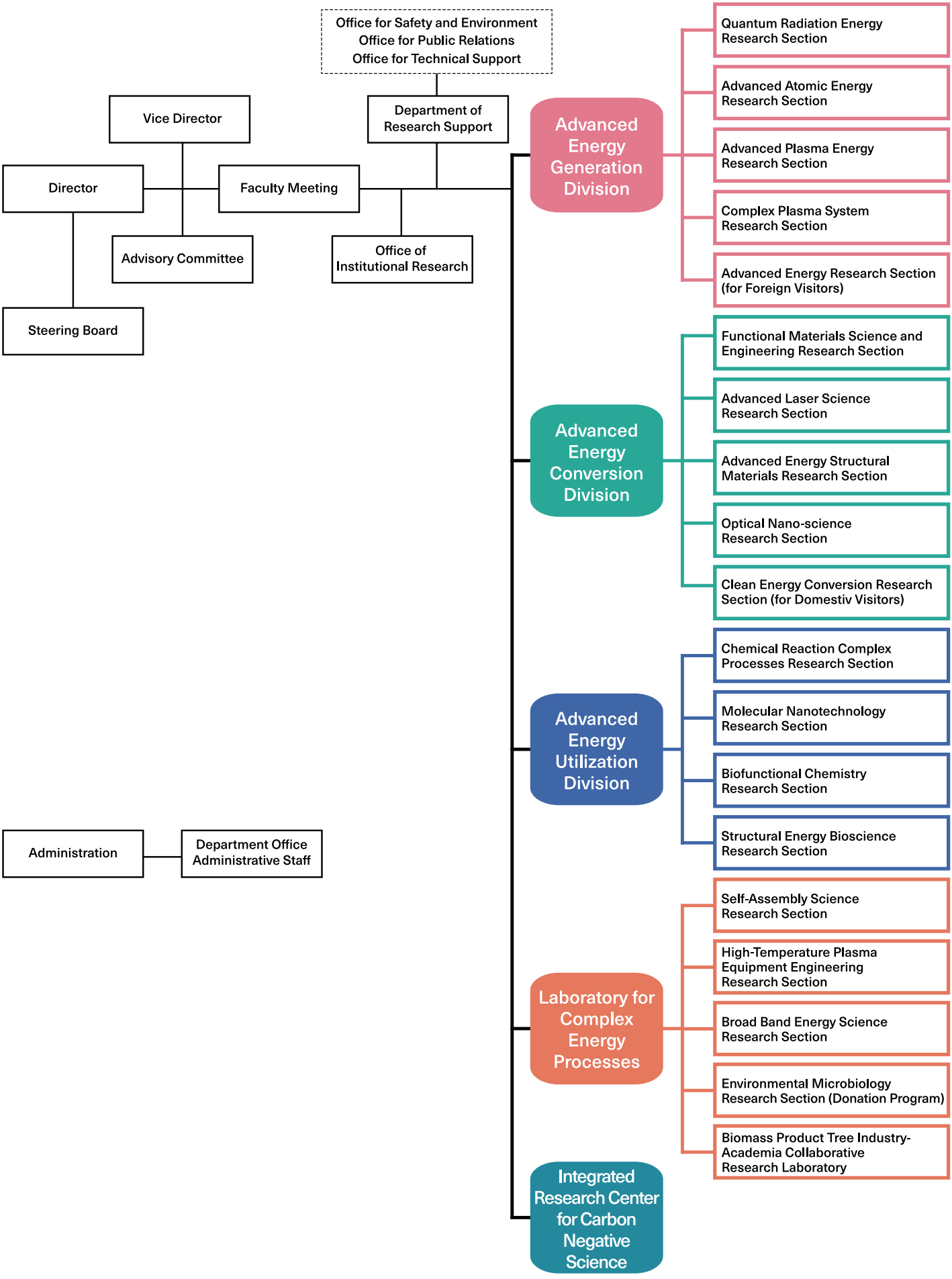
Japan has also set the goal of “virtually eliminating greenhouse gas emissions by 2050,” and carbon neutrality is now a goal for societies worldwide. The IAE is committed to a wide range of research into Zero-Emission Energy, which will play an increasingly important role in achieving carbon neutrality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

This annual report summarizes the major research achievements of each IAE’s research divisions for FY2022 (April 2022-March 2023) 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 2023

Takashi MORII
Director
Institute of Advanced Energy
Kyoto University

2. ORGANIZATION CHART



3. RESEARCH ACTIVITIES

3-1. RESEARCH ACTIVITIES IN 2022

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 turnability for basic researches 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).

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. Currently a copper cathode is used and the electron bunch charge is small and the FEL intensity is not so high. The cathode will be exchanged to CsTe to increase the FEL intensity.

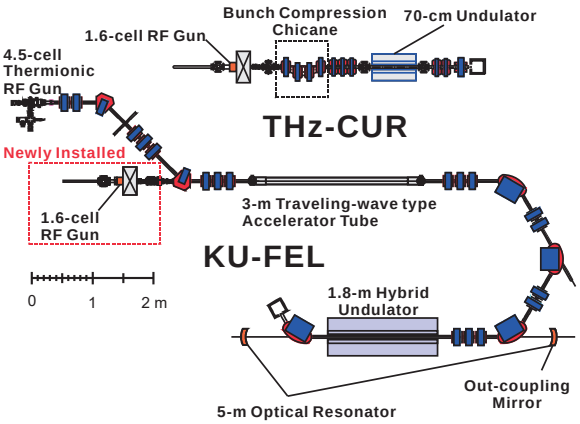


Fig. 1 Schematic drawing of the KU-FEL and THz-CUR

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 JFY2022, 18 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. As a next prototype of this type of undulator, we have developed new prototype consists of a new solenoid whose maximum field was 6 T and GM cryocooler. In order to reduce field amplitude fluctuation and to increase field strength, hybrid structure with vanadium permendur has been tested (Fig. 3).

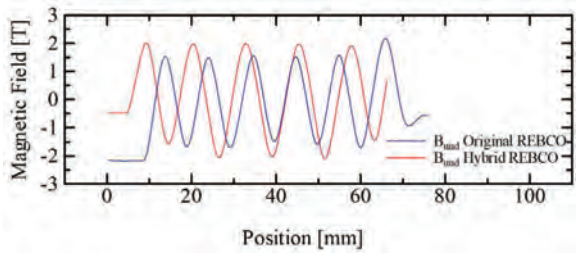


Fig. 3 Unduloator field using the GdBaCuO bulk superconductor and vanadium permendur (red line: Hybrid REBCO) is stronger than that of conventional GdBaCuO bulk superconductor (blue line: Original REBCO). Fluctuation of peak field strength is slightly reduced.

4. Isotope Imaging for Nuclear Safety and Security

We have proposed the F-LCS beam which has broader energy bandwidth with a small beam size and a spatially uniform energy spectrum. By using a helical undulator installed in a storage ring, such as the APPLE-II undulator in the BL1U beamline of UVSOR synchrotron facility, a circular motion of electrons stored in the storage ring can be excited. This circular motion of electrons widens the electron beam size and divergence. Due to the LCS interaction principle, broader bandwidth and a wider spatial distribution of the scattered gamma-ray beam can be expected. A simulation with EGS5 code has been performed and the proof of principle experiment carried out in the BL1U of UVSOR.

5. Social aspects of energy use

Despite the enormous efforts, more than 775 million people remain without electricity in 2023, of which 31 million live in Southeast Asia. Electrification can positively influence poverty eradication and development as well as exacerbate already existing inequalities in those communities. Our group investigates such effects with a perspective focused on quality of life, comparing the process and results of different electrification systems in rural contexts in SE Asia (Fig. 5). Applying qualitative techniques, our most recent studies have found that PV systems have improved the capabilities for education in rural households, reduced reliance on kerosene lamps and car batteries, and helped social and family interaction. Also, how the system's capacity can limit economic development or create concerns about the shift in lifestyle and sleep cycles, given the extended use of lighting at homes.

Fig. 5 Rural electrification survey sites 2016-2022

In urban contexts of ASEAN, our group has analysed how household roles affect efficient appliance purchasing intention. Finally, in the context of Latin America, we also study geographical and socio-cultural characterizations of household energy services.

Acknowledgment

All our research work have been supported by the KAKENHI, Q-LEAP(MEXT), JASTIP(JST), UVSOR Collaboration Research, The Heiwa Nakajima Foundation, The Murata Foundation, Hitachi Zaidan, CSEAS DASU (Kyoto University), and the Laboratory for Complex Energy Processes Collaboration Research (IAE).

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Advanced Atomic Energy Research Section

J. Yagi, Associate Professor
K. Mukai, Assistant Professor

1. Introduction

Main objective of our research section 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. Followings are main research achievements in the fiscal year of 2022.

- Finding electronic descriptors for predicting defect formation properties in Be intermetallics.
- Development and successful operation of liquid lithium lead droplet system for efficient recovery of hydrogen isotope using a heat and mass-transfer loop.
- Development of diffusion pump using sodium vapor for the divertor exhaust in a fusion system.
- Electrochemical purification of Bi in Li-Pb eutectic using chloride molten salt

2. Electronic descriptors for Be intermetallics

The use of an electronic descriptor is a high-throughput approach for predicting the chemical reactivities of various materials that has the potential to significantly facilitate the material design of Be intermetallic neutron multipliers for nuclear fusion applications. Herein, we perform first-principles calculations on 42 existing binary Be intermetallics to find an effective electronic descriptor. We demonstrate that the occupied Be *p* band center relative to the Fermi level is a bulk descriptor, correlating with the Be vacancy formation energy; a positive and linear correlation with R^2 = 0.85 was observed for $Be_{12}X$ (X: transition metal) as shown in Fig. 1. The upward shift in energy of the occupied Be *p* states with early or middle transition metals can reduce hydrogen solution energy, which could be attributed to the less filled anti-bonding state of interstitial hydrogen atom. It is confirmed that the bulk descriptor is an experimentally measurable scale, having the strong linearity (R^2 = 0.97) with the calculated.

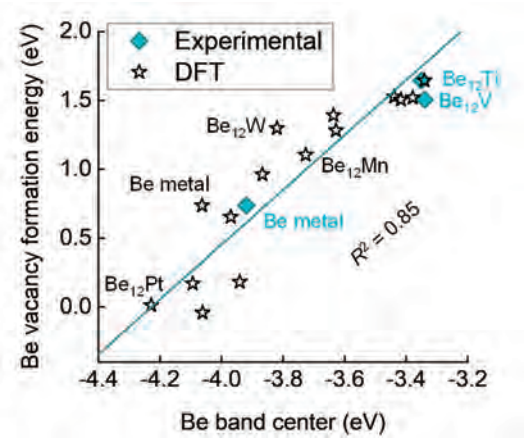

Fig. 1 Plots of vacancy formation energy in $Be_{12}X$ with occupied Be *p* band center

3. Development of hydrogen isotope (deuterium) recovery from liquid lithium lead droplet system

Lead lithium eutectic alloy (Pb-17at%Li, Pb-Li) is a candidate liquid breeding material with low chemical reactivity and good tritium breeding ratio. Effective tritium recovery method from the liquid must be developed for the blanket system with minimal tritium

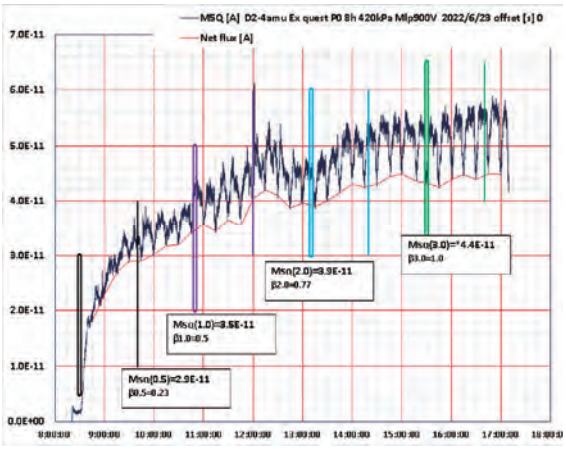

Fig. 2 The deuterium recovered from Pb-Li droplets while falling in a vacuum.

loss. The vacuum sieve tray (VST) method, tritium recovery from the liquid droplet surface falling in a vacuum, is a promising candidate developed in this section. This fiscal year, on a collaboration work with National Institute for Fusion Science (NIFS), the continuous operation campaign was performed. One of the recovery results is shown in Fig. 2. The deuterium dissolved in the Pb-Li loop system was successfully recovered at the VST test section.

4. Development of diffusion pump using sodium vapor for the divertor exhaust in a fusion system

Vacuum pump for the fusion system is quite important regardless of the confinement style, which must have high efficiency and resistance against tritium contamination and radiation. Additionally, it should work in strong magnetic field, without the release of high-Z element depending on the fusion system.

The diffusion pump which usually utilizes oil or mercury vapor to transfer the momentum, can be a candidate when the vapor source is replaced to the light alkali metal (such as Li or Na) which is free from radiation degradation. In this work, we tried to modify a commercial diffusion pump and the pumping speed is investigated. As the modification, the oil was replaced by sodium of the same volume, a voltage controller was added to the heater, and a cooling fan for the radiator-fin was replaced to a speed controllable one. Thermocouples to monitor the surface temperature of the pump were also attached.

Evacuation by Na vapor was obviously observed when the boiler temperature was close to or above 950 K. The heating of the boiler and the cooling of the radiator-fin showed a positive effect on the pumping speed (Fig. 3). So far, evacuation against He gas achieved 30L/s with Na vapor which is a bit slower than the one with oil vapor (~120 L/s) in the as received pumping system.

Considering these results and our past works on the purification of liquid metal, liquid alkali metal will be applicable for the vapor diffusion pump for fusion system.

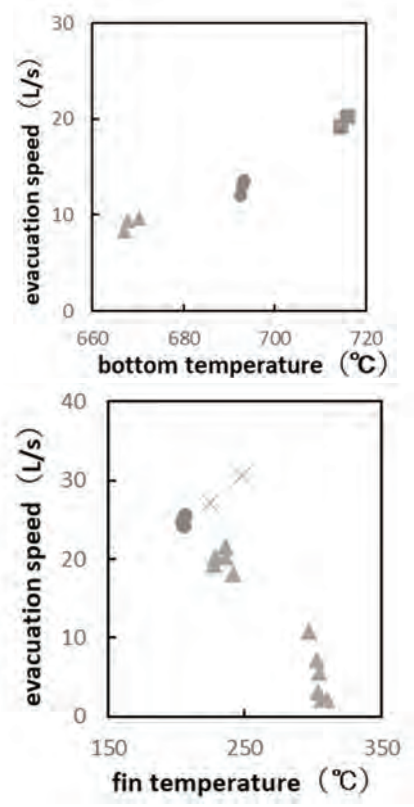

Fig. 3: Evacuation speed of Na vapor diffusion pump, changing the bottom boiler temperature (upside) and cooling fin temperature (downside)

5. Electrochemical purification of Bi in Li-Pb eutectic using chloride molten salt

Liquid lithium lead eutectic alloy (Li–Pb), a candidate of tritium breeding material in a fusion blanket, is easy to contain bismuth (Bi) as an initial impurity or transmutation product from lead (Pb). In neutron fields, Bi is transmuted to polonium (Po), a radioactive element. However, the extraction method for Bi has not yet been established.

In this research, an electrochemical method using chloride molten salt was employed to reduce Bi. This method has been suggested to have the potential to reduce several kinds of impurities. In this experiment, an electrochemical cell filled with chloride molten salt (LiCl 59.2 mol % – KCl 40.8 mol%) was prepared, and Li–Pb in an alumina crucible was placed in the chloride molten salt as the counter electrode. The working electrode was the liquid lead in a glass tube.

As a result of chrono-amperomety (CA) and ICP-MS analysis of the lead working electrode, transport of Bi into the lead electrode was confirmed when the potential of the electrode is around 1.5 V vs Li-Pb potential as shown in Fig, 4.

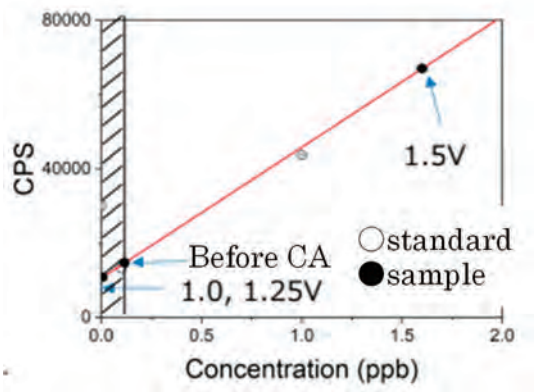

Fig. 4 Concentration of Bi in Pb electrode after chrono-amperometry (CA)

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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 FY2020 is reported focusing on transport characteristics regarding magnetic configurations, including the magnetic island effect, especially in (1) Transport analysis for high electron temperature plasmas fueled by high-intensity gas puffing and (2) development of multichannel 320 GHz interferometer system.

2. Transport analysis for high electron temperature plasmas fueled by high-intensity gas puffing[1]

High-intensity gas puff fueling (HIGP) is applied to the NBI plasma of Heliotron J to obtain high-performance plasmas to control fueling/edge recycling. A higher and more peaked electron temperature profile than conventional gas puffing-fueled (GP) discharge formed by HIGP is observed. From the analysis of the heat transport coefficient, an obvious improvement in electron heat transport is observed.

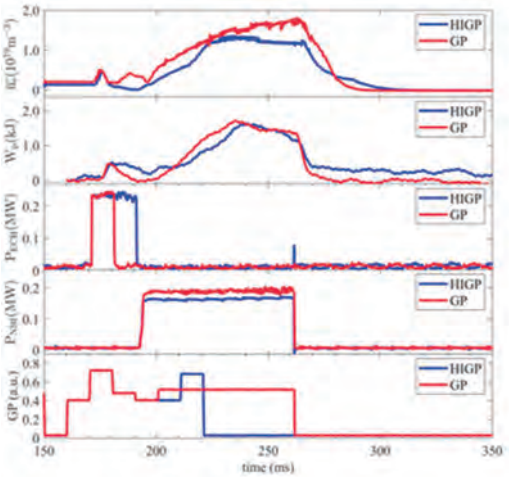

Fig. 1. Schematic diagram of the reflectometer system.

The experiment has been carried out under the configuration which has a low toroidal magnetic field component (low ε_t). The plasma parameters obtained in the HIGP and continuous GP-fueled plasmas are shown in Fig. 1. A 245kW ECH is applied to initiate the plasma with pre-gas puffing. Then NBI with the injection power of around 0.2MW is injected into the plasma after the termination of the ECH launch. The HIGP is applied from t = 210ms to 220ms while the GP is continuously puffed from 200ms to 260ms. In the experiments, the electron density with both the cases was set around 1.5×10^{19}m^{-3}.

The toroidal 15-sightline charge exchange recombination spectator (CXRS) and Nd:YAG Thomson scattering system are used to obtain the temperature profile and density profile. As shown in Fig. 2, a higher and more peaked electron temperature profile than GP discharge formed by HIGP fueling is

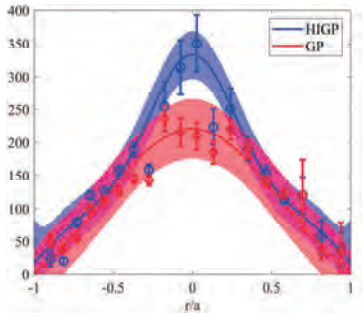

Fig. 2 Electron temperature profile obtained by HIGP and continuous gas fueling plasmas.

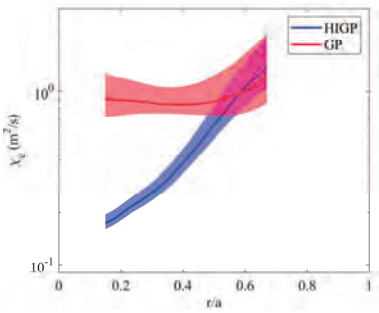

Fig. 3 Comparison of effective heat transport coefficients between HIGP and continuous GP plasmas.

observed. At the core region -0.5 < r/a < 0.5, the maximum T_e difference is up to 150eV.

Based on the profile obtained by the diagnostics, we evaluated the effective heat transport coefficient χ as follows,

$$\chi_j \sim \frac{\int P_j V' dr}{\langle \nabla r^2 \rangle n_j \nabla T_j} \quad (1)$$

where, n, T, P, V, and r are the density, temperature heating power density volume, and radial position, respectively. The subscription j denotes the particle species. The terms, P and χ, are calculated using FIT-3D and TR-SNAP codes. A significant improvement in electron heat transport is observed. As shown in Fig. 3, at the region of $r/a \sim 0.2$, the reduction of the effective electron heat transport coefficient is up to 80%.

3. Development of multichannel 320 GHz interferometer system in Heliotron J[2]

Density profile diagnostic with a high time resolution is essential to understanding the particle transport in fusion plasma experiments. The single-channel 320 GHz interferometer system developed in Heliotron J has been upgraded to a multi-channel system by extending the probing beam to the sheet beam to enable the measurement in Heliotron J. In this section, we report on the development of the multichannel 320 GHz interferometer system in Heliotron J.

The new interferometer is adopted heterodyne Michelson-type interferometer with a cutoff density n_e = 1.27×10^{21} m^{-3}, and the beam propagation depends on the quasi-optical techniques. Two separate solid-state oscillators (VDIE0029, AMC 630, Virginia Diodes, Inc.) are used as microwave generators. The sources are compact and easy to control. Each source delivers a maximum of 50 mW output power. The output frequency of one source is fixed at 320 GHz, whereas the other is tunable in the frequency range of 312–324 GHz. The frequency difference between the two sources can be easily changed to control the IF frequency. The time resolution of the interferometer is determined by the IF frequency of the system. Therefore, this system may obtain a high time resolution of less than 1 μs to measure density fluctuations. The submillimeter wave source and its optical bench are placed ~3 m away from the Heliotron J coils to avoid the influence of the magnetic field on the sources. A submillimeter wave beam was transmitted to another optical bench shown in Fig. 4 with oversized dielectric waveguides with an inner diameter of 76 mm. After the transmission to the bench, the probe beam was injected from outside the Heliotron J vacuum chamber port into the plasma and was reflected by a retroreflector array installed on the inner vacuum chamber wall. The beam was mixed with the local beam and detected by a single-ended mixer (WR-2.8FM, Virginia Diode, Inc.) on the optical bench.

To extend the probing beam to a sheet beam, a pair of off-axis parabolic (OAP) mirrors were used. As shown in Fig. 4, the OAP system converts the probing beam to the parallel sheet beam to inject into the vacuum chamber. The sheet beam is reflected on the retroreflector array on the wall of the vacuum chamber. Simply setting the detector after the beam splitter enables multi-channel measurements.

During the last experimental campaign, the multichannel interferometer system has successfully measured electron density using two channels. The results of electron density measurements at the center and edge of the plasma cross-section are shown in Fig. 5. The waveforms of the electron density obtained by the two channels of the 320 GHz interferometer agreed well with the 130 GHz microwave interferometer during the ECH modulation experiment. The electron density from the two channels of the 320G Hz interferometer will be analyzed whether the measured density profile is consistent with the density profile data obtained by the YAG Thomson Scattering system.

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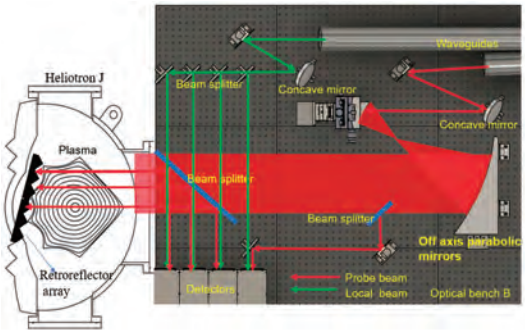

Fig. 4. Schematic illustration of a multi-channel Interferometer in Heliotron J.

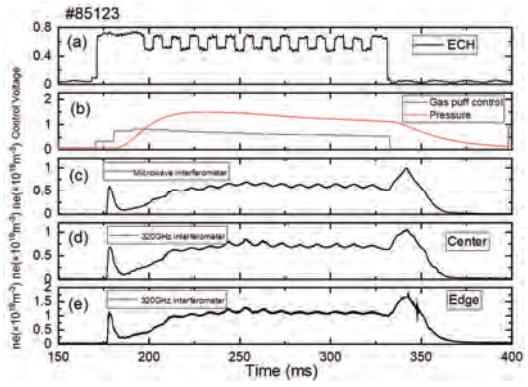

Fig. 5. Time trace of (a) heating power, (b) gas puff, (c) electron density measured with the microwave interferometer, (d) electron density measured with the center channel of 320GHz interferometer, and (e) electron density measured with the edge channel of 320GHz interferometer.

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

長﨑百伸, 西南物理研究所（中国）, IPP, Greifswald（ドイツ）, University of Wisconsin（アメリカ）, 先進ヘリカルシステムにおける反射計を用いた電子密度・揺動解析

長﨑百伸, IPP, Greifswald（ドイツ）, 先進ヘリカルシステムにおける電子サイクロトロン電流駆動

大島慎介, 長﨑百伸, 南貴司, 小林進二, Wisconsin University（アメリカ）, CIEMAT（スペイン）, Max-Plank Institute（ドイツ）, 先進ヘリカルシステムにおける周辺揺動解析

長﨑百伸, 大島慎介, 南貴司, 小林進二, Stuttgart Univ., CIEMAT（スペイン）, 先進ヘリカル磁場配位の最適化に向けたネットワーク拠点形成

小林進二, 長﨑百伸, 大島慎介, CIEMAT（スペイン）, Kurchatov Institute（ロシア）, ORNL（アメリカ）, 先進ヘリカル磁場配位の最適化に向けたネットワーク拠点形成

小林進二, IPP, Greifswald（ドイツ）, Kharkov Institute（ウクライナ）, 非共鳴マイクロ波による確率的電子加速とプラズマ着火への応用研究

長﨑百伸, 核融合科学研究所一般共同研究, 捕捉粒子制御による高エネルギー励起 MHD 不安定 性の励起・減衰

長﨑百伸, 核融合科学研究所・双方向型共同研究, Heliotron J における高速カメラ観測と磁気プローブ計測によるプラズマ解析

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長﨑百伸, 核融合科学研究所・双方向型共同研究, Heliotron-J における ECH によるトロイダル流駆動の検証

長﨑百伸, 核融合科学研究所・双方向型共同研究, ヘリオトロン J における X-mode 多チャンネル反射計の開発

長﨑百伸, 核融合科学研究所・双方向型共同研究, ヘリオトロン J におけるマルチパストムソン散乱計測

長﨑百伸, 核融合科学研究所・双方向型共同研究, レーザーブローオフ法を用いたヘリオトロン J プラズマにおける不純物輸送研究

長﨑百伸, 核融合科学研究所・双方向型共同研究, 磁場分布制御を活用したプラズマ構造形成制御とプラズマ輸送改善

長﨑百伸, 核融合科学研究所・双方向型共同研究, 伝送系途上での RF パワー計測法の研究

長﨑百伸, 核融合科学研究所・双方向型共同研究, 波動加熱による高速電子生成成時の非熱的放射機構の研究

長﨑百伸, 核融合科学研究所・双方向型共同研究, 乱流輸送低減に対する磁場配位依存性の研究

小林進二, 核融合科学研究所・双方向型共同研究, ヘリオトロン型磁場配位を利用した統計加速の実験室シミュレーションの検討

小林進二, 核融合科学研究所・双方向型共同研究, 磁場閉じ込めプラズマにおける複合粒子補給制御を用いた高密度化（ヘリオトロン J における高密度プラズマ生成と輸送特性）

小林進二, 核融合科学研究所・双方向型共同研究, 燃焼炉心プラズマ研究に向けた高エネルギー粒子物理と熱化粒子新古典理論の統合

小林進二, 核融合科学研究所一般共同研究, 高エネルギー粒子による波動励起と外部制御に関する研究

Financial Support

1. Grant-in-Aid for Scientific Research
長崎百伸, 基盤研究(A), 外部アクチュエータを用いた高エネルギー粒子励起 MHD 不安定性の制御

小林進二, 基盤研究(B), 先進ヘリカル配位のベータ効果が対称性と熱・乱流輸送に与える影響の実験的検証

小林進二, 基盤研究(A), 外部アクチュエータを用いた高エネルギー粒子励起 MHD 不安定性の制御（分担金）

2. Others

長﨑百伸, 自然科学研究機構, 2022 年度双方向型共同研究

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Complex Plasma Systems Research Section

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

1. Introduction

Nuclear fusion energy has some attractive features as a future option for the base-load electrical power source. 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, (3) exhaust ash and impurities. We are tackling these issues by understanding their physical processes by experiment using a magnetic confinement device Heliotron J.

Results in FY2022 featured in this report are about the plasma fluctuation and magnetic configuration control which are regarded as key issues for characterizing the heat transport and improvement of the control ability of confinement in fusion-relevant magnetized plasmas.

2. Observation of magnetic fluctuations

In order to confine high pressure plasmas stationary by using magnetic field, the plasma pressure should be balanced by the magnetic pressure. Stability of magnetically confined plasma is thus one of the important issues to be understood to realize magnetic fusion.

Toroidal magnetic fusion device forms closed magnetic flux surfaces by giving the rotational transform to field lines and confines high pressure plasmas. When magnetic field fluctuations cause the magnetic field lines to cross different magnetic flux surfaces, the plasma is transported out of the confinement region by the motion along the magnetic field lines. Thus, the characteristics of magnetic field fluctuations and their causes must be understood. In the FY2022 experimental campaign of Heliotron J, we observed excitation of magnetic fluctuations, which frequency is higher than previously observed [1]. Figure 1 shows typical temporal behavior of magnetic fluctuation. Plasma is generated at 150 ms by electron cyclotron resonance heating and auxiliary heated by neutral beam injection from 300 ms. Power spectrum of the magnetic fluctuation is broad and incoherent before beam injection. High frequency (90 kHz and 250 kHz) modes are excited during beam injection. We analyzed time-series data obtained simultaneous multi-points measurement with multi-magnetic-probes. Cross-power spectra indicates that both modes have the same spatial structure, i.e. toroidal mode number is 4 and poloidal mode number is 8. Frequency of both modes decreases with increase in the electron density and absolute values of frequency are explained by Alfven velocity. From these results, these modes are Alfven mode driven by energetic beam ions.

In addition, abrupt excitation of magnetic fluctuation is also observed. As shown in Fig. 2, a probe signal indicates that fluctuation grows at 270 ms abruptly. Here, fluctuations in the frequency range of 30-50 kHz increase. However, the life-time of this mode is very short, of the order of 10 ms. During excitation of this mode, background plasma parameter, e.g. plasma density, plasma pressure and heating power, are almost unchanged and thus it is very difficult to predict the onset of this mode. It is significant to elucidate this phenomenon because prediction of abrupt phenomena is one of the important issues in the future fusion reactor.

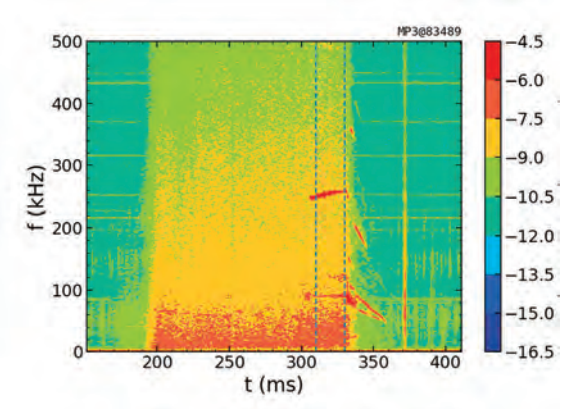

Fig.1 Typical temporal evolution of power spectrum of magnetic fluctuation. High frequency coherent fluctuations appear for 310-330 ms when co-directional neutral beam is injected.

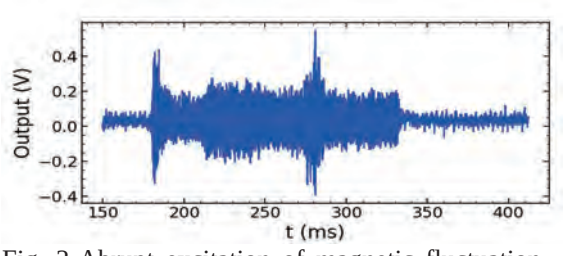

Fig. 2 Abrupt excitation of magnetic fluctuation. Fluctuation amplitude increases abruptly at 270 ms.

3. Configuration control experiment for confinement characterization against rotational transform

The study of confinement scaling law is of great importance for predicting future fusion reactor performance and is a key basis for the design of fusion reactor. Interestingly, the scaling laws in both tokamaks and stellarators indicate confinement improvement with the increase of rotational transform ι, a fundamental parameter characterizing a magnetic configuration of toroidal plasmas. The physical origin of this dependence, however, is not clear. This dependency should be thus reconsidered. There are many parameters that characterize magnetic configuration, e.g. magnetic well-depth and effective helical ripple ε_{eff}. In the stellarator, ε_{eff} is a stellarator-specific parameter and is considered very important for comparison confinement ability with tokamaks. Configuration parameters are widely spread due to the variety of configuration concepts of stellarator. Despite this, it is very difficult to change the parameters independently. For this reason, a large data base and advanced statistical analysis are required to obtain the configuration parameter dependence. This problem also makes optimization of magnetic configuration difficult.

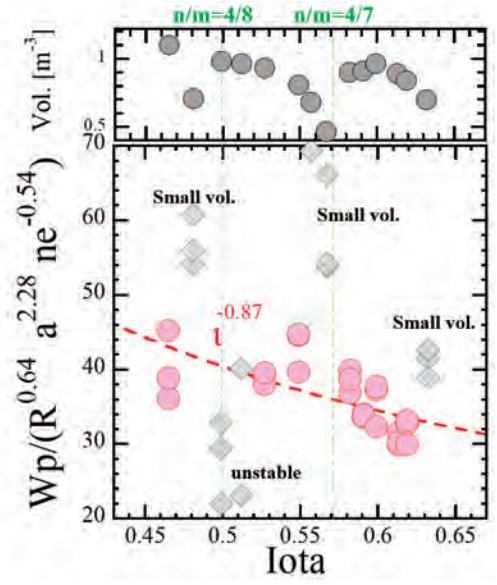

Fig. 3 Iota dependence of $W_p/R^{0.64}a^{2.28}n_e^{-0.54}$, normalized by the plasma size factors in ISS04. The normalized W_p exhibits a trend to decrease against iota (red circles). The grey square indicates *W*p with small volume configuration or unstable discharges with MHD perturbation.

The Heliotron J is a flexible stellarator and thus can perform configuration parameter scan experiment in a single machine. In FY2022 experimental campaign, a trend of confinement degradation against ι was discovered. The experiment was performed at a fixed density with the electron cyclotron resonance heating, and the rotational transform ι was controlled by altering the coil current ratio of the helical coil to toroidal coils. The observed degradation is different from the scaling laws in both tokamaks and stellarators. The stellarator scaling (ISS04: $\tau_E \propto a^{2.28}R^{0.64}P^{-0.61}n_e^{-0.54}B^{0.84}\iota^{0.41}$) indicates that the energy confinement time is proportional to $\iota^{0.41}$. Figure 3 shows the dependence of stored energy W_p on rotational transform. The stored energy is proportional to τ_E when input power is kept constant. Although the plasma size factors ($a^{2.28}R^{0.64}$) and density dependence ($n_e^{-0.54}$) are normalized, the stored energy demonstrated a negative dependence of $\iota^{-0.87}$. Here small volume experiments are excluded because transport channel in small volume plasma is considered to be different from large volume plasmas.

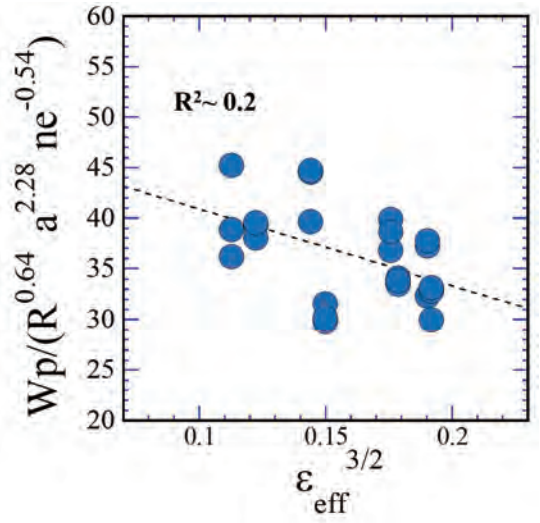

Fig. 4 Normalized stored energy $W_p/R^{0.64}a^{2.28}n_e^{-0.54}$ against effective helical ripple ε_{eff}, indicating ε_{eff} is not a prominent explanatory variable of Wp values.

The ι is independent for configuration parameter scan experiment? As mentioned above, the ι is coupling with other parameters. Although other parameters don't appear in the ISS04 scaling, plasma physics indicates the significance of other parameters. The ε_{eff} is a parameter to characterize neoclassical transport in a stellarator, and thus the normalized stored energy is compared with ε_{eff}. As shown in Fig.4, experimental data indicate weak negative dependence to ε_{eff}, however, the data-points are significantly dispersed, and the regression analysis results in a determination coefficient $R^2 \sim 0.2$, and therefore ε_{eff} is not a good explanatory variable for the W_p. This indicates that the ι dependence observed in this experiment is not originating from the neoclassical transport, but rather through other mechanisms such as turbulence transport.

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Collaboration Works

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大島慎介, 長﨑百伸, 南貴司, 小林進二, Wisconsin University（アメリカ）, CIEMAT（スペイン）, Max-Plank Institute（ドイツ）, 先進ヘリカルシステムにおける周辺揺動解析

長﨑百伸, 大島慎介, 南貴司, 小林進二, Stuttgart Univ., CIEMAT（スペイン）, 先進ヘリカル磁場配位の最適化に向けたネットワーク拠点形成

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南貴司, 核融合科学研究所・ＬＨＤ計画共同研究, 高機能高速密度干渉計測のための位相検出器の新展開

南貴司, 核融合科学研究所一般共同研究, 高度核融合プラズマ分布情報創出のための統合型レーザートムソン散乱計測データ処理システムの開発

門信一郎, 核融合科学研究所・双方向型共同研究, ドレスト重水素原子輝線スペクトルを用いたプラズマ中のマイクロ波電場計測

門信一郎, 核融合科学研究所・双方向型共同研究, ヘリオトロン J における EUV 分光を用いた不純物発光線強度比データの蓄積

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Financial Support

1. Grant-in-Aid for Scientific Research

稲垣滋, 基盤研究(B), ２流体プラズマ中に現る正準フラックスチューブの可視化検出とそれへの凍結仮説の検証（分担金）

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2. Others

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Advanced Energy Research Section

Sakhorn Rimjaem, Foreign Visiting Researcher
(Assistant Professor in Department of Physics and Materials Science, Faculty of Science, Chiang Mai University, 239, Huay Kaew Road, Muang District, Chiang Mai 50200, Thailand)

1. Summary

The author spent three months (Sep. 1, 2022-Nov. 30, 2022) as a guest associated professor at the Uji campus of Kyoto University, hosted by the Prof. H. Ohgaki's group.

Here the author reports about an investigation on study of solvation structure and dynamics of room-temperature ionic liquids using MIR free-electron laser.

2. Introduction

The unique set of properties of room-temperature ionic liquids (RTILs) has made them promising materials for modern electrochemical energy storage devices. One topic that has been under an intense debate is the free-charge carrier density in RTILs, which is one key to improving the efficiency of the devices. This quantity is strongly related to the short-range ion interactions and short-life interaction between ions and the surrounding molecules. Solvation structure, solvation dynamics, and hydrogen bond network are expected to be the key to a better understanding of such physical process, which is usually in the time scale of picosecond to femtosecond. Under the light of the MIR-FEL pump-probe (PP) experiment at KU FEL, the observation of interaction structure, interaction dynamics, and ion relaxation can be expected. Interpretation of experimental results can be done with the support from computational simulations.

3. Methodology

(1) Sample preparation

In this work we aimed to study the interaction lifetime and orientational decay of the ionic liquid 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ions ([Emim][NTf2]) when mixed with molecular solvent dimethyl sulfoxide (DMSO). In order to observe the effect of mixing ratio, [Emim][NTf2] (>98% HPLC, Merck KGaA) and DMSO (>99.9% anhydrous, Merck KGaA) were mixed to form binary mixtures with [Emim][NTf2] mole fraction XIL = 1.0, 0.9, 0.75, 0.5, 0.25, and 0.1 (the sample set includes sole DMSO, XIL = 0). Both chemicals were used as purchased and the samples were quickly prepared in ambient laboratory environment. The mixtures were kept in tightly closed glass vials and only few hundred μL of liquid sample was taken using a micropipette for each experiment. The sample was sandwiched between two diamond windows of an IR liquid cell with PTFE spacers for pathlength control. The pathlength was varied between 50 – 250 μm to obtain optimized signal.

(2) MIR-FEL pump-probe spectroscopy optical design and setup

The polarization selective PP setup was designed as shown in Figure 1. The FEL enters the setup and divided by a ZnSe beam splitter (BS) to form a pump beam and a probe beam. The pump beam is guided by the flat mirrors (M1 & M2) and is focused on the sample by a an off-axis parabolic mirror (OAP1). The probe beam is delayed by the optical delay line composed of two flat mirrors in retroreflector (RR) configuration. The computerized translational stage is used for optical path difference adjustment, which is in the range of 3 – 90 mm, to cover the required time delay of 10 – 300 ps. The probe beam is then reflected by the mirror (M3) and is focused by the OAP1 to spatially overlap with the pump beam in the sample volume. The transmitted pump beam is focused by OAP2 on the pyroelectric detector to collect as a pump-probe signal. The crossing angle between pump and probe beams at the sample is in the range of 10° – 20°. Two linear wire-grid polarizers are added for setting the polarization of the pump beam (P1) and for detecting the probe polarization (P2). The polarization angle of the probe beam can be switched between +45° and – 45° w.r.t. the probe polarization. Then, the ray optics simulation was carried out to determine all the required optical elements. The simulation was done based on the cloud-based software (3DOptix). An example of the ray simulation result and the 3D drawing of this setup made with a software FreeCAD are shown in Figure 2.

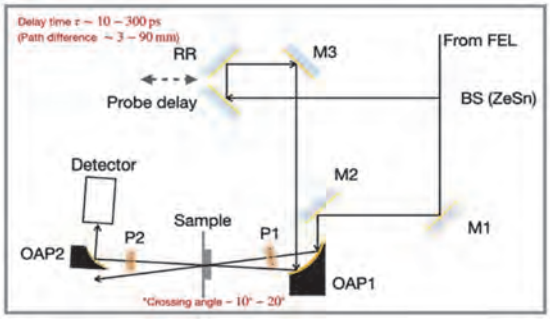

Fig. 1, Schematic design of the MIR-FEL polarization selective PP spectroscopy setup.

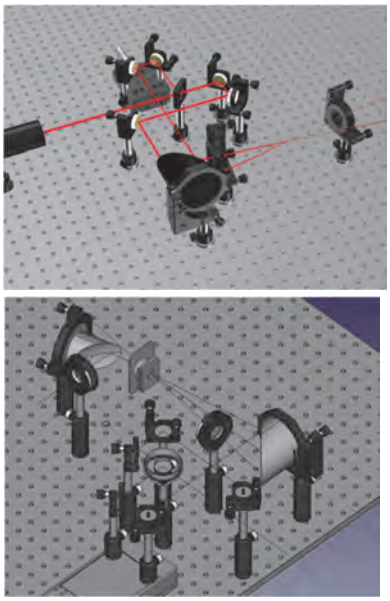

Fig. 2, (Top) A ray optics simulation to determine the specification of all optical elements. (Bottom) The 3D view of the designed setup.

The actual experimental setup at KU-FEL was set based on this drawing. The specifications of the key elements are OAP1 (90o, 3-in dim., 9-in. EFL), OAP2 (90o, 1-in dim., 2-in. EFL), flat mirrors (1-in dim.), and the crossing angle is 16^{o}.

4. Results and Discussion

The samples were first studied with FTIR spectroscopy to observe the absorption regions. The spectra show relatively much higher absorption on the fingerprint region (500 – 1500 cm^{-1}) than on the others. All absorption peaks look similar for all mixture samples and exhibit the combination of the [Emim][NTf2] and DMSO characters. The absorption of some [Emim][NTf2] peaks decrease with the mole fraction at wavenumber ~3160 cm^{-1}, which is the C–H stretches of the imidazolium ring alkyl or alkyl side chains. This shift is more pronounced when more DMSO is added. The shift indicates the existence of interaction between added solvent molecules and the cations. By using polarization selective PP spectroscopy with the FEL wavelength tuned to this vibrational mode at KU-FEL, we expect to be able to measure the lifetime of such interaction and probably the orientational decay of the ions.

The KU-FEL generated IR lasers at fundamental wavelength centered at ~6 μm (5.8 – 6.3 μm bandwidth). To obtain the desired wavenumber of ~3160 cm^{-1}, the second-harmonic generation (SHG) was applied by passing the FEL through the SHG crystal, which yielded the wavelength of ~3 μm (2.9 – 3.1 μm bandwidth). This wavelength corresponds to the required wavenumber of 3460 – 3185 cm-^{1}. The pump pulse energy was measured to be around 0.2 μJ prior the liquid cell. The pump-probe signal was measured by detecting the probe signal in comparison with the pump signal at varied optical delay path. We began the measurement with the pure [Emim][NTf2] at ~3160 cm^{-1} absorption line and there was no decay signal observed. We suspected the absorption at this wavelength is too low as shown by the IR spectrum. Therefore, we decided to try the measurement at higher IR absorption wavelength of ~1200 cm^{-1}. At this wavenumber the pump-probe signal also could not be detected but we observed the gas bubble formation in the sample liquid bulk, which is the indication of thermal dissipation as laser beam heated up the sample. We then tried to measure the response at ~1200 cm^{-1} in the mixture sample with XIL = 0.5, with the hope that the effect of strong absorption will be reduced to some level. Unfortunately, the expected exponential decay of the pump-probe intensity still could not be observed. Our postulate is the change in the probe signal is low since the population of the sample in the low vibrational state is low due to the excitation of the pump pulse.

With the FEL repetition rate of about 2856 MHz, the time between the consecutive pulse is about 0.3 ns. This is much shorter than the thermalization time of the liquid sample, meaning that the sample does not have enough time to relax. This issue has also been pointed out by [Novelli et al., PCCP, 2022]. They applied the THz FEL polarization selective pump-probe spectroscopy to study the dynamics of water with the setup similar to ours. For water having thickness of 50 μm, the thermalization time can be estimated to be in the order of 20 ms. With this in mind, the technique to modify the laser pulse train to have lower repetition rate is needed. Optical technique like plasma mirror is one option to allow ultrafast and high intensity beam to be selectively reflected. With such development, the pump-probe spectroscopy based on MIR-FEL light source may be achievable.

4. Conclusion

The experimental study to investigate the dynamics of ion interaction in ionic liquid/solvent mixtures using MIR-FEL polarization selective PP spectroscopy has been proposed. The work includes design and construction of the optical setup in pump-probe configuration. This setup alignment was carried out at KU-FEL to fit the beamline end station and used in the measurement. There was no observable pump-probe signal detected in any of the sample. This difficulty is attributed to the low absorption of the sample at the interested vibrational mode and too high repetition rate of the MIR-FEL. However, there was a positive indication showing that the designed setup is actually functioning. It seems from the current findings that additional optical technique may be required in the future to perform such experiment using the MIR-FEL.

[1]. Novelli F. et al 2022 *Phys. Chem. Chem. Phys.* 24 653

Advanced Energy Research Section

Josefine H.E. Proll, Foreign Visiting Researcher
(Assistant Professor at Eindhoven University of
Technology, Eindhoven, The Netherlands)

1. Summary

The author spent three months (Jan 01 2023 -Mar. 31, 2023) as a guest professor at the Uji campus of Kyoto University, hosted by the Heliotron J group.

Here the author reports about successes in turbulence modelling for Heliotron J.

2. Introduction

Recent successes in stellarator optimisation have allowed for the construction of neoclassically optimised stellarators such as Wendelstein 7-X and HSX. Experiments have shown [1,2] that the now dominant transport channel is turbulence. Thanks to the large space of available 3D magnetic field shapes, optimising also for turbulence is a possibility and might allow for stellarator and heliotrons configurations to be serious candidates for a DEMO reactor. Especially electrostatic turbulence driven at the ion scale, i.e. ion-temperature-gradient modes (ITG) and trapped-electron modes (TEM), have been found to significantly contribute to turbulent transport and have thus been studied in analytical theory and simulations in stellarator geometry. In so-called maximum-J configurations, of which W7-X is an approximation, it was shown analytically [3] that the classical electron-driven TEM was absent, which was shown to lead to low levels of turbulent heat flux (see Figure **2**) [4].

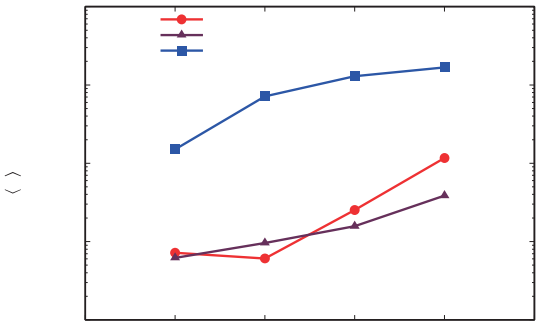

Figure 2: Normalised heat flux Q for grad-n-driven turbulence for different configurations. a/Ln is the density gradient scale length.

While HSX, a quasi-symmetric configuration and decidedly non-maximum-J, does not benefit from reduced linear growth rates (see Figure **1**), it does boast a similarly low turbulent heat flux. This unexpected nonlinear stabilisation has been attributed to the very low global shear of HSX and the subsequent increasedpool of subdominant and stable eigenmodes,

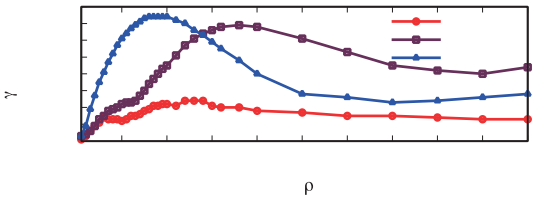

Figure 1: Linear growth rates of TEMs driven by a density gradient of a/Ln=3 in different configurations

to which energy can be transferred to reach saturation.

The question now is whether a configuration like Heliotron J, which is also approaching maximum-J-ness (albeit to a lesser degree than the high-mirror configuration of W7-X studied previously), and also has very low shear almost as low as HSX, can benefit from both mechanisms – the reduction of TEM thanks to maximum-J *and* improved saturation thanks to the low shear, and boast even lower heat fluxes. This would be a very interesting avenue to pursue for optimisation, as fully maximum-J configurations can be hard to achieve, especially over the full plasma radius. As an additional consequence of the absence of classical TEMs in W7-X, other types of modes can arise. Very recently, the so-called universal instability [5] has been identified in simulations in W-X geometry [6] and has been linked to potentially lower heat fluxes. Also in Heliotron J, the universal instability is expected to appear thanks to the postulated reduction of TEMs. During the research stay, several of these questions were addressed.

3. Gyrokinetic simulations for Heliotron J

To investigate whether the universal instability (UI) is indeed found in the different configurations of Heliotron J, linear simulations using the GENE code [7] were performed. Because the universal instability is predominantly driven by a density gradient, the temperature gradients of both ions and electrons were set to zero, and only a normalised density gradient of $a/L_n=3$ (with a being the minor radius and L_n the density gradient scale length) was chosen. Interestingly, in all configurations investigated, the universal instability is found to be dominant over a large range of low wave numbers (see Figure **4**), indicating that, similar to the case in Wendelstein 7-X, the UI might dominate the nonlinear transport and showcase enhanced saturation properties. Whether this is indeed the case is currently being investigated with nonlinear simulations. It is

remarkable that the UI is seen in ALL configurations of Heliotron J. In the ultra-high-bumpiness case ("5 to 0" in Figure **4** and Figure **3**) or the high-bumpiness case ("5 to 1"), the stability of the classical TEM and the subsequent emergence of the UI is somewhat expected, because these two configurations are approaching quasi-isodynamicity the most, whereas the standard configuration ("5 to 2") and the low-bumpiness configuration ("5 to 3") are less quasi-

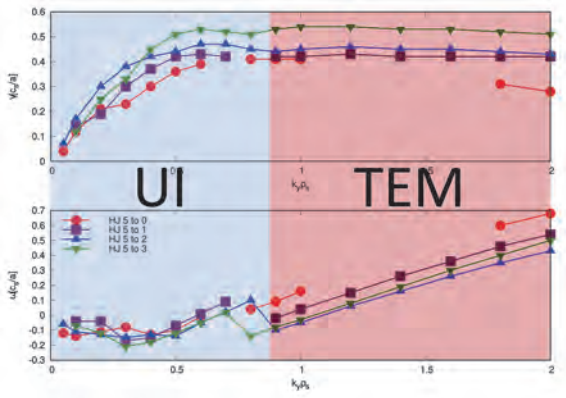

Figure 4: Linear growth rates of TEMs driven by a density gradient of a/Ln=3 in different configurations of Heliotron J, from low bumpiness (5 to 3) to ultra-high bumpiness (5 to 0)

isodynamic. However, it seems that even the lower degree of quasi-isodynamicity in the standard configuration and the low-bumpiness configuration is sufficient to stabilise the TEM. The theoretically predicted trend of higher degree of quasi-isodynamicity leading to lower TEM growth rates is seen regardless. These simulations are for pure density gradient with vanishing temperature gradients, which is very far from what is observed experimentally. To also perform computationally demanding nonlinear simulations (especially those with an electron-temperature-gradient require a lot of computing resources because the electron-scales need to be resolved, too), a joint proposal for computing time at IFERC was written between J. Proll and A. Ishizawa. The entire computing time asked for was granted, so that these investigations can continue full force in the coming months.

4. Available energy as a metric for turbulence

While the simulations above did show that a higher degree of quasi-isodynamicity (through a higher degree of bumpiness) leads to lower growth rates, we would need a nonlinear measure to assess whether also the actual levels of turbulence are reduced. To this end we can use the novel metric of available energy [8–10], a fully nonlinear expression which adheres to energy conservation and which has been shown to correlate remarkably well with the electron heat flux caused by trapped-electron modes. In our investigations, it was found (Figure **3**) that the available energy is generally reduced the higher the bumpiness is. While the available energy in its current form [10] is only that of the trapped electrons, and it is questionable that it would also faithfully represent turbulence driven by the passing-electron-driven UI, the results agree well with the linear results from the

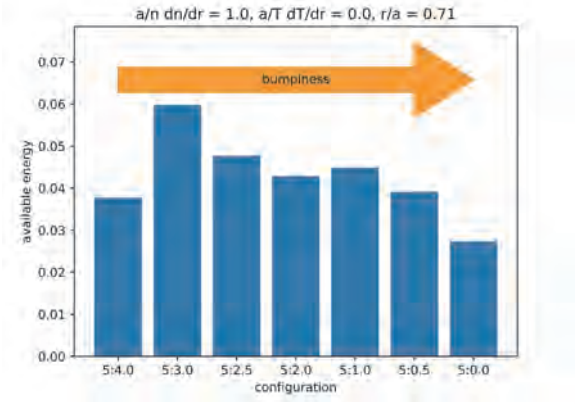

Figure 3: Available energy calculated for the different configurations of Heliotron J for a density gradient a/Ln=3.

previous section, and predict that the higher the bumpiness, the lower the turbulence. This would also explain the experimental findings where a higher bumpiness reported better overall confinement. A publication which compares the experimental results and the simulations and available energy calculations is in preparation. Moreover, work has begun to use the available energy as a metric to find turbulence-optimised configurations in the configuration space of Heliotron J, which might be used in one of the upcoming experimental campaigns.

6. Summary

We have confirmed that turbulence driven by TEMs is generally weak in Heliotron J and that higher bumpiness leads to enhanced stabilisation. Also the universal instability was found, as expected due to the high degree of quasi-isodynamicity. Work confirming the findings with nonlinear simulations is under way.

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Functional Materials Science and Engineering Research Section

Y. Miyauchi, Professor
T. Nishihara, Assistant 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 (CNTs), two-dimensional (2D) 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 2022.

2. Statistical verification of anomaly in chiral angle distribution of air-suspended carbon nanotubes

CNTs have long attracted attention due to their distinct optical, mechanical, electronic, and thermal properties, which are beneficial in the development of various future technologies. In addition, their potential to be generated from carbon dioxide has extended their importance in terms of present social demands to reduce carbon dioxide emissions. Among CNTs, single-walled CNTs (SWCNTs) have excellent functionalities that are sensitively dependent on their chiral structures, which are determined according to their diameter and chiral angle. However, large-scale bulk synthesis of SWCNTs with an on-demand chiral structure is still difficult and clarifying their growth mechanism in detail toward structure-controlled bulk synthesis is of central importance in nanomaterials fields. To date, theoretical studies have predicted that the configurations of the opening tube edge composed of armchair- and zigzag-shaped sites have significant impact on the SWCNTs' growth rate and the resultant structure abundance distribution. However, lack of sufficient statistical data on the chiral structure distribution of both metallic and semiconducting SWCNTs has prohibited rigorous experimental verification of such theoretical predictions.

In this study, we reported statistical verification of the chiral structure distribution of as-grown, air-suspended individual SWCNTs that are unaffected by various nonideal effects, including interactions with other nanotubes in bundles and with the substrate [1]. We determined the chiral structures of 413 air-suspended SWCNTs using broadband Rayleigh spectroscopy. Our statistical analyses have revealed that the fractional abundance as a function of chiral angle shows a linear increasing trend with an anomaly in the derivative at the chiral angle of approximately 20° (refer to Fig. 1). From this critical result, we have clarified that the consecutive armchair site (red edge in the inset) is a key edge configuration strongly influencing the growth preference of each SWCNT structure. These findings on the anomalous abundance distribution and the proposed model accounting for the chiral angle dependence of the growth rate are expected to allow us to obtain deeper understanding of the growth mechanism of SWCNTs.

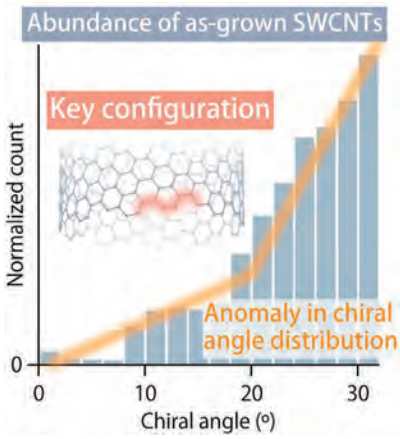

Fig. 1 Normalized chiral angle distribution of as-grown, air-suspended individual single-walled carbon nanotubes (SWCNTs) [1].

3. Directional exciton-energy transport in a lateral heteromonolayer of WSe_2–$MoSe_2$ (Fig. 2)

Excitons, in particular those in low-dimensional semiconducting nanomaterials are expected as next generation energy and/or information carriers for future energy/information devices. For these devices, controlling of the direction of exciton energy flow is one of the most important challenges. Generally, spatial asymmetry is required to induce a directional flow of quasi particles. As for charged particles like electrons, generation of such a flow is simply achieved by introducing potential asymmetry using an external electric field. However, for generating a directional

flow of neutral particles such as excitons, electric field cannot be a direct driving force. Therefore, finding a method to directionally drive excitons laterally in an ultrafast time scale has been strongly desired.

We reported observation of directional exciton energy transport across the interface in the WSe_2-$MoSe_2$ lateral heterostructure [2]. Space and frequency resolved photoluminescence (PL) and PL excitation measurements revealed exciton energy transfer in the lateral direction induced by asymmetric energy landscape bult-in at the sharp interface of the two different 2D semiconductors. The results suggest that excitonic devices using this type of lateral heterostructure is promising in applications for energy/information devices using fast exciton energy transport.

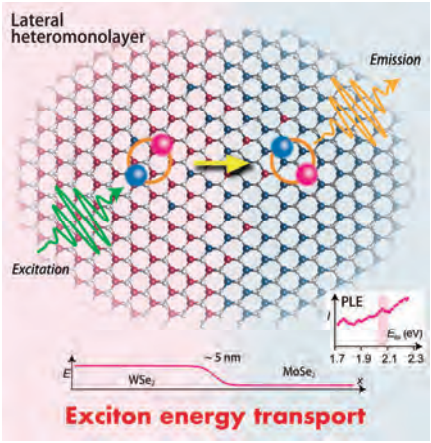

Fig. 2 Directional exciton-energy transport in a lateral heteromonolayer of WSe_2–$MoSe_2$ [2].

4. Anisotropic exciton drift-diffusion in a monolayer WS_2xSe_{2-2x} alloy with a gradually changing composition

In addition to the demonstration of the unidirectional transport of excitons using lateral heterostructure monolayer with a sharp one-dimensional heterojunction [2], we also demonstrated anisotropic exciton drift-diffusion in a $WS_{2x}Se_{(2-2x)}$ alloy monolayer with gradually changing composition ratio extended over micrometers [3]. The significant observation was that the spatial profile of the PL image became anisotropic under the finite exciton energy gradient under isotropic laser excitation. We confirmed that the degree of asymmetry had a strong correlation with the energy gradient. The results were successfully interpreted based on the simulation results considering drift and diffusion of excitons under the finite exciton energy gradient.

5. Polarized Raman spectroscopy on topological semimetal $Co_3Sn_2S_2$

In the last few years, the ternary ferromagnetic compound $Co_3Sn_2S_2$ has been identified as a topological semimetal, which can host a Weyl semimetal phase. To date, electronic properties of this material has attracted growing attention because it provides a desirable platform to study Weyl fermion physics near the Weyl point that acts as a source or sink of the Berry curvature field, which is one of the central interests of the current condensed matter physics. Moreover, Weyl semimetals is expected as a candidate material for nonreciprocal thermal emitters that break Kirchhoff's law, which may lead to a breakthrough in the radiative heat transfer technologies. In contrast to the intensively studied electronic properties, however, phonon properties of $Co_3Sn_2S_2$ have yet to be clarified experimentally; even the most fundamental information, phonon frequencies and their symmetries have unidentified. The lack of the Raman spectral fingerprint in the literature has hindered a quick experimental identification of the crystal structure, as well as confirmation of the validity of ab-initio calculations on $Co_3Sn_2S_2$ by comparing the calculated phonon frequencies with the experimental ones.

In this study, we clarified polarized Raman spectra of the topological semimetal $Co_3Sn_2S_2$ [4]. Two major phonon Raman peaks were observed at 289 cm^{-1} and 386 cm^{-1} over continuous background emission signals, and attributed to Γ point phonon modes with E_g and A_{1g} symmetries, respectively, according to the group theory and Raman tensor analysis. Line shape analyses revealed that the high-frequency A_{1g} mode exhibited asymmetric peak feature suggesting the Fano resonance between the A_{1g} phonon scattering with the continuous electronic background. The clarified phonon energies and symmetries, as well as the electronic contribution to the Raman scattering, will not only be useful as a fingerprint to readily verify the experimentally grown or theoretically calculated crystal structure, but also suggest importance of Raman spectroscopy as an effective tool to study low energy excitations and their interactions in $Co_3Sn_2S_2$.

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Advanced Laser Science Research Section

T. Nakajima, Associate Professor
K. Ando, Program-Specific Assistant Professor

1. Introduction

Laser is a versatile technique to probe various dynamics and also fabricate various devices. This year we have developed a few different techniques to probe the electrochemical processes during hydrogen evolution, fabricate the functional metal surfaces, and modify the size and shape of nanoparticles for the utilization toward green energy.

2. Influence of liquid viscosity and temperature on the morphologies of laser-induced microstructures

Laser materials processing is a useful technique to fabricate micro/nanostructures on the material surface, and performed not only in air but also in liquids in some cases to fabricate desired surface morphologies. How and how much the property of the liquid influences the surface morphology of the laser-irradiated target is not yet completely understood. This is particularly true in terms of liquid viscosity. To clarify the role of liquid viscosity in laser materials processing we undertake the study to ablate the metal target in different liquids at different temperatures and compare the morphology of the ablation crater. The liquids we employ in this study are water (H_2O), ethanol (ET), ethylene glycol (EG), and glycerol (GOL) at room temperature (RT), and additionally EG and GOL at 100 °C, since their viscosities significantly change at different temperatures. Representative results with Ni targets are shown in Fig. 1. In Fig. 1(a) we clearly see the confinement effects. From Fig. 1(b), we notice that the diameter of the crater in each liquid linearly increases with laser fluence, and at a given laser fluence, the crater diameters are air < ET < water < EG at 100 °C < EG at RT < GOL at 100 °C < GOL at RT. Similar is true for the volume (Fig. 1(c)). To explain the different ablation efficiencies in different liquids at different temperatures we consider the pressure exerted to the target under the confined geometry by laser-induced plasma, and estimate the plasma-induced recoil pressure. The relative pressures exerted to the target during the laser pulse are found to be 1:0.78:1.09:1.20:1.26 in water, ET, EG at RT, GOL at RT, and GOL at 100 °C, respectively, and this order is in good agreement with those of the experimentally obtained diameters and volumes of ablation craters shown in Fig. 1(b) and (c). This clearly shows that it is not the liquid viscosity but the plasma-induced recoil pressure that plays an important role on the ablation efficiency in liquids.

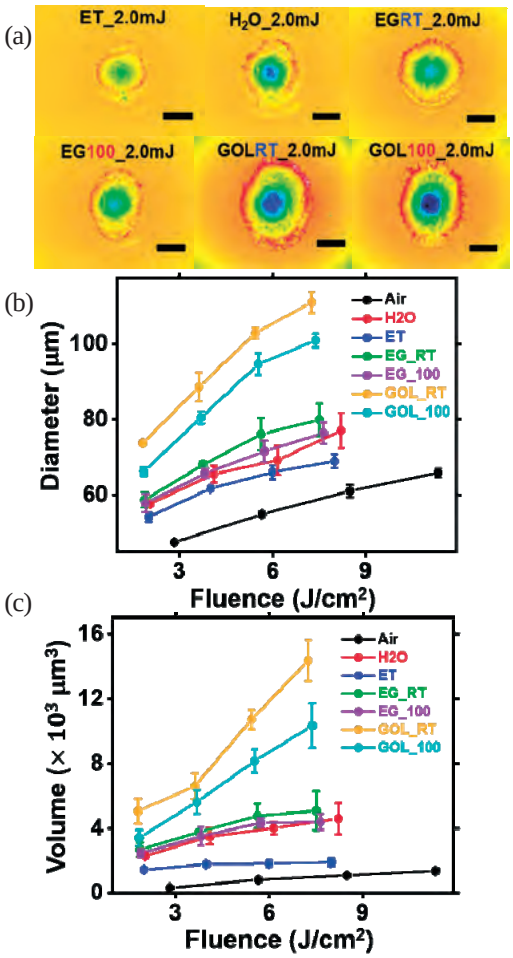

Fig. 1 (a) Morphologies of the ablation craters in air and various liquids at different temperatures. Variation of (b) diameters and (c) volumes of ablation craters as a function of laser fluence.

3. Correlation between the bubble forming sites and micro/nanostructures on the electrode surface during hydrogen evolution

Production of hydrogen gas through water electrolysis using the excess electricity is one of the promising candidates for green energy. For the efficient production and transportation of hydrogen gas through water electrolysis it is very important to

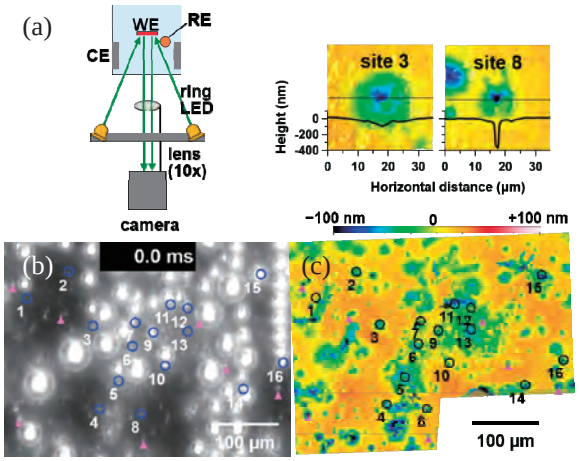

Fig. 2 (a) Experimental setup. (b) Optical image of hydrogen bubbles where all bubble forming sites are numbered. (c) Corresponding false-colored surface profile of the electrode. The figures above panel (c) are the blow-ups of the surface profiles at sites 3 and 8.

know where on the electrode the hydrogen bubbles are formed, since the deeper understanding of formation mechanism will enable us to design the surface morphology of the electrode. For this purpose we optically monitor the formation of hydrogen bubbles on a Ni disk cathode from the front side (Fig. 2(a)) to identify the bubble forming sites (Fig. 2(b)), and correlate them with the surface profile with ~μm accuracy (Fig. 2(c)). We notice that the bubble forming sites are located at the shallow structures, but their structures are not necessarily similar, as shown by the surface profiles of bubble forming sites 3 and 8. To better understand the local bubble dynamics we analyze the optical images of the bubbles at sites 3 and 8 using many successive images taken with the time interval of 1 ms, and obtain the temporal variations of the squared radius, R^2, and rising velocities, v, of the bubbles formed at sites 3 and 8 (Fig. 3). We find that the growth rates and formation periods of the bubbles are completely different at those sites, and the formation period is very long at site 8. The

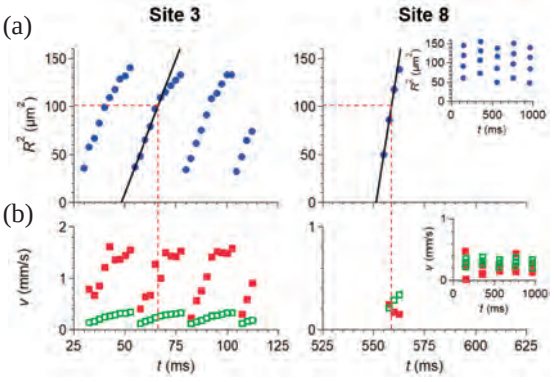

Fig. 3 (a) Temporal variations of the squared radius, R^2, and (b) experimental (closed squares) and theoretical (open squares) rising velocities, v, of the bubbles formed at sites 3 and 8.

difference of the experimental and theoretical rising velocities of the bubble at site 3 implies the presence of local convection flowing upward near site 3 since the theoretical rising velocity is obtained using the Stokes law without taking into account the convection. In contrast, there is practically no local flow near site 8. These results suggest that, although sites 3 and 8 are only ~120 μm apart, the dynamics of the bubbles as well as the local convections at those sites are very different. This is the first study to correlate the bubble forming sites and surface morphologies of the electrode and clarify the dynamics of bubbles.

4. Dynamics of hydrogen bubbles formed at a laser-induced microstructure on the electrode during hydrogen evolution

What we have learned from the study described in the previous section is that, although there is a clear correlation between the bubble forming sites and their local surface morphologies, the local surface morphology itself does not seem to determine the bubble dynamics. Knowing this, we fabricate a single microstructure on a polished Ni electrode by single-shot laser irradiation, and study the formation of hydrogen bubbles at a laser-induced microstructure through the optical detection. The results are summarized in Fig. 4. From the optical image of the laser-induced microstructure with bubbles shown in Fig. 4(a) we notice that the bubbles are never formed at the central area of the microstructure, and all the bubble forming sites numbered 1-7 are located at the periphery of the microstructure where there are bumps (Fig. 4(b)) with so many micro/nanostructures (Fig. 4(c) and (d)). It is interesting to point out that the growth rates and formation periods of the bubbles under the constant current operation are different at different bubble forming sites. This finding clearly implies that a subtle local structure within a single microstructure strongly influences the bubble forming activity of the individual sites, although they are only a few tens of μm apart.

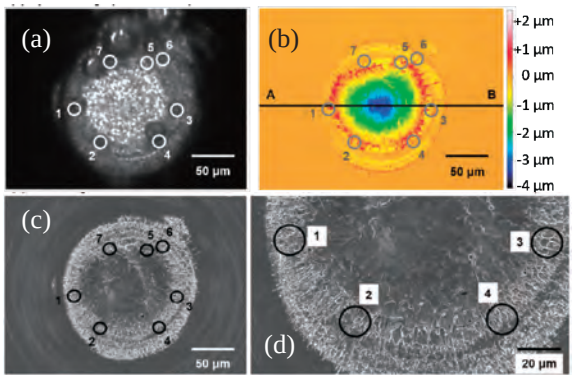

Fig. 4 (a) Optical image of the laser-induced microstructure with bubbles and (b) surface profile of the corresponding area. (c) SEM image of the microstructure and (d) its blow-up.

Financial Support

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Advanced Energy Structural Materials Research Section

K. Morishita, Associate Professor
K. Yabuuchi, Assistant Professor
A. Kimura, Researcher

1. Introduction

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

(1) Theory, modeling, numerical simulation and data-driven science & technology of irradiated materials

Radiation damage processes in materials during irradiation occur at a wide variety of time and length scales. To understand this process, 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 molecular dynamics, ab-initio quantum calculations, kinetic Monte-Carlo, rate-equation theory analysis, FEM and CFD. Recently, additional efforts have also been devoted to this research using machine learning, AI (artificial intelligence) and data-driven techniques.

(2) Plant integrity analysis

Structural integrity of a reactor pressure vessel (RPV) during a pressurized thermal shock (PTS) events is of critical importance in the quantitative assessment of reactor safety. We evaluate this using three-dimensional computational fluid dynamics (3D-CFD) and the finite element method (FEM). Through this evaluation, the risk of the RPV function loss is quantified and it 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 point defects is responsible for the evolution of the microstructure, which may cause degradation, (or development), 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. Mechanism of non-equilibrium point defect 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. 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 MD technique was used to simulate displacement cascades in Fe. Fig. 1 shows a simulated example of the time evolution of this process initiated from a 50 keV recoil atom.

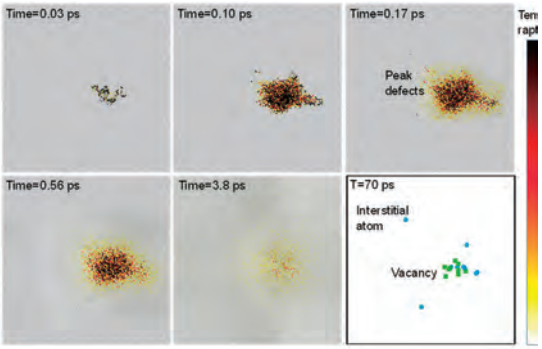

Fig. 1: Our molecular dynamics simulation shows the time evolution of athermal defect production process in Fe during irradaition.

As shown in the figure, at about sub-ps after the primary recoil atom starts to move, a large number of displaced atoms are formed with a very high density. In the central region, the kinetic energies and arrangement of the atoms exhibit a quasi-molten state. As time evolves, the cascade core cools down gradually, during which the displaced atoms in the molten zone return to their lattice point positions and annihilate. Almost all of the displaced atoms are annihilated (disap-

peared) during this cooling phase, but some still remain. These can be described as lattice defects (i.e., interstitial atoms) that are athermally introduced into the material by the effects of incident neutrons. Interestingly, some of these interstitial atoms are isolated at this time, while others are grouped together to form clusters. Such information is highly valuable, as whether the interstitial atoms thus produced are isolated or clustered can have a significant impact on subsequent defect reactions.

The mechanism of defect production demonstrated here is quite different from the conventional one employed by the NRT model for evaluating *dpa*. A more detailed model construction is underway.

3. Size and temperature dependence of point defect binding free energy to defect clusters in Fe

Size and temperature dependence of the point defect binding free energy has numerically evaluated for self-interstitial atom (SIA) clusters and vacancy clusters in bcc Fe by using continuum models based on thermodynamics and linear elasticity. The estimated binding free energy of SIAs to SIA-clusters is much higher than that of vacancies to vacancy clusters, indicating that SIA-clusters are more thermally stable than vacancy clusters. For relatively small clusters, the estimated binding free energy at 0 K is comparably consistent with atomistic calculation data; and then, the SIA biding free energy at 850 K is averagely about 35 % lower than that at 0 K, while the vacancy binding free energy is about 6 % lower; which may remarkably affect the formation kinetics of those defect clusters under irradiation. These kinds of information will be one of the basic parameters for a theoretical model of the microstructural evolution of Fe-based materials in the nuclear fusion DEMO environment.

This work was performed in the collaboration with Dr. Watanabe et al. at of National Institutes for Quantum Science and Technology (QST).

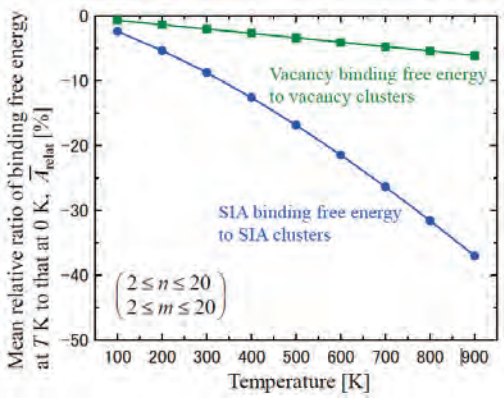

Fig. 2: Temperature dependence of the free energy of point defects to small defect clusters in Fe.

4. Development of new power device "DISTAR"

With the aim of developing new energy devices with higher functionality, we prototyped a small device (Distar) that combines a light-receiving element (LED) and a light-emitting element (solar panel), which is inspired by the operating principle of a conventional bipolar transistor. By applying positive feedback to the current flowing through the circuit, our prototype device showed a current amplification factor of about 1000. Then, this prototype circuit was modeled theoretically, and a simulation model was constructed so that the relationships between the current, voltage, resistance, etc. of the circuit could be understood. It was found from the model calculations that although the current amplification factor reaches 1000, the Joule heat in the resistor is very large, and the energy efficiency of the entire circuit is extremely low (90 percent of input energy is lost). Based on this fact, it is currently concluded that further efforts are necessary to improve energy efficiency. This research is a joint research with Professor Emeritus Kensho Okamoto of Kagawa University.

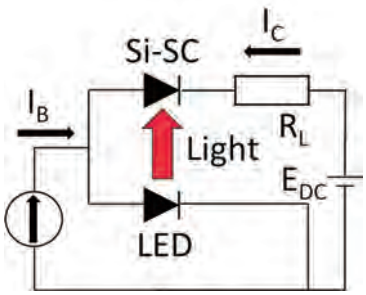

Fig. 3: DISTAR circuit

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.

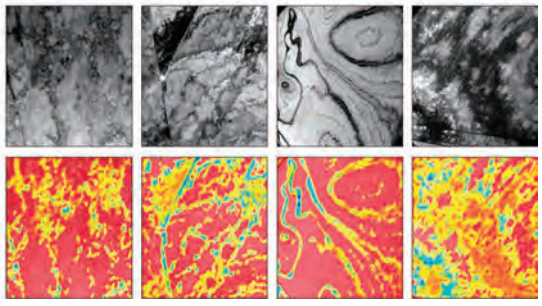

Fig. 4: Image analysis using AI

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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 2022.

1. Valley Relaxation of the Moiré Excitons in a $WSe_2/MoSe_2$ Heterobilayer

Due to their unusual physical properties and ability to function as extreme two-dimensional (2D) systems, atomically thin materials such as graphene and semiconducting transition-metal dichalcogenides (TMDs) and their van der Waals (vdW) heterostructures have gained increasing attention. The physical properties of atomically thin materials originating from a particular atomic arrangement are significantly altered by emerging moiré superlattices made up of lattice- or angular-mismatched vdW heterostructures. The moiré superlattice is gaining attention for its ability to engineer optically excited, tightly bound electron-hole pairs (excitons) and can result in exciton trapping through in-plane periodic moiré potentials in twisted semiconducting TMDs heterobilayers. The quantum confined zero-dimensional (0D) as a two-level system created by the moiré exciton trapped in the moiré potentials is encouraging for the development of quantum optics and quantum information processes.

The confinement of moiré potential of exciton alters the optical characteristics of the system. Under low-excitation power density conditions, the moiré exciton results in the appearance of sharp peaks in the low-temperature photoluminescence (PL) spectrum. Additionally, the moiré pattern (atomic registry) has a significant impact on the optical selection rule of the exciton. The intrinsic valley degrees of freedom control the optical properties of monolayer TMDs. The K and -K valleys at the edge of the Brillouin zone are inequivalent but energetically degenerate due to the strong spin-orbit interaction and lack of inversion symmetry. The optical selection rule and corresponding circular polarized light emission are both valley-dependent due to the inherent coupling of the valley and spin degrees of freedom.

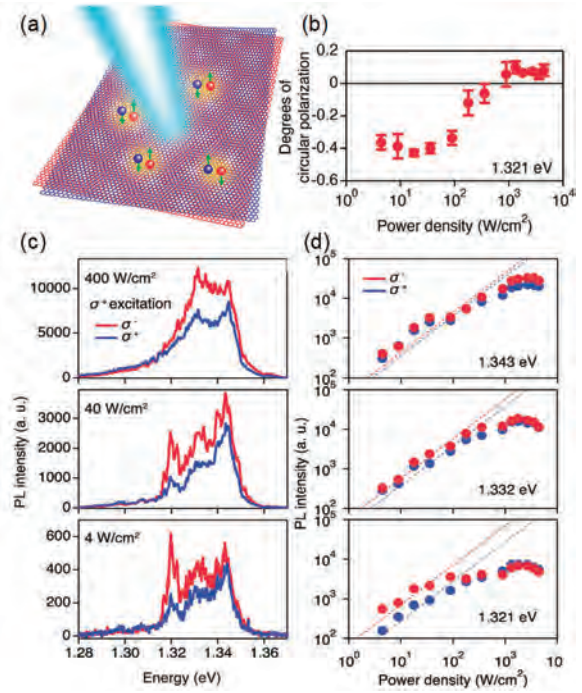

Fig. 1 (a) Schematic of moiré exciton in $WSe_2/MoSe_2$ heterobilayer. (b) Degree of circularly polarization as a function of excitation power density. (c) Low-temperature circularly polarized PL spectrum under σ+ circularly polarized excitation (1.676 eV) with different excitation power densities. The σ+ and σ– circularly polarized components are shown as the blue and red lines, respectively. (d) Excitation power density dependence of the PL intensity monitored at 1.321, 1.332, and 1.343 eV in the polarization-resolved PL spectra.

Contrary to monolayer TMDs, the optical selection rule of moiré superlattice also influences the circularly polarized light emission due to the atomic registry's C_3 symmetry and the valley degrees of freedom. The fascinating optical and electrical properties requires an understanding of the intra- and intervalley relaxation processes. The valley relaxation process in monolayer TMDs has thus been successfully explained and controlled through extensive experimental and theoretical studies. Electro-static carrier doping techniques were used to continuously control the valley relaxation process by altering the electron-hole exchange interaction. It has been discovered that momentum-dependent long-range electron-hole exchange interactions dominate the valley relaxation of neutral excitons in monolayer TMDs. On the other hand, it is still unclear how

the valley relaxation process in the moiré superlattice works, where the reduced dimensionality might also have an impact.

Here, we used circularly polarized PL and photoluminescence excitation (PLE) spectroscopy to investigate the intra- and intervalley relaxation of the moiré excitons in a twisted $WSe_2/MoSe_2$ hetero-bilayer. Contrary to 2D monolayer TMDs, the experimentally observed circularly polarized emission is strongly dependent on the excitation power density. The excitation power density dependence of circularly polarized emission leads to the inter-valley relaxation of the moiré exciton, which are originated from Pauli blocking due to the low density of states typical of 0D systems. The intravalley relaxation of the moiré exciton states from the triplet to singlet state via Γ_5 phonon emission is also revealed by the resonant PLE measurement. Circularly polarized quantum light emitter may be used in quantum optics and information processing as a result of our discoveries regarding the valley relaxation of moiré excitons.

2. Dynamics of Moiré Exciton in a Twisted $MoSe_2/WSe_2$ Heterobilayers

Studies in artificial vdW heterostructures made of two atomically thin 2D materials have received a lot of attention. A number of distinct physical phenomena, such as superconductivity, ferromagnetism near 3/4 filling, correlated insulator phases, and Hofstadter butterflies in graphene moiré superlattices, have new pathways thanks to the recent discovery of moiré superlattices at the interface of vdW hetero-structures with small lattice mismatches or twist angles between two monolayers. When optically generated electrons and holes in a spatially separated layer interact via Coulomb interactions, an interlayer exciton is created. This exciton is then contained within the moiré trap potential and spatially organized as a moiré exciton ensemble. The dense array of coherent quantum emitters is one application of the moiré trapped exciton that has great potential for many-body physics. However, little is known about the discrete excitonic states and dynamics of the confined exciton within the moiré potential.

The excitons can be divided into optically active bright excitons and inactive dark excitons in semiconductors. The dipole-allowed bright exciton exhibits radiative recombination during the emission process and directly couples to light via strong light-matter interaction. Optical absorption and PL spectroscopy makeit possible to observe and track the dynamic behaviors of bright excitons. However, due to the weak light-matter interaction and reduced oscillator strength, optical access to the dark exciton is challenging. Dark excitons can be used in research on spin storage and long-lived qubits. The dark exciton state in monolayer 2D materials exhibits nonequilibrium dynamics as well as optical responses, and studies have shown that

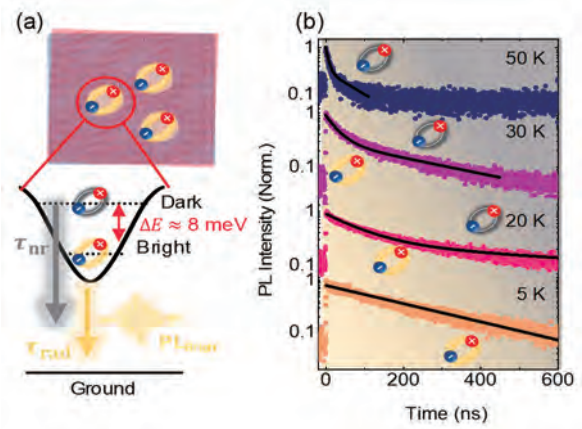

Fig. 2 (a) Schematic of moiré excito states confined in the potential. The splitting of bright and dark moire exciton states is about 8 meV. (b) PL decay profiles at various temperatures. The contribution of bright and dark moiré exciton states is changed from low to high temperature.

it is energetically inferior to the bright exciton state.

The energy structures and characteristics of the bright and dark moiré exciton states in the moiré potential, however, may raise important and crucial questions. Therefore, it is essential to conduct experiments to demonstrate the existence of dark exciton within moiré potential. The dynamics of bright and dark moiré excitonic states in twisted semiconducting vdW heterobilayers requires further research in order to fully understand their revolutionary significance for fundamental moiré physics and potential quantum optics applications in the novel platform of moiré exctonic systems.

Here, we used PL spectroscopy and rate-equation analysis to investigate the moiré exciton states and their dynamics in twisted $MoSe_2/WSe_2$ heterobilayers. The experimental results demonstrate the existence of a dark moiré exciton state above the lowest emissive bright singlet exciton state, and the dynamics of bright excitons are determined by radical recombination and transition to the dark exciton state with the aid of phonons. In-depth information is provided regarding the dynamics and nature of moiré exciton states.

Our findings lay the groundwork for further investigation into quantum phenomena in moiré physics for use in quantum optics while illuminating novel aspects of quantum states of moiré excitons and fascinating moiré exciton dynamics.

Collaboration Works

松田一成，University of Bordeaux（フランス），単一ナノ物質における先端分光

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1. Grant-in-Aid for Scientific Research

松田一成，基盤研究(S)，原子層人工ヘテロ構造におけるバレースピン量子光学の開拓と応用

松田一成，学術変革領域研究(A)，２.５次元構造の分析技術開発

松田一成，挑戦的研究（萌芽），バレースピン制御とデバイス応用：バレートロニクスに向けた課題と挑戦

松田一成，学術変革領域研究(A)，２.５次元物質科学の総括（分担金）

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2. Others

篠北啓介，創発的研究支援事業，半導体モアレ超構造を用いた量子電磁力学の創生

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Clean Energy Conversion Research Section

Kenji Kitayama, Visiting Professor
(Daicel corporation)

1. Introduction

As a senior research scientist, the author is responsible for "improving technical capabilities" and "problem solving" in the field of organic synthesis in our company. In particular, he has focused on "developing high-performance catalysts" and "establishing organic synthesis technology using simple materials as raw materials" to improve the technology.

For example, as an example of a high-performance catalyst, a system that can use a safe oxidizing agent in an epoxidation reaction, and as an example of organic synthesis technology using simple raw materials as raw materials, consider the organic synthesis technology using molten sulfur that is a by-product in the factories.

Since 2017, as a senior research scientist, he has expanded his expertise from organic synthesis to forest science and has achieved some results. We will also introduce its contents. At the same time as signing a comprehensive collaboration agreement with Kyoto University in October 2021, Daicel established an industry-academia collaborative research laboratory in the Uji area as a base for the fusion of research fields and industry-government-academia collaboration. We believe that these efforts will lead to the realization of a sustainable society.

2. Efforts of the senior research scientist

The author, as a senior research scientist, is making efforts to "improve technical capabilities" and "solve problems" in the organic synthesis field of our company. In particular, he focused on "developing high-performance catalysts", "establishing organic synthesis technology using simple materials as raw materials", and "early acquisition and practical application of new technologies" as key points for technological improvement. In this paper, we will introduce related research such as epoxy compounds, which are organic synthesis products of our company, in relation to these points. In terms of "developing high-performance catalysts," we are working to develop high-performance catalysts for the production of epoxy compounds, which are our main products. Specifically, as a safe and environmentally friendly method, we have conducted the joint research with some university to construct an electrolytic epoxidation system. This is a system in which oxidation (epoxidation) is carried out on the positive electrode and reduction is carried out on the negative electrode. However, although it is oxidized on the positive electrode, we thought it would be difficult to oxidize the olefin to the epoxides directly on the electrode. We therefore decided to investigate the electrochemical generation of the oxidant. After studying various electrolytes, it was found that peroxides were produced when hydrogen carbonates or carbonates were used, and it was also confirmed that olefin epoxidation would proceed in the presence of a suitable catalyst[1].

In "Establishing organic synthesis technology using simple materials as raw materials", we are investigating organic synthesis technology using molten sulfur produced as a by-product in factories. As an ultimate goal, we expect to be able to develop functional materials such as thiirane. Finally, we have not yet succeeded in introducing elemental sulfur into organic compounds using elemental sulfur itself as a reaction reagent. This is also the subject of joint research with a university, but first, in order to get used to working with organic sulfur compounds, we started to develop a new organic synthesis method using thiols. We have been able to publish several joint results in papers[2], the most interesting of which is the catalytic addition reaction of thiols to alkynes. Using a nickel catalyst, a sulfur atom was introduced on the same carbon and the dithioacetal was synthesized in good yields with high regioselectivity.

In "Early acquisition and practical application of new technology" we are looking at the industrialization of new organic synthesis technology using microreactor or microwave processes. Many excellent research results have been published in these areas, but commercialization is not possible unless the reactor and process conditions are taken into account at the same time. We don't think it's possible to start the research on our own. That is why we are working closely with the leading scientist who can guide us in building together from the basics, while gathering information and conducting internal reviews.

As a part of our efforts to create a sustainable society, we have been working on the use of woody biomass. For example, we have tried to produce hydrogen by dehydrogenation from cellulose, a component of woody biomass[3], and to introduce functional groups into saccharides by substitution of hydroxyl groups with carbon groups[4].

We believe that this category includes the

electrosynthesis and photochemical reactions mentioned above, and we are looking for good topics to propose.

3. Summary

Based on the author's experience in synthetic organic chemistry, which is his specialty, he talked about the importance of pursuing a doctoral degree based on his experience in leading product development (development of monomers for electronic materials) and leading to commercialization. This talk will encourage undergraduate students and master's students. I also hope that it will be explained in a way that is easy to understand for them with different fields of expertise.

Finally, I would like to take this opportunity to express my gratitude to all the mentors, superiors, subordinates, seniors, and juniors who participated in the research.

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Clean Energy Conversion Research Section

Shigeru Kashiwagi, Visiting Associate Professor
(Tohoku University)

1. Introduction

Terahertz (THz) radiation sources have attracted considerable interests because of their potential applications in fields such as material science, medical imaging, and high-speed communication. The coherent THz radiation having polarization control ability can be used for various types of scientific investigation and applications. Vibrational circular dichroism (VCD) measurements in the THz region are extremely sensitive to conformational changes in proteins. THz source capable of switching left and right circular polarizations with high speed is very useful for biological analysis and is in great demand. As described above, THz waves is traditionally used as probes for characterization, or spectroscopic means for "observation". Furthermore, high-field THz waves from the short electron bunches allow "control" of the molecular arrangement.

We are developing an accelerator-based THz radiation sources using the test accelerator (t-ACTS) [1] at Tohoku University and the THz-CUR of KU-FEL facility [2] at Kyoto University. In particular, the research is being conducted on the generation mechanism and polarization/amplitude control of a coherent undulator radiation (CUR) from extremely short electron beams.

2. THz coherent undulator radiation

The relativistic and short electron bunches passing through an undulator is capable of generating high intensity, coherent, and narrowband radiation in THz wavelength region. The radiation spectrum from the electron bunch can be written as

$$\left.\frac{d^2I}{d\omega d\Omega}\right|_N = \{N + N(N-1)|F_{3D}(\boldsymbol{k})|^2\} \cdot \left.\frac{d^2I}{d\omega d\Omega}\right|_1 \quad (1)$$

where N is the number of electrons in the bunch, I radiation intensity, ω radiation frequency, Ω solid angle of the radiation. The three-dimensional form factor is defined by

$$F_{3D}(\boldsymbol{k}) = \int S_{3D}(\boldsymbol{r})\, e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} d\boldsymbol{r}. \quad (2)$$

$\boldsymbol{k}$ and $S_{3D}(\boldsymbol{r})$ are the wave vector towards the observation point and the three-dimensional charge distribution of the electron bunch, respectively. If the form factor is sufficiently large, the radiation intensity from the electron bunch is proportional to the square of the electron number N.

As a relativistic electron beam propagates through an undulator, under the condition that the pulse length of the electron beam is sufficiently shorter than the resonance wavelength of the undulator radiation, the radiation will have temporal coherence. The temporal profile of the electric field of the undulator radiation shows an almost sinusoidal wave with a cycle of the number of undulator periods. The frequency spectrum of the CUR were measured by the Michelson interferometer with pyro-electric detector at t-ACTS. In this experiment, electron beam energy was 30 MeV and the pulse length of electron beam was approximately 80 fs. A 2.5 m long undulator with 25 periods and a peak magnetic field of 0.41 T was utilized to generate the CUR [3].

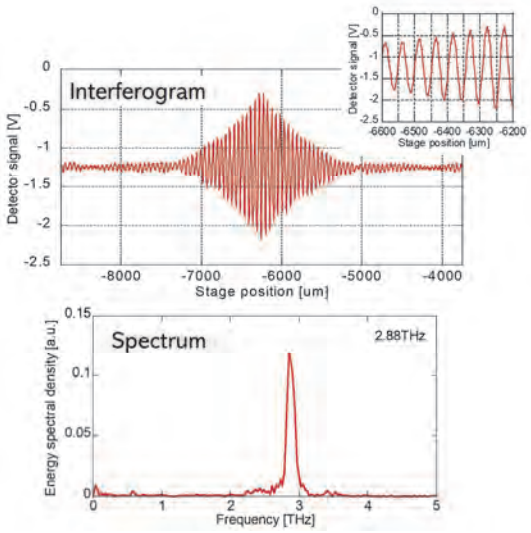

Fig.1: (Up) Measured interferogram of CUR; (Down) derived frequency spectrum from interferogram with K=3.6 [3].

3. Variable polarized coherent THz source

We have demonstrated to produce arbitrary polarization states from the linearly polarized CUR with a frequency of 1.9 THz at the t-ACTS at Tohoku University. Figure 2 shows a variable polarization manipulator (VPM) using a Martin–Puplett interferometer [4,5]. The VPM consists of a beam-splitter wire-grid and two rooftop mirrors, with one rooftop mirror mounted on a movable stage. The CUR from a planar undulator is linearly polarized. An incident beam of the CUR is split into two orthogonal linear polarizations by the beam-splitter wire-grid, and the reflected and transmitted beams travel to the rooftop mirrors. The two beams rotated by 90° using the rooftop mirrors are polarized and superimposed at

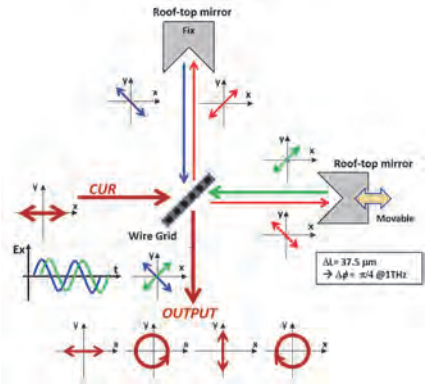

Fig.2: Variable polarization manipulator (VPM) using a Martin–Puplett interferometer.

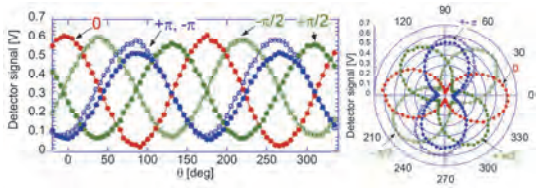

Fig.3: Measured intensity of the CUR as a function of rotating angle of the polarizer wire-grid. The phase difference (δ) between two orthogonal linear polarizations are 0, $\pm\pi$, $\pm\pi/2$, respectively.

the splitter wire-grid. The relative phase (δ) between the two orthogonal linearly polarized beams is adjusted using the movable stage. By using the VPM, it is possible to produce various polarization states by simply adjusting the relative phase. All polarization states of linearly polarized, elliptically polarized, and left and right circularly polarized states can be realized by moving the interferometer stage. In other words, the left and right circular polarization can be switched by simply shifting the movable stage by half a wavelength of the CUR. The VPM can realize high-speed switching the left and right circular polarization at several-hundred-Hz using a piezoelectric actuator stage. In addition, the VPM has the advantage of high transmission efficiency in the interferometer. The results of the polarization measurement using the wire-grid polarizer and quarter-waveplate clearly showed that variable polarized states were created from the CUR (Fig.3). Stokes parameters were measured using a polarizer to derive the degree of polarization.

5. CUR stacking using optical cavity

To generate intense terahertz pulses, we are conducting research on the superposition of CUR pulses using an optical resonator as shown in Fig.4. The THz CUR pulse stacked in an optical cavity are extracted using plasma mirror. Test experiments were carried out using the THz-CUR source at Kyoto University (Fig.5). It was confirmed that the transmittance was almost 100% when the Si-plate was placed at Brewster's angle to the CUR pulse. Using an Si-plate and a nanosecond time duration of Nd:YAG

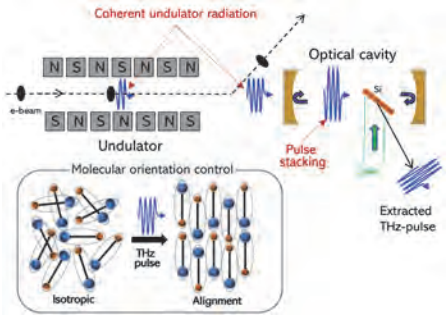

Fig.4: Generation of a high field THz CUR pulse using optical resonator and plasma mirror.

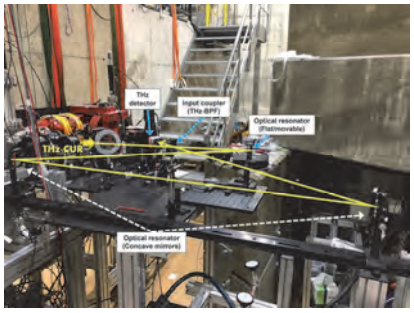

Fig.5: Optical resonator at THz-CUR source.

laser, we were able to reflect THz CUR pulses by a plasma mirror. In the experiment, the electric field superposition in the optical resonator was confirmed by changing the resonator length and measuring the interference pattern, however it was not sufficient enhancement. As next step, it will be necessary to improve the injection optics of the CUR into the optical resonator.

5. Summary

High-intensity THz sources based on CUR are being developed at Tohoku University and Kyoto University. We were able to establish a variable polarization THz source using VPM. For further THz pulse enhancement, we continue basic research on pulse stacking of CURs using optical resonators and plasma mirrors. This research is supported by the Joint Usage/Research Program on Zero-Emission Energy Research, IAE, Kyoto University (ZE30C-08, ZE31C-12, ZE2020A-30, ZE2021A-33, ZE2022A-19).

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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 recycling processes, new metal plating processes, and new rechargeable batteries.

In this fiscal year, we have researched a new recycling process for rare earth elements from magnet scraps using molten salt electrolysis and alloy diaphragm. We have also studied a silicon film plating process using molten salts, and dual carbon batteries using ionic liquids.

2. Development of New Recycling Process for Rare Earth Elements from Magnet Scraps Using Molten Salt Electrochemical Process and Alloy Diaphragm

Dy-doped Nd–Fe–B magnets are utilized in many important applications such as high-performance motors for electric vehicles. However, heavy rare earth (RE) elements such as Dy are difficult to supply stably. Thus, it is necessary to develop an efficient recycling process for RE elements. We have proposed a new recycling process for RE elements from magnet scraps using a molten salt electrochemical process and an alloy diaphragm [1]. Our previous studies have mainly used solid alloys as diaphragms, whereas in recent years we have focused on liquid alloys, which are expected to diffuse RE much faster than solids [2]. In this fiscal year, we investigated the electrochemical RE (RE = Nd and Dy) –alloying behaviors of Fe in molten LiF–CaF_2–NdF_3–DyF_3 systems at 1123 K.

To confirm the formation of liquid alloys, we performed potentiostatic electrolysis of the Fe plate electrode at 0.10 V vs. Li^+/Li for 1 hour. After electrolysis, the cross-section of the sample had a metallic luster and swelled into a drop-like shape, confirming the formation of liquid alloys. Fig. 1a shows the cross-sectional SEM image of the sample after potentiostatic electrolysis at 0.10 V for 5 minutes. A Nd-rich composition is confirmed. Fig. 1b shows the cross-sectional SEM image of the sample after potentiostatic electrolysis at 0.10 V for 5 minutes (1st-step), followed by changing the potential to +0.215 V for 30 minutes (2nd-step). The composition of the alloy is Dy-rich. From these results, we expect that controlling the RE dissolution potential from the liquid alloy diaphragm will enable its application as a selective permeation diaphragm for Nd.

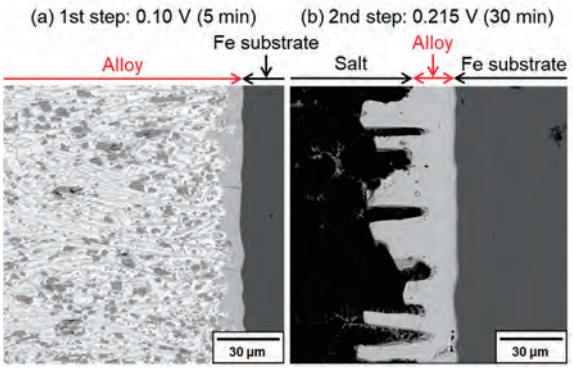

Fig. 1. Cross-sectional SEM images of the samples after potentiostatic electrolysis in molten LiF–CaF_2–NdF_3 (0.5 mol%)–DyF_3 (0.5 mol%) at 1123 K.

3. Development of Si film Plating Process Using Molten Salt Electrolyte: Fabrication of p-n Junction Si

To manufacture solar cells with fewer steps, plating n- and p-type Si directly on the substrate is a promising method. We have already proposed a new electrodeposition process of Si utilizing molten KF–KCl as an electrolyte and $SiCl_4$ as a Si ion source [3]. So far, we have reported the electrodeposition of dense and smooth Si films in KF–KCl at 923–1073 K [4,5]. Further, we have reported n-type Si electrodeposition in KF–KCl–K_2SiF_6 [6] In this fiscal year, we investigated the fabrication of p–n junction Si films by two-step electrodeposition. Furthermore, we measured the solar cells characteristics of the obtained p–n junction Si film.

We electrodeposited a p-type Si film as the first layer on a graphite substrate in KF–KCl–K_2SiF_6 with 5 mol ppm of KBF_4 at 1023 K. Subsequently, an n-type Si film was electrodeposited as the second layer in KF–KCl–K_2SiF_6 at 1023 K. Fig. 2 shows the cross-sectional SEM image of electrodeposited p-n junction Si film. A dense Si film with a thickness of around 40 μm was obtained. There was no clear boundary between p-type and n-type Si, indicating good interface formation. Fig. 3 shows the current–voltage characteristic of the electrodeposited p–n junction Si film under light illumination. A high short circuit current density (J_{sc}) of 21.1 mA cm^{-2} flowed. On the other hand, V_{oc} was much smaller than the desired

value, which might be caused by impurities in Si films. Therefore, further improvement of the electrodeposition method is needed.

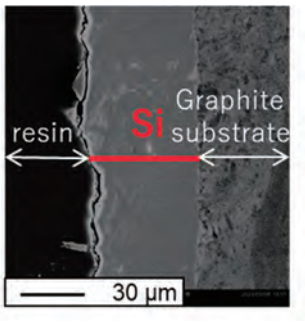

Fig. 2. Cross-sectional SEM image of the electrodeposited p-n junction Si film in KF–KCl molten salt at 1023 K.

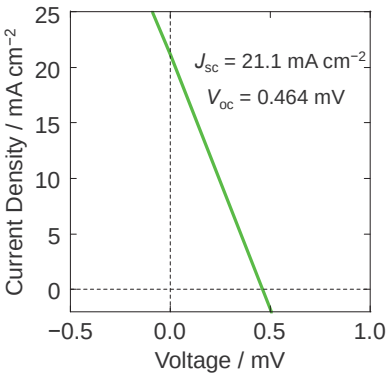

Fig. 3. A current–voltage characteristic of the electrodeposited p-n junction Si film under light illumination.

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

The establishment of carbon neutral society is one of our urgent matters, and large-scaled energy storage devices are required toward the wide spread use of renewable energy. Although current lithium-ion batteries (LIBs) are the candidates owing to their high energy densities, the usage of scarce lithium and cobalt resources and flammable organic solvents are potential barriers to further distribution as large-scaled batteries. Thus, our group has focused on novel rechargeable batteries utilizing abundant sodium and potassium resources as charge carriers and ionic liquids (ILs) as safe electrolytes [7].

We explored the feasibility of dual-carbon batteries, which is composed of carbon-based materials as both positive and negative electrodes [8]. In general, cations and anions are involved with electrode reactions at negative and positive electrodes, respectively. In the case of conventional organic solvent-based electrolytes, several issues remain unsolved such as aluminum corrosion and solvent co-intercalation. In contrast, ILs are composed of only ions, which suppress the depletion of charge carriers and side reactions at the electrode/electrolyte interface.

In this fiscal year, we investigated the anion intercalation/deintercalation behavior of graphite positive electrodes in amide-based ILs containing FSA^- or FTA^- anion (FSA = bis(fluorosulfonyl)amide, FTA = (fluorosulfonyl)(trifluoromethylsulfonyl)amide). As the results of charge–discharge tests of M/graphite (M = Li, Na, K) half-cells using various ILs, K[FTA]–[C_4C_1pyrr][FTA] was found to be a promising electrolyte. Fig. 4 shows charge–discharge curves of graphite positive electrodes in K[FTA]–[C_4C_1pyrr][FTA] IL electrolyte at 298 K. Initial charge and discharge capacities are 115 and 87.6 mAh g^{-1}, respectively, with a coulombic efficiency of 76%. Multistep voltage plateaus are observed, suggesting FTA^- intercalation between graphene layers to form graphite intercalation compounds (GICs). According to X-ray diffraction analysis, stage 1 FTA-GIC was detected at the full-charged state. After the 2nd cycle, the discharge capacities of ca. 90 mAh g^{-1} are maintained up to 50th cycle.

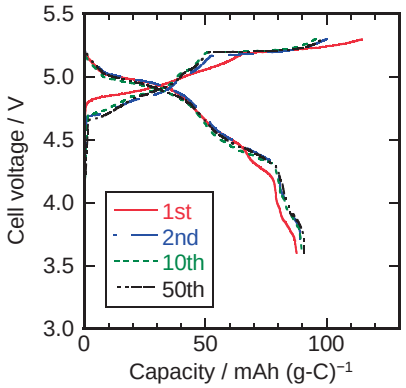

Fig. 4. Charge–discharge curves of K/graphite half-cells in K[FTA]–[C_4C_1pyrr][FTA] IL electrolyte at 20 mA g^{-1} at 298 K.

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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 2022 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. 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-to-tale 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 30V, 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.

5. Manifold dynamic non-covalent interactions for steering molecular assembly and cyclization

Non-covalent interactions that govern many chemical and biological processes are crucial for the design of supramolecular and controlling molecular assemblies and their chemical transformations. However, the characterization of weak interactions in complex molecular architectures at the single-bond level has been a longstanding challenge.

we employed bond-resolved scanning probe microscopy combined with an exhaustive structural search algorithm and quantum chemistry calculations to elucidate multiple non-covalent interactions that control the cohesive molecular clustering of well-designed precursor molecules and their chemical reactions. The presence of two flexible bromo-triphenyl moieties in the precursor leads to the assembly of distinct non-planar dimer and trimer clusters by manifold non-covalent interactions, including hydrogen bonding, halogen bonding, C-H$\cdots\pi$ and lone pair$\cdots\pi$ interactions. The dynamic nature of these weak interactions allows for the transformation of the arrangement of monomers in the assembled clusters as molecular density increases, which alters the reaction pathways in the subsequent on-surface synthesis of cyclized products. Our findings highlight a vital route for controlling on-surface supramolecular assemblies and steering their chemical transformations through the manipulation of manifold dynamic non-covalent interactions.[3]

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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. Nature has developed fantastic solutions to convert solar energy to chemical energy and to utilize them in exceptionally efficient manners for almost 3 billion years. It is our challenge to understand the efficient bioenergetic processes of nature and to construct bio-inspired energy utilization systems. The research interests in our group focus on the design of biomacromolecules and their assemblies for molecular recognition, catalysis, and signal transduction in water, the solvent of life. We take synthetic, organic chemical, biochemical and biophysical approaches to understand biological molecular recognition and chemical reactions. Proteins and protein/nucleic acids 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 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 followings are the main research achievements in the fiscal year 2022.

2. Controlled assembly of fluorophores inside a nanoliposome

Cellular compartmentalization plays an essential role in organizing the complex and multiple biochemical reactions in the cell. An artificial compartment would provide powerful strategies to develop new biochemical tools for material production and diagnosis, but it is still a great challenge to synthesize the compartments that encapsulate materials of interest while controlling their accurate locations, numbers, and stoichiometry. Chemical characteristics of a liposome-encapsulated compartment, which has great potential to locate various materials of interest with precise control of their locations and numbers in the compartment, were evaluated. A nanoliposome was constructed inside a ring-shaped DNA origami skeleton and further equipped with a double-stranded DNA platform to assemble molecules of interest in the nanoliposome (Fig. 1). Upon formation of the nanoliposome, a pH-sensitive fluorophore on the bridged platform showed little or no response to the pH change of the outer buffer, ensuring that the molecules assembled on the platform are effectively shielded from the outer environment. The ring-shaped DNA skeleton equipped with a double-stranded DNA platform allows spatial assembly of several functional molecules inside the nanoliposome to isolate them from the outer environment.

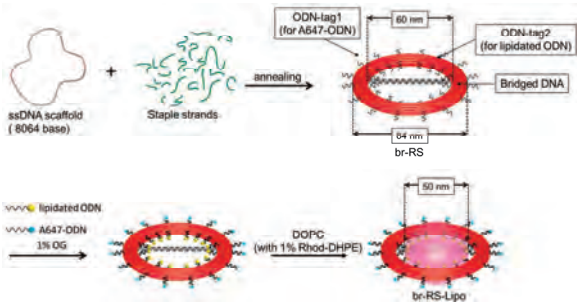

Fig. 1 Design of a bridged ring-shaped DNA origami skeleton that guides formation of a nanoliposome.

3.Dynamic assembly of cascade enzymes by the shape transformation of a DNA scaffold

Within cells, the close spatial arrangement of cascade enzymes facilitates the channeling of intermediates and enhances cascade reaction efficiency. Reconfigurable DNA nanostructures, owing to their structural controllability and precise spatial addressability, are promising tools for mimicking such processes. In this study, a 3D DNA origami scaffold, with a dynamic shape transformation from its open boat form to a closed hexagonal prism induced by toehold-mediated strand displacement, is designed to investigate the enzyme cascade reaction of xylose reductase and xylitol dehydrogenase from D-xylose metabolic pathway. Enzymes are assembled on the DNA scaffold in its open state, which is subsequently closed by the assistance of DNA sequence-specific closing keys. The enzyme cascade efficiency is much higher in the static encapsulated closed state than in the open state due not only to the enzyme proximity but also the environmental factors of 3D DNA structure (Fig. 2 and 3). These results provide novel insights into controlling enzyme

cascade reactions by inducing the shape transformation of DNA nanostructures and how environmental factors affect the action of multi-enzyme complexes in the cell.

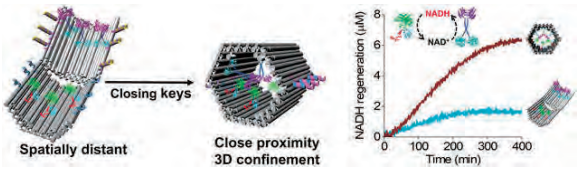

Fig. 2 Schematic representations of the cascade reaction of XR and XDH from a part of xylose metabolic pathway was loaded on 3D DNA scaffold with the shape transformation.

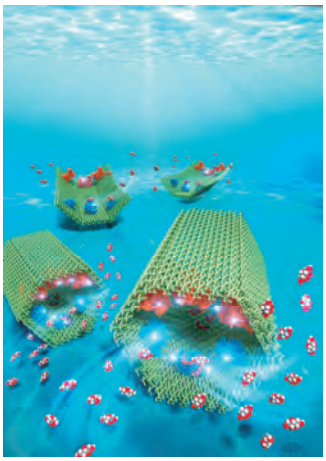

Fig. 3 The image of the cascade reaction of XR and XDH on 3D DNA scaffold with the shape transformation.

4. FRET-based cathepsin probes for simultaneous detection of cathepsin B and D activities

Fluorescent cathepsin probes were prepared by modification of peptidic substrates for cathepsin B (CTSB) and cathepsin D (CTSD) with FRET pairs (Fig. 4). Fluorophores with distinguishable emission characteristics were applied to CTSB and CTSD probes with their appropriate quenchers to simultaneously monitor the activity of CTSB and/or CTSD. Conjugation of both the CTSB and CTSD probes with short single-stranded DNA drastically increased their reactivity to cathepsins over the parent probes possibly by improving their solubility. The activity of CTSB and CTSD were simultaneously detected by using these orthogonal FRET-based cathepsin probes.

Fig. 4 DNA conjugated FRET-based probes for cathepsin B (CTSB) and cathepsin D (CTSD) were designed to simultaneously detect the activity of both cathepsins.

5. A two-step screening to optimize the signal response of an auto-fluorescent protein-based biosensor

Auto-fluorescent protein (AFP)-based biosensors transduce the structural change in their embedded recognition modules induced by recognition/reaction events to fluorescence signal changes of AFP. The lack of detailed structural information on the recognition module often makes it difficult to optimize AFP-based biosensors. To enhance the signal response derived from detecting the putative structural change in the nitric oxide (NO)-sensing segment of transient receptor potential canonical 5 (TRPC5) fused to enhanced green fluorescent protein (EGFP), EGFP-TRPC5, a facile two-step screening strategy, *in silico* first and *in vitro* second, was applied to variants of EGFP-TRPC5 deletion-mutated within the recognition module (Fig. 5). In *in silico* screening, the structural changes of the recognition modules were evaluated as root-mean-square-deviation (RMSD) values, and 10 candidates were efficiently selected from 47 derivatives. Through *in vitro* screening, four mutants were identified that showed a larger change in signal response than the parent EGFP-TRPC5. One mutant in particular, 551-575, showed four times larger change upon reaction with NO and H_2O_2. Furthermore, mutant 551-575 also showed a signal response upon reaction with H_2O_2 in mammalian HEK293 cells, indicating that the mutant has the potential to be applied as a biosensor for cell measurement. Therefore, this two-step screening method effectively allows the selection of AFP-based biosensors with sufficiently enhanced signal responses for application in mammalian cells.

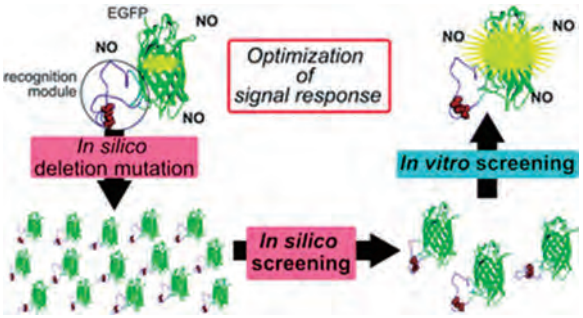

Fig. 5 Schematic representations of a two-step screening to optimize the signal response of AFP based biosensor (NO sensor).

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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 2022.

2. The base-pair opening dynamics of nucleic acids in living human cells

DNA and RNA are polymers having not only genetic information but also functions such as regulating gene expression, catalyzing reactions, and so on. The structure, dynamics, and interactions of nucleic acids, which are related to these funations, might be different under in vitro and cellular conditions. A base pair is a fundamental unit of nucleic acids structures. However, studying the base-pair opening dynamics inside living cells had been challenging. In this study, we investigated the base-pair opening kinetics inside living human cells using the in-cell NMR technique. We determined the exchange rate constant (k_{ex}) of the imino proton involved in hairpin and G-quadruplex (GQ) structures with the proton of solvent water. It was deduced by the obtained k_{ex} values that at least some G-C base pairs of the hairpin structure and all G-G base-pairs of the GQ structure open more frequently in living human cells than in vitro. In vitro NMR analysis using various crowding agents suggested that interactions with endogenous proteins, especially positively charged ones, could be responsible for the increase in frequency of base-pair opening. This study demonstrated a difference in dynamics of nucleic acids between in-cell and in vitro conditions. Finally, we assume that partially unfolded structures that are supposed to be present inside cells can be targeted by drugs. Our in-cell NMR technique can be applied for the development of these drugs.

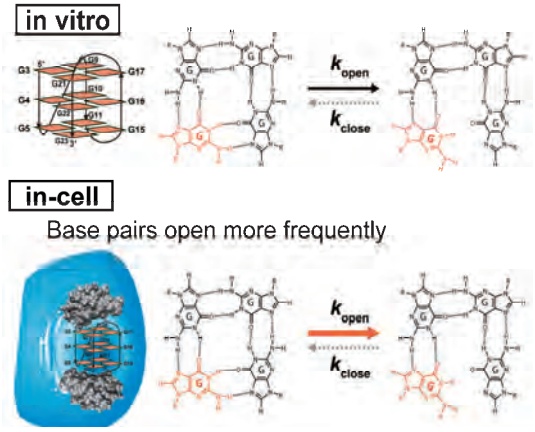

Figure 1. All G-G base-pairs in the GQ structure open more frequently in living cells than *in vitro*.

3. The first heteronuclear 2D in-cell NMR spectra of nucleic acids in living human cells

To investigate the structure, dynamics and interaction of biomolecules in living cells, in-cell NMR is a powerful tool. In in-cell NMR, living cells containing the biomolecule of interest are put into the NMR magnet and the NMR signal of the biomolecule in living cells are directly recorded. We have been developing the methodology of the in-cell NMR for nucleic acids. This year, we succeeded in recording the first heteronuclear 2D in-cell NMR spectra of RNA aptamer. To obtain milligram quantities of ^{13}C, ^{15}N-isotopically labeled RNA cost-effectively, we adopted a tRNA-scaffold system. In this system, the RNA of interest is transcribed in *E. coli* as a chimeric transcript, in which the RNA of interest being inserted into tRNA via two hammerhead (HH) ribozymes. tRNA protects entire RNA from degradation by RNases, while HH ribozymes enable the RNA of interest to be cleaved from the tRNA-scaffold during the purification procedure. The prepared isotopically labeled RNA aptamer for HIV Tat protein was incorporated into living human cells. Then, we successfully recorded the first 2D ^{1}H–^{13}C and ^{1}H–^{15}N HMQC in-cell NMR spectra of the RNA aptamer in complex with the ligand. The development of this methodology has the

following advantages. Firstly, the signals of the introduced nucleic acids can be clearly distinguished from those of the intracellular endogenous molecules and/or of the molecules in the medium. Secondly, in the 2D ^{1}H–^{15}N HMQC and 2D ^{1}H–^{13}C HMQC in-cell NMR spectra, the resolution of the signals of the introduced nucleic acids are improved as compared in the 1D ^{1}H in-cell NMR spectrum. Thirdly, the ^{15}N and ^{13}C chemical shift values of the introduced nucleic acids could be used as new sources to monitor the state of the nucleic acids, in addition to the ^{1}H chemical shift values. Therefore, it is expected that the developed methodology will be widely applied in the field of nucleic acids research.

4. Structure-function relationship of a feruloyl esterase that targets a variety of substrates

Woody biomass comprises cellulose, hemicellulose, and lignin. Hemicellulose is a branched heteropolysaccharide consisting of hexoses and pentoses. Hemicellulose is also linked with modification groups and lignin through covalent bonds. Decomposition and isolation of these components are attractive because they are regarded as valuable biorefinery precursors. Feruloyl esterases (FAEs) are the enzymes that hydrolyze ester bonds connecting hemicellulose with the modification groups and lignin. Fungal FAEs belonging to subfamily (SF) 6 are known to catalyze decomposition of woody biomass and produce ferulic acid derivatives. The molecular mechanisms underlying substrate recognition and catalysis by SF6 FAEs are still elusive. Here, we selected SF6 FAE of *Aspergillus sydowii* (*As*FaeE), which was shown previously to exhibit higher activity towards variety of substrates; most of SF6 FAEs are known to target only a certain substrate. We obtained a recombinant *As*FaeE and investigated the specific activity towards a variety of model substrates. We then determined the crystal structure of

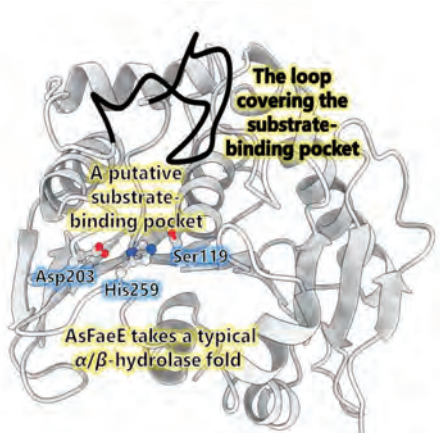

Figure 2. The determined crystal structure of *As*FaeE.

*As*FaeE. *As*FaeE took a typical α/β-hydrolase fold with a canonical serine-histidine-aspartate catalytic triad. *As*FaeE was found to have a loop covering the substrate-binding pocket, which is a unique feature among others; this loop should play a key role in substrate binding and/or recognition. We are currently carrying out structure-based functional mutagenesis and further structural analyses. These studies should give a clue to engineering functionally advanced FAEs in the future.

5. Structure and interaction analysis of human origin recognition complex subunit 1

Human origin recognition complex (hORC) initiates the DNA replication from particular loci in genomes called replication origins. Our previous study suggested that hORC recognizes the replication origin in a G-quadruplex (GQ) structure-dependent manner. However, the mechanism how hORC recognizes a GQ-forming DNA is not clear. Here, we analyzed the interaction between the GQ-binding region of the subunit 1 of hORC, hORC1(GQ), and DNA that forms GQ structure (GQ-DNA). Firstly, we prepared the ^{13}C, ^{15}N-labeled hORC1(GQ) and assigned most amide proton signals by heteronuclear multidimensional NMR experiments. NMR and CD analyses indicated that hORC1(GQ) is mostly disordered in both free and complex with GQ-DNA. The chemical shift perturbation analysis for hORC1(GQ) upon binding of GQ-DNA indicated that the specific basic amino acids and polar amino acids of hORC1(GQ) are responsible for binding GQ-DNA. The obtained structural insight is helpful for understanding how hORC1 recognizes the position of replication origin.

6. Dynamics of DNA in the nucleic acid-nucleic acid condensate

Currently, the condensate of biomolecule, such as a protein and nucleic acid (NA) is an emerging target. Although, there are abundant studies on the protein-protein or protein-nucleic acid condensate, studies on NA-NA condensate is limited. We used one of the reported NA-NA condensate-forming system. In the system, three DNA strands having partially complimentary sequences to each other form Y-shape structure and the base pairs were formed at the ends of Y-shape DNAs. That causes the formation of Y-DNA condensate. We carried out NMR analysis on the dynamics of oligo DNAs forming G-quadruplex structure (GQ-DNA) introduced into the Y-DNA condensate. The translational motion of GQ-DNA inside the Y-DNA condensate was affected by surrounding environment. Interestingly, on the other hand, the rotational motion of GQ-DNA inside the Y-DNA condensate was not affected by the condensate. Our dynamics analysis gives us the spatial information inside the Y-DNA condensate and it is useful to develop the reaction field by NA-NA condensate.

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Self-Assembly Science Research Section

A. Rajendran, Junior Associate Professor

1. Introduction

In recent years, DNA origami has emerged as a novel technique for constructing materials ranging from nano to micrometer scale, with sub-nanometer addressability.[1] This technique has been utilized in various applications, including chemical, biological, and materials science. DNA origami has also been used for organizing enzyme cascades, and studies have shown that it can enhance the efficiency and rate of sequential reactions.[2] However, the use of DNA origami for templating biomass-related enzymes is hindered by their poor stability under various conditions. For example, origami materials tend to melt around 50°C when subjected to thermal treatments.[3,4,5] Furthermore, origami materials such as origami cuboid can break even under mild forces, which are applied during structural analysis by force-based methods such as atomic force microscopy (AFM).[6] Biomass often undergoes chemical pretreatments using strong acids or bases to break down the lignin. 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. The samples can be stored in pure water for several applications.[8] However, the triangular origami exhibits several defective sites in pure water. Additionally, the origami undergoes digestion against nucleases such as DNase I, which is the most abundant nuclease in blood and plasma, either in vitro or in cell culture medium, and T7 endonuclease I. Most origami synthesis buffers contain 5-20 mM Mg^{2+}, as origami cannot be folded without Mg^{2+}. However, when the folded origami is exchanged into an Mg^{2+}-free buffer, its structural integrity changes depending on its super/globular structure and buffer composition. For example, the 6-helix bundle retains its folded structure when exchanged into Tris, Tris-acetic acid-EDTA (TAE), and phosphate buffers, while the 24-helix bundle remains intact only in Tris buffer. Similar results were observed for a tubular origami, which retained its folded structure when exchanged into the crystallization buffers of various proteins, such as HEPES, PEPES, and 2-(N-morpholino)ethanesulfonic acid (MES). The presence of phosphate buffers and EDTA in TAE can competitively replace the origami-bound Mg^{2+}, thereby destabilizing the structure. The structure-dependent denaturation of origami in low magnesium tissue culture medium was also reported. Regarding other cations, origami is unstable in the presence of K^+, Ca^{2+}, and NH_4^+, which are usual supplements in protein crystallization buffers. Overall, these findings indicate that Mg^{2+} is necessary to ensure the folded structure, while the ionic strengths in physiological conditions are much lower than needed to ensure origami stability. The typical Mg^{2+}, Na^+, and K^+ concentrations in cell culture media are 0.04-0.8, 150, and 5.5 mM, respectively, making this environment unsuitable for origami materials. Not only in biological applications, but also in material applications such as spray coating, low magnesium is required. Therefore, it is essential to develop methods to stabilize DNA origami nanomaterials for diverse applications, especially when dealing with enzymes involved in biomass energy conversion.

2. Approaches to increase the stability of DNA origami nanomaterials

The presence of nicks in the phosphate backbone of staple strands is one of the primary reasons for the instability of origami materials. While increasing the length of the staple strands could improve thermal stability, it could also create practical challenges, such as higher synthetic costs, decreased product yield and purity, and limitations on the maximum length of synthetic oligo DNAs. Several methods have been attempted to address the stability issues of origami materials. Some methods that have been reported include photo-cross-linking by 8-methoxypsoralen[3] and the formation of cyclobutane pyrimidine dimers[7] to introduce covalent linkages. However, these methods are not suitable 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. Additionally, coating with lipid bilayers, virus capsids, other proteins, cationic polymers, and spermidine has been attempted. In addition to these non-natural treatments, we have demonstrated the optimal conditions for enzymatic ligation of staple nicks in 2D origami. However, this method resulted in only 31-55% ligation efficiency, and thermal stability improved by only 5-20°C,

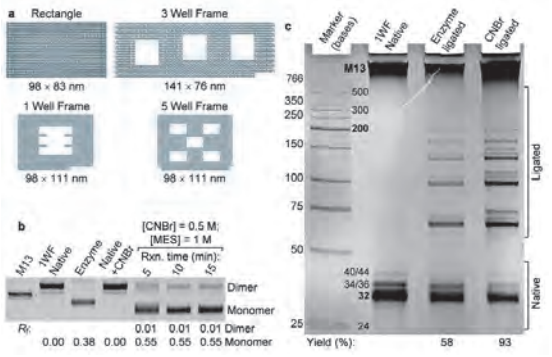

Figure 1. a) DNA origami nanomaterials used in this study. b) Characterization of the chemical ligation by AGE. c) Estimation of the ligation efficiency by PAGE.

depending on the structure. The only other ligation method reported for full-size origami is chemical ligation by *N*-(3-dimethylaminopropyl)-*N'*-ethylcarbodiimide (EDC). Despite being an interesting demonstration, this method requires tedious processes. Batch modification of the 3'-end of all the ~226 staples is necessary, amino-modified ddNTPs and terminal deoxynucleotidyl transferase are required in addition to T4 polynucleotide kinase (PNK), and the method also releases isourea as a by-product. Moreover, this method creates an unnatural backbone linkage with an amino group at each ligation site that can be readily cleaved upon treatment with mild acids. Thus, to improve the stability of DNA origami, we have recently performed enzymatic ligation[9] and cosolvent-assisted enhancement in enzymatic ligation. However, these methods do not work for 3D DNA origami and require overnight for the reaction to complete. Thus, we aimed to perform the chemical ligation of DNA origami. To carry out this research, we collaborated with Prof. Takashi Morii's group at the Biofunctional Chemistry Research Section of the Advanced Energy Utilization Division.

3. Chemical ligation of DNA origami nanomaterials

The chemical ligation process was carried out using CNBr on four different types of 2D square lattice DNA origami, including rectangle (Rec),[1] 1 (1WF),[10] 3 (3WF),[11] and 5 well-frame (5WF),[12] as shown in Figure 1a. Agarose gel electrophoresis (AGE) was used to characterize the ligation reaction. As illustrated in Figure 1b, the chemically ligated origami migrated faster compared to the native and enzymatically ligated origami. This clearly indicates that the chemical ligation method is more efficient compared to the other methods mentioned above. Moreover, the chemical ligation reaction was completed within 5 min, highlighting the advantage over enzymatic ligation, which typically requires overnight reaction time for saturation. To optimize the ligation yield, reaction conditions were carefully adjusted. As a result, the highest possible ligation efficiency, exceeding 90%, was achieved under the optimized conditions (Figure 1c). This ligation method not only improves the thermal stability up to 30ºC but also enhances stability during electrophoresis and subsequent extraction, as well as 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.

4. Conclusions

In summary, our study demonstrates the use of chemical ligation as an efficient method for nick ligation in DNA origami nanomaterials. By optimizing the reaction conditions, we were able to ligate staple nicks in origami with near-quantitative yields. This method was successfully tested on four different 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 this method enhances its stability against thermal treatments, during electrophoresis and purification, as well as providing resistance against nuclease and cell lysate. Overall, our findings suggest that chemical ligation is a highly effective method 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, and on axis undulator field measured at 10 K is shown in fig. 2. This is the world highest level of the periodic magnetic field.

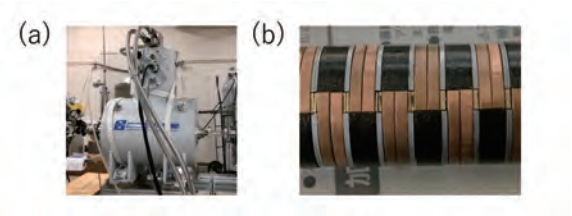

Fig. 1 (a) Photograph of the new unduloator prototype and (b) the new hybrid stacked array.

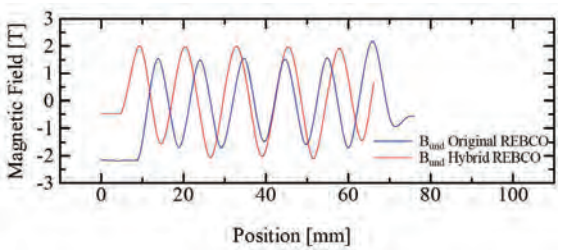

Fig. 2 Unduloator field using the hybrid array of GdBaCuO bulk super conductor and vanadium permendur (red line: Hybrid REBCO) is stronger than that of conventional GdBaCuO bulk superconductor array (blue line: Original REBCO). Fluctuation of peak field strength is slightly reduced.

3. Direct sampling ECE radiometer for investigate avalanching transport in magnetized plasmas

The magnetic confinement nuclear fusion is one of the promising energies to realize a sustainable society. Over many years, the study of plasma confinement has been the central issue of magnetic fusion research. The widely known problem is called power degradation: the degradation of energy confinement time (τ_E) against heating power (P), i.e., $\tau_E \propto P^{-0.6\pm0.1}$. Due to the power degradation, the plasma heating for achieving fusion reaction becomes inefficient. The origin of power degradation is caused by turbulence, which is present a broad range of scales. Although the variety of dynamics due to the nonlinearity of turbulence makes the system complex, the recent studies predict the significant amount of avalanching transport, which is based on the self-organized criticality [1,2]. In this year, we have work on the study of turbulence and avalanching transport in the experimental device, Heliotron J.

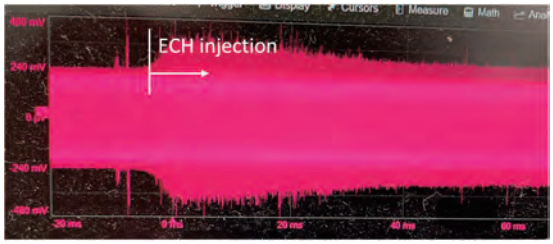

Fig. 3 A waveform of ECE obtained by the GHz sampling DSO.

The electron cyclotron emission (ECE) is one of the promising diagnostics to measure electron plasma temperature (T_e). Because avalanching transport ranges from micro to macro scale, the high spatial resolution is necessary for the measurement. In this year, we tested the direct sampling of the intermediate frequency (IF) of ECE radiometry. This technique has advantages to the previous filter-bank type of radiometer in the point that the spatio-temporal resolution and signal-to-noise ratio (SNR) can be adjusted after the data acquisition [3]. The GHz sampling digital storage oscilloscope (DSO) with a sampling rate of 80GHz, a band width of 36GHz and a record length of 2Gpts are tested for the measurement. At the front-end, the local oscillator of 56GH is used for down-converting the radio frequency (RF) waves to IF with single-side-band. Thus, the RF waves from 56GHz to 98GHz (f_{IF} = 0-36GHz) are simultaneously measured by the DSO (Fig. 3). The relation between spatio-temporal resolution and SNR, which is based on the radiometer equation, was confirmed from the measurement data. We also investigated the effect of noise from electron cyclotron heating (ECH). The correlations between ECH radiation (70GHz) and other IF channels show no-correlation, which indicates the ECE system is not directly suffered by the ECH noise.

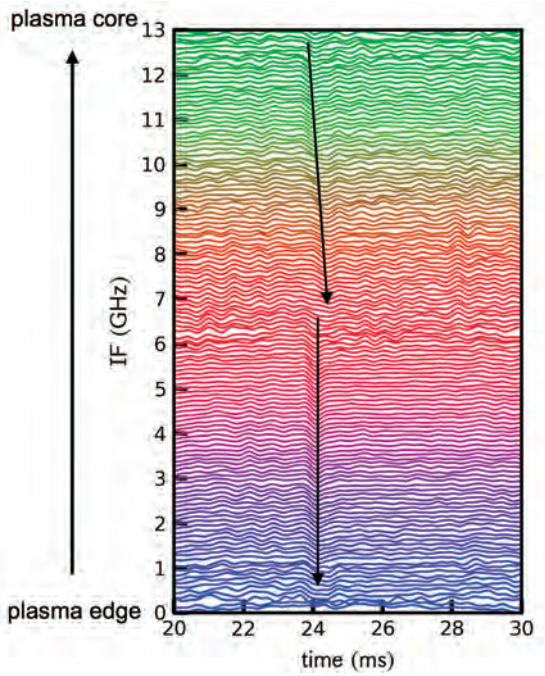

Fig. 4 Temporal evolution of direct sampling ECE radiometer observed in Heliotron J. The large-scale avalanche-like dynamics is indicated as the black arrow.

Figure 4 shows the spatio-temporal evolution of ECE fluctuations. The interval of IF frequency, which corresponds to the spatial location, is set to 0.1 GHz. This is roughly equivalent to the spatial resolution of $\Delta(r/a) \sim 0.008$. As shown in Fig. 4, the large scale (almost half of the plasma radius) of avalanche-like events are shown with slowly propagating (~160 m/s) and rapidly propagating (almost simultaneous) features. The temporal dynamics of avalanches are found as a signature of *1/f* type of ECE spectrum. We also found the *1/f* spectrum is increased against the increases of heating power, which suggest the cause of power degradation.

Acknowledgement

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Environmental Microbiology Research Section

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

1. Introduction

There is a very close relationship between energy resource consumption and environmental protection, becoming an essential research issue for developing a sustainable society. We still heavily rely on fossil energy, and there is concern that emitted greenhouse gases break the harmony of the global environment. Besides, we need a great deal of energy to fix environmental pollution that continues to be the shadow of civilization's progress due to the energy consumption of fossil fuels. As one of the solutions, we will develop a practical method using 'enzymes' derived from environmental microorganisms with high energy utilization efficiency in catabolism. Also, we are remarking on sustainable food production methods, which are the energy of life. We are globally working with academics, biotechs, and university start-ups to network research toward the social implementation of our technologies.

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

Polychlorinated biphenyls (PCBs) are well-known environmental pollutants broadened in all living environments. Biphenyl dioxygenase (BDO) plays a crucial role in the degradation of PCBs. BDO catalyzes the incorporation of two oxygen atoms into the aromatic ring of PCB, which induces the aromatic ring cleavage. Significantly, we developed the composite type of catalytic enzyme consisting of the two BDOs

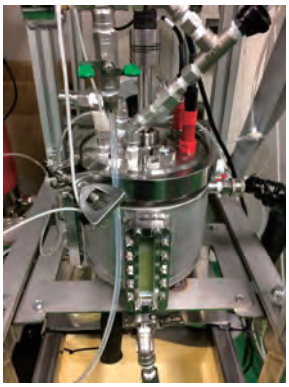

Figure 1. The composite BDOs-microbial catalyst was evaluated in the dedicated experimental bioreactor with the device of oxygen microbubble generation.

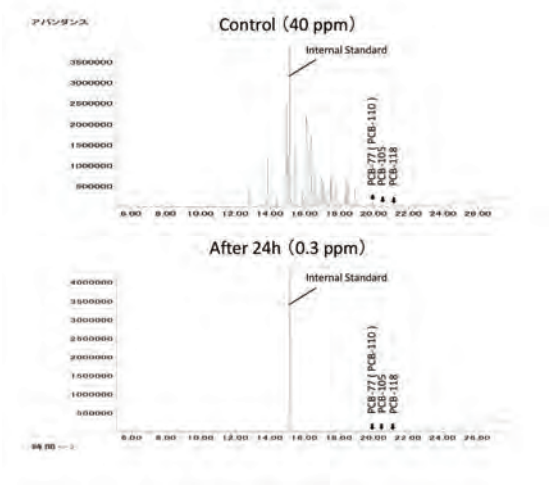

Figure 2. The data from the gas chromatography-quadrupole mass spectrometer showing the PCBs degradation by the composite BDOs-microbial catalyst.

with different substrate specificities; moreover, we developed the bioreactor for generating oxygen microbubbles that enhance the enzymatic activities BDOs (Figure 1). As a result, we succeeded in constructing the practical system that degraded 99.3% of 40 mg L^{-1} of major commercial PCBs (Kenechrol KC-300 and KC-400) in 24 hours (Figure 2). Moreover, this result achieved the waste disposal standard defined by the Ministry of the Environment Government of Japan.

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

To extend further the composite degrading reaction of PCBs, we have been trying to create a unique artificial enzyme that dechlorinates PCBs by two-electron reduction. Here, we collected fresh-water sediments from the contaminated site with PCBs in the Osaka area and investigated whether the bacteria associated with PCBs dechlorination exist. As a result, it was estimated that *Dehalobacter* sp. and *Desulfitobacterium* sp. by 16S rRNA gene phylogenetic analysis. Wang and He (Environ Sci Technol, 2013) reported that '*Deharobacter*' dechlorinates penta-/hexachlorinated biphenyls and '*Desulfitobacterium*'

dechlorinates tetra-chlorinated biphenyls hydroxylated at the para position. We succeeded in preparing the media for growing these particular bacterial species and their cultivation method. Besides, we also observed that these two bacterial species reduce PCBs in the artificial model of the polluted environment. Even today, repeated long-term observation is being made to confirm whether the result is correct.

3-1. Discovery of a novel anti-filamentous fungal protein secreted by *Rhizoctonia solani*.

Rhizoctonia solani is a filamentous fungus belonging to the phylum Basidiomycota and displays a polyxeny plant-necrotizing pathogenicity that is well known to cause severe diseases in many crops, including rice sheath blight which seriously damages paddy-rice production. The infection mechanism of this phytopathogenic filamentous fungus has not yet been fully elucidated, but when wheat bran is added to the growth medium, it is characterized by the secretion of glycosidases that lyse the cell walls of plants and fungi. We discovered a novel protein with a molecular weight of approximately 10 kDa that exhibits anti-filamentous fungal activities in the secretion of *R. solani* cultured with wheat bran as a solid medium. The results were reported for the first time this year 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; moreover, it was suggested that this protein also inhibited conidium formation and germination of *F. fujikuroi*. However, this protein did not inhibit the growth of *Saccharomyces cerevisiae*, a yeast that belongs to the same phylum Ascomycota as *F. fujikuroi* but is different from filamentous fungi. A BLAST search of this protein's partial amino acid sequence revealed by amino acid sequence analysis suggested that it is a protein of unknown function. Likewise, the whole genome sequence of the *R. solani* strain producing this protein was analyzed, and a BLAST search of the deduced full-length amino acid sequence also suggested that it is a protein of unknown function. Based on the above process and sequence analysis of the cDNA encoding this protein, this protein's complete amino acid sequence was 122 residues, and the amino acid sequence of the mature protein, excluding the presumed signal peptide sequence, was 88 residues. As a result, the molecular weight of this protein was estimated to be 9648.24. This mature protein's primary amino acid sequence has a unique structural feature that has never been reported. Specifically, this protein consisting of 88 residues had a double-repeat structure of 41 residues with extremely high homology (92%) across the central 6 amino acid residues. The functional role of such repetitive sequences is generally still poorly understood. We named this anti-filamentous fungal protein "**Double-Repeating Homologous Sequence Anti-Fungal Polypeptide (DRHS-AFP)**."

3-2. Preparation of a recombinant DRHS-AFP and evaluation of its anti-filamentous fungal spectrum.

We constructed a genetically recombinant protein expression system for DRHS-AFP. The DRHS-AFP gene encoding the 88 residues of the mature protein with the additional initiation methionine was amplified by using PCR. Then, the DRHS-AFP expression plasmid, pEp10, was constructed by inserting the DRHS-AFP gene into the *E. coli* expression vector pET-15b and *E. coli* host strain BL21(DE3) was transformed with pEp10. The anti-filamentous fungal activity of the recombinant DRHS-AFP was evaluated against some plant pathogenic filamentous fungi, *F. fujikuroi* (Figure 3), *Fusarium solani*, *Pyricularia oryzae*, *Trichoderma viride* (from the phylum Ascomycota), *Pythium* sp. (the phylum Oomycota), *Rhizoctonia solani* (the phylum Basidiomycota), and *Rhizopus microsporus* (the phylum Zygomycota). As a result, it was shown that the genetically recombinant DRHS-AFP had a growth suppressive effect only on 4 strains of filamentous fungi belonging to the phylum Ascomycota and that the genetically recombinant DRHS-AFP had an anti-filamentous fungal activity comparable to that of the native DRHS-AFP.

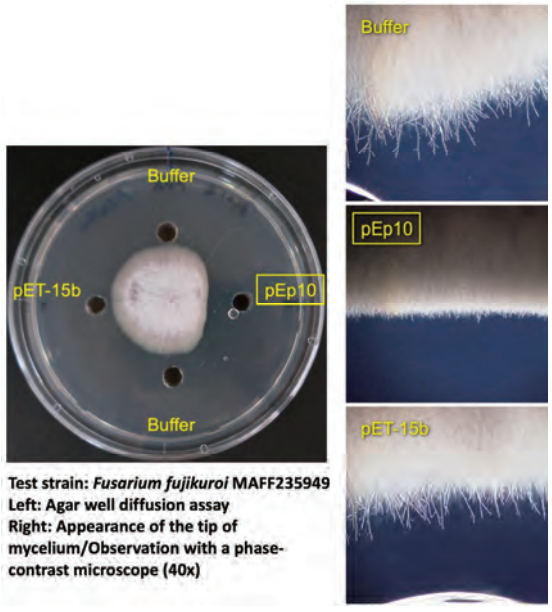

Figure 3. The anti-filamentous fungal activity of genetically recombinant DRHS-AFP.

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Integrated Research Center for Carbon Negative Energy Science

T. Nohira, Professor
K. Kondo, Program-Specific Associate Professor

1. Introduction

To achieve carbon neutrality in 2050, it is necessary to create a new energy system which includes an active carbon dioxide fixation process in addition to "zero emission" technology. In this research center, we are investigating such carbon negative technologies. Specifically, we are engaged in research to convert carbon dioxide into useful materials using renewable energy, biomass, etc.

In this fiscal year, we have investigated the conversion of CO_2 into diamond by molten salt electrochemical process. We have also studied the activity of fungal glucuronoyl esterase to cleave ester linkages in lignin-carbohydrate complex.

2. Conversion of CO_2 into diamond by molten salt electrochemical process

As a carbon negative technology, not only the CO_2 capture and storage (CCS) but also the CO_2 capture and utilization (CCU) will play an important role in the future. Here, electrochemical CO_2 conversion technology in molten salt is considered to be one of the promising candidates for CCU [1,2]. In this study, we aimed to convert CO_2 into diamond, which is one of the most valuable carbon materials. As a first step, we investigated the electrochemical synthesis of diamond in molten LiCl–KCl systems containing K_2CO_3 and KOH, based on the premise that CO_2 dissolves as CO_3^{2-} in molten salts containing O^{2-}. We used micro-Raman spectroscopy and scanning electron microscopy (SEM) to confirm that the deposits obtained by electrolysis were diamond. As a second step, we attempted the electrochemical synthesis of diamond using CO_2 as the actual raw material. Here, we also bubbled H_2O into the molten salt to produce KOH.

Cyclic voltammetry and potentiostatic electrolysis were performed after adding K_2CO_3 and KOH to LiCl–KCl eutectic melts under an Ar atmosphere at 973 K. The working electrode was a Ni flag (Φ 3 × 0.1 mm) or Ni plate (5 mm × 10 mm × 0.1 mm), the counter electrode was a glass-like carbon rod, and the reference electrode was an Ag^+/Ag electrode. The potential was calibrated with Li^+/Li potential. After electrochemical measurements were performed, samples were prepared by potentiostatic electrolysis using the Ni plate electrodes. In the case where CO_2 was used as a raw material, LiCl–KCl eutectic molten salt containing Li_2O was prepared, and CO_2 and H_2O were bubbled into it in predetermined amounts, respectively. After electrochemical measurements, potentiostatic electrolysis was performed to prepare samples. The obtained samples were analyzed by SEM, EDX, and micro-Raman spectroscopy.

First, electrochemical measurements in baths containing only K_2CO_3, only KOH, or both indicated that carbon deposition and hydrogen evolution proceed simultaneously in the potential range more negative than 1.2 V. Then, samples were prepared by potentiostatic electrolysis using Ni plate electrodes at 1.0 to 1.2 V (vs. Li^+/Li). As an example, the surface SEM image of a deposit obtained at 1.1 V is shown in Fig. 1a. The EDX analysis of this area showed that only C and Ni from the substrate were detected. The result of micro-Raman spectroscopy of the sample is shown in Fig. 1b, which shows a spectrum characteristic of diamond with a sharp peak at 1332 cm^{-1}. Based on the results of these three analyses, the electrochemically synthesized angular particles were identified as diamond.

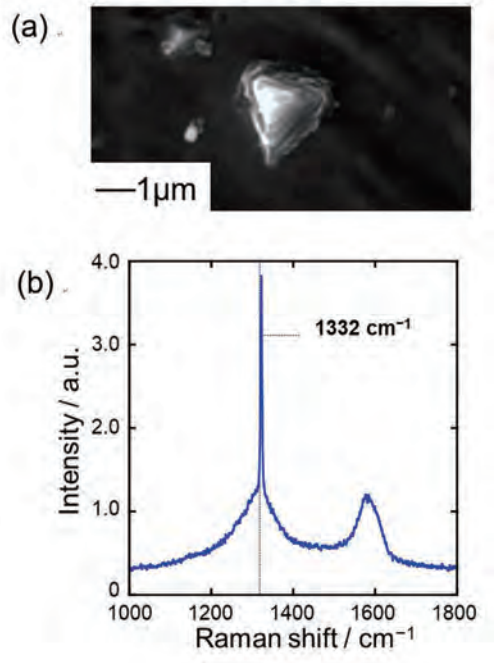

Fig. 1 (a) An SEM image and (b) a Raman spectrum of the sample obtained by potentiostatic electrolysis of a Ni plate electrode in molten LiCl–KCl–K_2CO_3–KOH at 973 K.

Second, CO_2 gas and H_2O gas were introduced in molten LiCl–KCl containing O^{2-} ions. After that, potentiostatic electrolysis was performed at 1.0 to 1.2 V (vs. Li^+/Li). In samples prepared at 1.2 V, we observed a peak at 1332 cm^{-1} attributed to diamond, as well as broad peaks attributed to the D-band and G-band of amorphous carbon. The obtained deposits are considered to be a mixture of diamond and amorphous carbon.

3. Activity of fungal glucuronoyl esterase to cleave ester linkages in lignin-carbohydrate complex

A major component of woody biomass is a lignin-carbohydrate complex which is formed by associations of lignin, hemicellulose, and cellulose. Lignin is an attractive aromatic resource for the production of various materials. Hemicellulose and cellulose can also be utilized to produce biofuels and multiple materials. However, the recalcitrant structure of the lignin-carbohydrate complex is an obstacle to the efficient utilization of woody biomass. In the lignin-carbohydrate complex, the association of lignin and hemicellulose is strengthened by covalent cross-linkages such as ether, ester, and phenyl glycoside linkages. Among these linkages, ester linkages formed between lignin and glucuronoxylan are often found in hardwood biomass, where glucuronoxylan is a main hemicellulose component. Glucuronoyl esterase (GE) is an enzyme that catalyzes the hydrolysis of the ester linkage, thereby weakening the association of lignin and glucuronoxylan (Fig. 2).

We previously identified a fungal GE which exerts high catalytic efficiency toward a model substrate, benzyl glucuronate. Although the GE can be prepared by yeast expression system, its yield (0.16 mg/L-culture) was insufficient for the investigation of GE activity toward natural substrates. This year, we improved the purification procedure for the GE. As a result, the yield of the GE reached 3.65 mg/L-culture. Therefore, a 28-fold increase in the yield was achieved.

We then investigated the activity of the GE toward ester linkage in the natural woody biomass. Firstly, a biomass fraction rich in the ester linkage was extracted from beech wood powder. From the extracted fraction, multiple signals of ester linkage were observed by NMR spectroscopy, which suggested the existence of various structures of lignin or hemicellulose proximal to the ester linkage (Fig. 3a). Next, enzymatic reaction by the GE toward the extracted fraction was performed. Intensities of some ester linkage signals were reduced by the reaction (Fig. 3-2b, labeled with asterisks), which indicated successful cleavage of ester linkages catalyzed by the GE. Exceptionally, the intensity of one ester linkage signal was not changed by the reaction (Fig. 3b, labeled with an arrow head). This result suggested that GE could not cleave the ester linkage giving this signal. The proximal structure of lignin or hemicellulose to this ester linkage may prevent GE activity due to steric hindrance. Our NMR analysis demonstrated the GE activity to cleave ester linkages in the lignin-carbohydrate complex extracted from natural beech wood. In addition, an insight into the preference of substrate structure for GE activity was obtained.

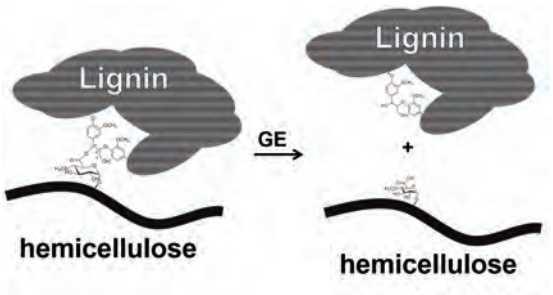

Fig. 2. Cleavage of ester linkage between lignin and hemicellulose.

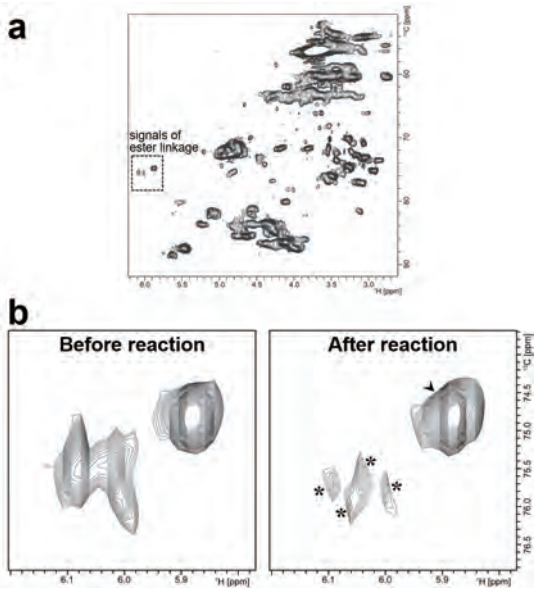

Fig. 3. NMR spectrum of extracted lignin-carbohydrate complex fraction (a) and ester linkage signals before and after the reaction by the GE (b).

Acknowledgement

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Collaboration Works

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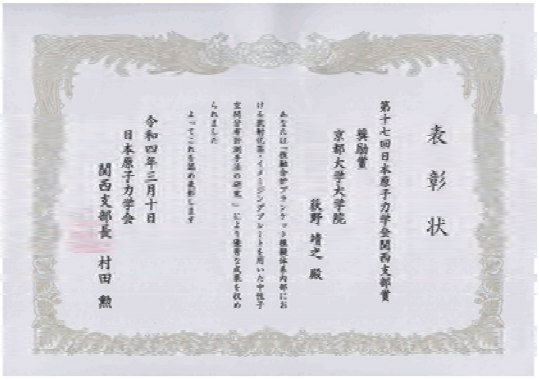
3-2. AWARD

Incentive Award in the 17th AESJ Kansai meeting

Advanced Atomic Energy Research Section
Yasuyuki Ogino (D3)

The 17th Atomic Energy Society of Japan (AESJ) Kansai meeting, which was sponsored by the Kansai Branch of AESJ, was held on 10th March 2022 online. This event provides young researchers and students in the field of nuclear fission and fusion science and engineering and surrounding area an opportunity to present their works.

Mr. Yasuyuki Ogino (D3) attended and made an oral presentation on the title of "Methodology research of neutron distribution measurement inside the fusion blanket mock-up using activation foils and an imaging plate". He presented the method and analysed results of neutron distribution measurement inside the fusion blanket mock-up using various material foils, an imaging plate, and the compact DD fusion neutron source. In this meeting, he received the Incentive Award from the Kansai Branch of AESJ.


表彰状

第十七回日本原子力学会関西支部賞

奨励賞

京都大学大学院

荻野 靖之 殿

令和四年三月十日

日本原子力学会

関西支部長 村田 熱

Poster Award in the 2nd IAE Student Research Presentation meeting

Advanced Atomic Energy Research Section
Fu Nomoto (M2)

The 2nd IAE Student Research Presentation meeting, which was sponsored by the Institute of Advanced Energy (Kyoto University), was held on December 16 (Fri.).

Mr. Fu Nomoto (M2) attended and made a poster presentation on the topic of "Electrochemical purification in fusion liquid blanket (in Japanese)". The following is an overview of presentation.

Liquid lithium lead eutectic alloy (Li–Pb), a candidate of tritium breeding material in a fusion blanket, is easy to contain bismuth (Bi) as an initial impurity or transmutation product from lead (Pb). In this research, an electrochemical method using chloride molten salt was employed to reduce Bi.

He received the Poster Award from Institute of Advanced Energy, Kyoto University. The criteria for judging posters are as follows. 1. Is it easy to understand for people in other fields? 2.Positioning of the research 3. Questions and answers 4. Poster Preview Presentation.

Shimadzu Research Promotion Award (Shimadzu Science Foundation)

Functional Materials Science and Engineering Research Section
Yuhei Miyauchi (Professor)

Professor Yuhei Miyauchi was awarded Shimadzu Research Promotion Award from Shimadzu Science Foundation on February 20th, 2023. The award is given to researchers under the age of 45 belonging to research institutions in Japan who have achieved original results in basic research and applied/practical research in the fields of science and technology, mainly in the area of scientific instrumentation, and whose research is expected to be further developed. He was awarded the award on the achievements of "Measurements of Novel Thermal Effects in Exciton Emission of Carbon Nanotubes".

In his award lecture, which was held on February 20th, 2023 at Hotel Okura Kyoto, he presented his achievements on clarifying mechanism of thermalization suppression and brightening of excitons in carbon nanotubes (CNTs) on dimensionality modification, discovery of thermal up-conversion luminescence phenomena and ultra-narrowband exciton thermal radiation phenomena in CNTs. These achievements opened new opportunities for applications of carbon nanotubes in future quantum photonics, bioimaging, and energy engineering fields.

Iijima Award for Young Scientists in the 63rd Fullerenes-Nanotubes-Graphene General Symposium

Functional Materials Science and Engineering Research Section
Akira Takakura (Program-specific researcher)

In the 63rd Fullerenes-Nanotubes-Graphene General Symposium which was held on August 31st-September 2nd, 2022 at Tokyo Metropolitan University, Dr. Akira Takakura made an oral presentation on the topic of "Efficient coalescence of carbon nanotubes with preserved chiral angles" and he received the Iijima Award for Young Scientists. The award was established by The Fullerenes, Nanotubes and Graphene (FNTG) Research Society in order to recognize superior symposium presentations by young researchers (in principle, 40 years of age or younger).

The 1st Place Award of the Engineering Ceramics Division (ECD) Best Poster Awards (The ECD of The American Ceramic Society)

Functional Materials Science and Engineering Research Section
Hiroyuki Sakai (M2)

The poster "Effect of eutectic reaction on RE-silicate formation by surface modification of SiC" presented during the 46th International Conference on Advanced Ceramics & Composites Virtual Meeting held in January 2022, has received the 1st Place Award of the ECD Best Poster Awards. The award consists of a $500 prize, a certificate and complimentary ACerS Global Graduate Researcher Network (GGRN) membership.

The award ceremonies were held during the plenary session of the 47th International Conference on Advanced Ceramics & Composites, held in Daytona Beach, Florida in January 2023.


The Engineering Ceramics Division
Best Poster Award: First Place
Is Presented To
Hiroyuki Sakai[*1] Tatsuya Hinoki[2]
[*1]Graduate School of Energy Science, Kyoto University, Japan
[2]Open Innovation Institute, Kyoto University, Japan

Award for Distinguished Activitiy (FY2022), Japan Society of Maintenology

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

Dr. Kazunori Morishita was awarded for his many years of distinguished activities from the Japan Society of Maintenology on July 13, 2022. This award is annually given to those who have made a remarkable contribution to the activities of the Society, both in Japan and overseas. It includes contributions to business promotion, business operation, membership services, education related to the maintenology, and human resource development. This year, his continuous research and educational activities on nuclear materials, his great contribution to the extensive management of the society, and also his recent special efforts to establish the West Japan Branch of the society, were highly acclaimed. The award ceremony was held on the first day of the annual meeting of the society held at Kyoto University Clock Tower Centennial Hall.

2022 Distinguished Achievement Award, Materials Scienece and Tehnology Division, Atomic Energy Society of Japan

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

Dr. Kazunori Morishita was awarded for his distinguished research activities from Materials Science and Technology Division, the Atomic Energy Society of Japan. This award is annually given to the member who has made outstanding contributions and achievements in the field of nuclear energy materials research. This year, his many years of great contributions to the research and education on nuclear materials, especially his unique multiscale modeling research efforts to elucidate the irradiation damage process in nuclear materials, were highly acclaimed. The award ceremony was held on September 8, 2022 at the annual division meeting held at Ibaraki University.

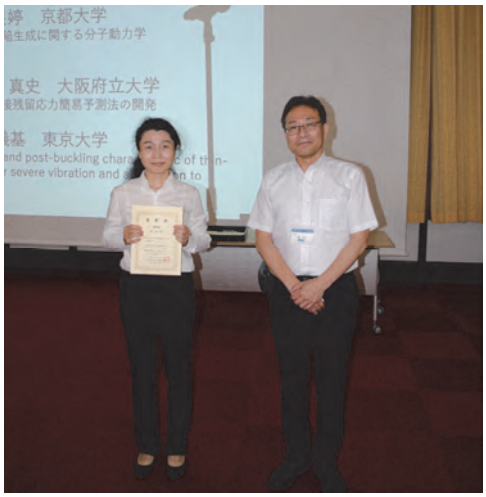

第５回日本原子力学会
材料部会 功績賞
森下 和功 殿
原子炉・核融合炉材料の照射劣化のマルチスケールモデリングに関する教育研究活動
あなたは長年にわたり原子力材料の研究と技術開発において大変優れた成果を上げるとともに材料部会の活動に多大なる貢献をされましたその功績を讃えるとともに今後のさらなる発展を期待して表彰します
令和４年９月８日
一般社団法人日本原子力学会
材料部会長 福元 謙一

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

Advanced Energy Structural Materials Research Section
Yuting Chen (D3)

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 2022 annual meeting of this society held at Kyoto University on July 15, 2022, Ms. Yuting Chen gave the oral and poster presentations on "Molecular dynamics simulation study of non-equilibrium defect formation in iron under Irradiation". Their efforts to find new defect generation mechanisms were highly evaluated, and her presentation eventually won the Student Session Award (“Prize for creativeness”).



Student Session Outstanding Achievement Award in the Japan Society of Maintenology (*Grand prize*)

Advanced Energy Structural Materials Research Section
Zhu Liangfan (D1)

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 2022 annual meeting of this society held at Kyoto University on July 15, 2022, Mr. Liangfan Zhu gave the oral and poster presentations on "Modeling on the formation of solute atom clusters in RPV steel due to irradiation”. Their efforts to explore the new methodology to establish irradiation correlation rules were highly focused, and his presentation eventually won the Student Session Award, “Grand prize”.

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

Advanced Energy Structural Materials Research Section
Yuuki Hamasaki (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 2022 annual meeting of this society held at Kyoto University on July 15, 2022, Mr. Yuuki Hamasaki gave the oral and poster presentations on "Challenges to develop the new device “dister” consisting of a LED and a light receiving element”. Their efforts to explore the new energy device were interested, and his presentation eventually won the Student Session Award (“Prize for encouragement”).

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

Advanced Energy Structural Materials Research Section
Zhu Liangfan (D1)

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 Spring Meeting held at the University of Tokyo, Mr. Zhu made a poster presentation on their effort on “Statistical evaluation of non-equilibrium defect formation in Fe under neutron irradiation”, and received the Student Session Outstanding Achievement Award for their creative research using statistics. (Photo below: Zhu is second from the right in the first row.

2022 Best Figure Prize, Materials Scienece and Technology Division, Atomic Energy Society of Japan

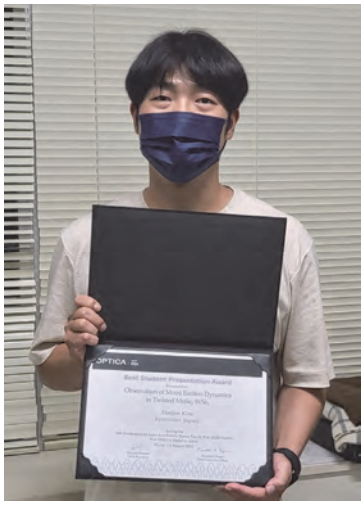
Advanced Energy Structural Materials Research Section
Yuting Chen (D3)

Ms. Yuting Chen was awarded for the 2022 Best Figure Prize from Materials Science and Technology Division, Atomic Energy Society of Japan. This award is annually given to those who have taken academic drawings that are considered to be a great impact on the progress of research on nuclear materials. This year, the movies captured in her molecular dynamics simulations in which the mechanism of athermal defect production in irradiated materials was investigated, were highly acclaimed. The award ceremony was held on March 15, 2023 at the annual division meeting held at the University of Tokyo.

OPTICA Best Student Presentation Award (The 15th Pacific Rim Conference on Lasers and Electro-Optics)

Optical Nano-science Research Section
Heejun Kim (D2)

Mr. Heejun Kim (D2) was awarded OPTICA Best Student Presentation Award in the 15th Pacific Rim Conference on Lasers and Electro-Optics (CLEO Pacific Rim, CLEO-PR 2022) on August 3rd, 2022. The OPTICA Best Student Presentation Award is given to students who have presented outstanding academic results in the field of lasers and electro-optics. He was awarded this prize on the achievements of "Observation of Moire Exciton Dynamics in Twisted $MoSe_2$ - WSe_2 Heterstrobilayer".



Young Scientist Poster Award in the 62th Fullerenes Nanotubes and Graphene Research Society General Symposium

Optical Nano-science Research Section
Duanfei Dong (M2)

Mr. Duanfei Dong (M2) was awarded Young Scientist Poster Award in the 62th Fullerenes Nanotubes and Graphene Research Society General Symposium on September 31th, 2022. The Young Researcher's Award is given to students and young researchers who have presented outstanding academic results in the field of material science of fullerenes, nanotubes and graphene. He was awarded this prize on the achievements of "Electrically tunable moire trions in twisted $WSe_2/MoSe_2$ heterobilayers" from the Fullerenes Nanotubes Graphene General Research Society. He was also selected Nanoscale Horizon Award from the Young Researcher's Award.

Best Student Award in the 13th International Symposium of Advanced Energy Science

Optical Nano-science Research Section
Masafumi Shimasaki (D6)

Mr. Masafumi Shimazaki (D6) was awarded Best Student Award in the 13th International Symposium of Advanced Energy Science on September 6th, 2022. The Best Student's Award is given to students and young researchers who have presented outstanding academic results in the field of advanced energy science. He was awarded this prize on the achievements of "Directional exciton energy transport via asymmetric energy landscape in lateral heteromonolayer WSe_2-$MoSe_2$".


CERTIFICATE
of the Best Student Poster Award
Masafumi Shimasaki

Research Encouragement Award at The 54th Symposium on Molten Salt Chemstry

Chemical Reaction Complex Processes Research Section
Wataru Moteki (D1)

The 54th Molten Salt Symposium, which was organized by the Molten Salt Committee of the Electrochemical Society of Japan, was held on 29th September, 2022. The purpose of this event is to provide researchers and students in molten salt chemistry and related fields with opportunities to present their work and to promote academic and industrial development in the field.

Mr. Wataru Moteki (D1) attended the symposium and made an oral presentation entitled "Electrodeposition of Crystalline Si in Molten KF–KCl–K_2SiF_6 Using Liquid Zn Electrode: Study Using Zn Film Electrodes Prepared on Graphite Plate Substrates by Electrodeposition". He received the Research Encouragement Award.

Student Presentation Award at The 90th ECSJ Spring Meeting

Chemical Reaction Complex Processes Research Section
Wataru Moteki (D1)

The 90th ECSJ Spring Meeting, which was sponsored by the Electrochemical Society of Japan, was held on March 27–29th, 2023. This event provides young researchers and students in the field of electrochemistry and its surrounding area an opportunity to present their works.

Mr. Wataru Moteki (D1) attended and made an oral presentation on the topic of "Electrodeposition of Crystalline Si in Molten KF–KCl–K_2SiF_6 Using Liquid Zn Electrode: Study with Zn Film Electrodes Prepared on Silicon Plate Substrates by Electrodeposition".

He received the Student Presentation Award from the Electrochemical Society of Japan.

4. JOINT USAGE/RESEARCH PROGRAM

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

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

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

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

We propose a new concept of Zero Emission Energy as a typical model of Advanced Energy. IAE Zero Emission Energy Research aims at the realization of environmentally friendly energy system for sustainable society with minimum emission of environmental pollutants and with maximum utilization of energy and resources. Since FY2011, we had operated a project, “Joint Usage/Research Program on Zero Emission Energy”, which is the program authorized by the MEXT. We have started the second term of the Program from FY2016 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 FY2022 Joint Usage/Research collaborations of total 110 subjects (including two workshop) on Zero Emission Energy were performed with more than 350 visiting participants from 31 all-Japan Universities and Institutions including graduate/undergraduate students. Researchers from 5 foreign Universities also participated in the program. The results of these collaborations are summarized in a report "IAE Joint Usage/Research Program on Zero Emission Energy 2022". The meeting to present some of remarkable results obtained in FY2022 was held online on March 10, 2023. If you have interest to this collection, please contact to the Office of Zero Emission Energy Research.

In addition to the Joint Usage/Research collaborations, we organized "Kyoto University 125th Anniversary Commemorative Event, The 13th International Symposium of Advanced Energy Science -Research Activities on Zero-Emission Energy Network-" on September 5–7, 2022. This symposium was held as a hybrid event due to the COVID-19. This symposium consists of oral and ZE poster sessions, and satellite meeting. 324 scientists and students including 5 foreign and 6 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 13th International Symposium

List of Zero Emission Energy Joint Usage/Research Subjects in FY 2022

(Subject, Principal Researcher, IAE Key Person)

NMR approach toward elucidation of superflat aluminum electrodeposition mechanism, Atsushi Kitada, Masato Katahira

Development of Interface Design for Improvement of High Temperature Oxidation Properties of High Melting Point Diborides, Ryuta Kasada, Keisuke Mukai

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

Deactivation of SiC Unpaired Electrons by Hydrogen Termination and the Effects on Anti-corrosion, Sosuke Kondo, Kiyohiro Yabuuchi

Evaluation of irradiation resistance of high entropy compound superconductors, Naoko Oono, Kiyohiro Yabuuchi

Elucidation of redox status-dependent mitochondrial temperature fluctuation towards the development of energy production system mimicking mitochondria, Reiko Sakaguchi, Takashi Morii

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

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

Fermentation of cellulase-aminating reagent via carbon fixation, Minoru Takeda, Masato Katahira

NMR analysis on regulation of the RNA-binding protein TLS-induced phase separation via methylated RNA, Riki Kurokawa, Masato Katahira

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

Combined effect of irradiation and corrosion on hydrogen isotope permeation behavior in functional coatings for fusion reactor blanket, Takumi Chikada, Kiyohiro Yabuuchi

Study of the surface modification layer of lithium ion electrolyte for electrodialysis, Kazuya Sasaki, Keisuke Mukai

Development of a low-density stacked CNT targets and generation of high-pressure gas by the high-power laser irradiation, Ryutaro Matsui, Kazunari Matsuda

Structure control of persistent materials by molecular vibrational excitation, Takayasu Kawasaki, Heishun Zen

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

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

In-vitro investigation of safety and carotenoid-synthesis of Bacillus strains isolated from shrimp gut by whole genome sequencing for development of biomaterials applied in shrimp aquaculture, Nguyen Thi Van Anh, Yumiko Takatsuka

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

Precision analysis of high-reactive β-1 structure in lignin for advanced biomass utilization, Yasuyuki Matsushita, Masato Katahira

Mid-infrared spectroscopy of Zintl-phase NaMgX (X=Bi,Sb) using Free-electron laser, Mamoru Kitaura, Heishun Zen

Structural basis of DNA recognision by the replication initiator ORC, Shou Waga, Masato Katahira

Study on optimization of alloying elements of tungsten alloys for improved irradiation tolerance, Shuhei Nogami, Kiyohiro Yabuuchi

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

Dependence of the hardness increase caused by hydrogenation on irradiation temperature in ion-irradiated tungsten, Koichi Sato, Kiyohiro Yabuuchi

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

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

Study for the development of functional peptides controlling cell proliferation mechanism using NMR method, Hideki Kusunoki, Takashi Nagata

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

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

Research on enzyme-free structural alteration of glycan by infrared free electron laser, Takashi Honda, Heishun Zen

Generation and sustainment of high-energy density plasmas via the interaction between high power laser and structured medium, Yasuaki Kishimoto, Hiroshi Sakaguchi

NMR analysis of artificial biomolecules that regulate the function of biomolecules, Taiichi Sakamoto, Takashi Nagata

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

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

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

Fabrication of functional organic thin films using infrared free electron pulsed laser deposition method, Takashi Nakajima, Heishun Zen

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

Analysis of processing mechanizum in h igh polymer material by using infrared free electron laser, Jun Fujioka, Heishun Zen

Study of solvation structure and dynamics of room-temperature ionic liquids using MIR free-electron laser, Sakhorn Rimjaem, Hideaki Ohgaki

Measurement of scintillation response by fast neutron, Ken Ichi Fushimi, Keisuke Mukai

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

Hydrogen and helium mixed plasma irradiation effects on tungsten materials with rhenium, Yoshio Ueda, Kiyohiro Yabuuchi

Design of physical properties of atomic layer materials by intelayr stacking arrangement, Susumu Okada, Kazunari Matsuda

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

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

Extension of operation regimes for advanced heliotron plasmas using stochastic electrostatic acceleration, Masayuki Yoshikawa, Shinji Kobayashi

Luminescent nanoporous diamond formed by anodization, Kazuhiro Fukami, Hiroshi Sakaguchi

Development of an RNA eiding oligonucleotide to regulate the production and utilization of biological energy, Masatora Fukuda, Takashi Morii

Nondestructive evaluation of residual elastic strain distribution around the interface between non-irradiated areas and ion irradiated area III, Tamaki Shibayama, Kiyohiro Yabuuchi

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

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

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

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

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

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

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

Counting the number of mode-selectively excited phonon by observation of anti-Stokes/Stokes Raman scattering, Kyohei Yoshida, Hideaki Ohgaki

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

Control of humidity sorption in porous molecular crystal by intense infrared rays, Hiroshi Yamagishi, Heishun Zen

Dissolution behavior and spectroscopic measurement of boron compounds in molten salt, Yumi Katasho, Yutaro Norikawa

Hydrogen isotope pick-up and retention in He-exposed W-Mo alloys, Enrique Jimenez Melero, Kiyohiro Yabuuchi

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

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

Impact of nonlinear effect on electron cyclotron current drive (ECCD) in tokamak fusion reactor, Kenji Tobita, Kazunobu Nagasaki

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

Study on living radical polymer production process toward development of highly durable film for lower environmental load, Yusuke Miyake, Hiroshi Sakaguchi

Investigation of wavelength converted thermal radiation based on the vibrationals strong coupling, Tomohiro Fukushima, Taishi Nishihara

Integrated Nano-Calcium Carbonate Enhanced With Rare Earth Phosphates-Lanthanide in Improving Solar Panel Efficiency, Nasrudin Bin Abd Rahim, Hideaki Ohgaki

Surface Modification and Microstructure Control of Magnesium Alloys for Bio-signal Responsiveness, Takeshi Yabutsuka, Kiyohiro Yabuuchi

Synegistic effects of electronic excitation and displacement damage in oxide/nitride ceramics, Kazuhiro Yasuda, Kiyohiro Yabuuchi

Heavy-ion irradiation and post-irradiation annealing effects in explosion-welded CuCrZr/316LN joints for ITER application, Somei Ohnuki, Kiyohiro Yabuuchi

High-Fluence Irradiation Behavior of Reduced Activation Fusion Reactor Materials and its Mechanical Property, Masami Ando, Kiyohiro Yabuuchi

Contribution of infrared laser irradiation to diabetes-related pancreatic dysfunctions, Kazuhiro Nakamura, Heishun Zen

Research and development of enzymatic activity control using VHH antibody, Akifumi Takaori, Takashi Nagata

Study of PV Hybrid Energy Systems for Rural Electrification in Cambodia, Vannak Vai, Hideaki Ohgaki

Study of phonon and thermal proerties of moire super lattice composed of layred materials, Shinichiro Mouri, Kazunari Matsuda

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

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

Comparative study for antimicrobial activities among antimicrobial cyclic lipopeptide fengycin analogs, Kenji Yokota, Tomijiro Hara

Study of optical property of atomically thin layered materials using near-field scanning optical microscope, Masaru Sakai, Kazunari Matsuda

Study on advanced ICT-based maintetance technology for zero-emmission energy infrastructure, Hidekazu Yoshikawa, Kazunori Morishita

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

Mechanical property evaluation of solid-state welded ODS alloys, Sanghoon Noh, Kiyohiro Yabuuchi

Hydrogen pickup of ion irradiated Zry alloys, Hideo Watanabe, Kiyohiro Yabuuchi

Evaluation of oxide formation process in alloy powder of high chromium ODS steels, Noriyuki Iwata, Kiyohiro Yabuuchi

Elucidation of the shrimp growth promoting mechanisms of dietary supplementation with Bacillus spores, Tsuyoshi Ohira, Tomijiro Hara

Supramolecular assembling regulation of bacterial cell division protein FtsZ on DNA nanostructures, Akira Onoda, Eiji Nakata

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

Development of Design Methods for Leading Small Molecules by RNA Aptamers, Yousuke Katsuda, Takashi Morii

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

Analysis of reaction meachanism of haloacid dehalogenase, Takashi Nakamura, Takashi Morii

Developmental research on microbial community structure analysis and biopest applications in medicinal plant cultivation, Makoto Ueno, Tomijiro Hara

Small scale water purifier system for pesticides removal: case study hill tribe at Chang Rai province, Thailand, Pannipha Dokmaingam, Hideaki Ohgaki

Evaluation of thermal resistance at the interface of candidate materials for fusion reactor divertor, Masafumi Akiyoshi, Kiyohiro Yabuuchi

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

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

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

Fluorescenct analyses of biomolecules and metals through signal amplification system, Ippei Takashima, Eiji Nakata

Interation of LHD divertor plasma and irradiated tungsten, Mingzhong Zhao, Kiyohiro Yabuuchi

Radial Correlation Analysis on Edge Plasma Tubulence in a Toroidal Plasma and Its Dependence on Plasma Confituration, Yoshihiko Nagashima, Shinsuke Ohshima

The effect of ion beam irradiation on the properties of hevily doped nanocrystals, Masanori Sakamoto, Kiyohiro Yabuuchi

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

Ionic conduction mechanism of lithium ion conductive LAGP-$LaPO_4$ composite, Shigeomi Takai, Takashi Morii

Effect of FEL irradiation on the efficiency of carbon dioxide fixation in bacterial cells, Tetsuro Kono, Hideaki Ohgaki

Analyses of Electroretinograms from Crayfish's Compound Eyes Evoked by KU-FEL Irradiation-2: Fast and Late Reaction, Fumio Shishikura, 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

Investigation for expeirimental simulation of space plasmas using magnetically confined configurations, Kenichi Nagaoka, Shinji Kobayashi

Public outreach activity of advanced energy science for carbon neutral, Hidekazu Yoshikawa, 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 2022, although the pandemic of COVID-19 still had a significant impact on the actual implementation of the collaborative activity, strong advancement of the collaboration was achieved.

Despite the difficulty in organizing the cooperative research program, however, 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. Although reduction of the risk of the infection was given the highest priority, 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, Solar Simulator, KU-FEL and various laser systems.

2. The cooperative research program

In the fiscal year of 2022, 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 FY2022 is shown in the next page.

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

The whole sum 5

Category			Total
A1	A2	A3	
4	1	4	9

The individual research subjects are as follows.

Supporting Activities on International and Industrial Collaborative Research

A1

"Organization of the 22nd young research seminar on NMR"

・ Y. Yamaoki, M. Katahira, T. Nagata, K. Kondo (Inst. Adv. Energy, Kyoto Univ.)

"Support of 11th International Workshop on Infrared Microscopy and Spectroscopy with Accelerator Based Sources (WIRMS2022)"

・ H. Zen, H. Ohgaki, T. Kii (Inst. Adv. Energy, Kyoto Univ.)
・ Y. Ikemoto (JASRI)
・ S. Kimura (Osaka Univ.)
・ E. Okamura (Kobe Univ.)
・ A. Paarmman (Fritz Haber Institute)
・ P. Dumas (Soleil Synchrotron)

"Support of the collaboration research on "Occurrence and Characteristics of Microplastic Waste from Surface Roadside Soil in Selected Areas of Mon State" invited by the JSPS Core to Core program, "Kansai-Asia Platform of Advanced Analytical Technologies (KAPLAT)"

・ T. Morii, E. Nakata, L. Peng, H. Ohgaki (Inst. Adv. Energy, Kyoto Univ.)
・ M.T. Tawng (Department of Chemistry, University of Yangon)

"Support for the collaborative activity on fusion plasma and energy science between Japan and Thailand"

・ K. Nagasaki, H. Ohgaki, S. Inagaki (Inst. Adv. Energy, Kyoto Univ.)
・ T. Onjun, S. Dangtip (Thailand Institute of Nuclear Technology).
・ S. Pivsa-art, S. Pavasupree (Rajamangala University of Technology Thanyaburi)

Cooperative Research

A2

"Identification of polarization of radiation from energetic electrons in a laboratory magnetized plasma"

・ S. Inagaki, S. Kobayashi, K. Nagasaki, H. Ohgaki, T. Kii (Inst. Adv. Energy, Kyoto Univ.)

Sprouting Research

A3

"Mechanistic aspects for the modulation of scaffolded enzyme activity on DNA nanostructures"

・ L. Peng, T. Morii, E. Nakata (Inst. Adv. Energy, Kyoto Univ.)
・ M. Nakabayashi, Y. Hui (Grad. Sch. Energy Sci., Kyoto Univ.)

"Energy flux control of nanocomposite materials for non-concentrated sunlight utilization"

・ T. Nishihara (Inst. Adv. Energy, Kyoto Univ.)

"Improvement of in-cell NMR technique utilizing isotopic labeling and dynamic nuclear polarization"

・ Y. Yamaoki, M. Katahira, T. Nagata (Inst. Adv. Energy, Kyoto Univ.)

"On- surface synthesis of asymmetric graphene nanoribbon at low temperature for energy conversion material"

・ T. Kojima (Inst. Adv. Energy, Kyoto Univ.)

The Laboratory Seminars

Laboratory Seminars

The Laboratory promotes topical academic seminars in order to strengthen the research activities in each research section and to enhance the mutual cooperation among a lot of academic fields. In the fiscal year of 2022 the aims and progress reports of five cooperative researches were presented and discussed, as summarized below. The Laboratory also planned a symposium on April 7, 2023 for presentation of the cooperative research results in FY2022.

(1) July 25, 2022
S. Inagaki
"Understanding the Universe with Millimeter Waves Radiated by High-Energy Electrons "
Inst. Adv. Energy, Kyoto Univ.

(2) August 31, 2022
L. Peng
"Mechanistic aspects for the modulation of scaffolded enzyme activity on DNA scaffold"
Inst. Adv. Energy, Kyoto Univ.

(3) September 21, 2022
T. Nishihara
"Energy flux control of nanocomposite materials for non-concentrated sunlight utilization"
Inst. Adv. Energy, Kyoto Univ.

(4) October 19, 2022
Y. Yamaoki
"Improvement of in-cell NMR technique utilizing isotopic labeling and dynamic nuclear polarization"
Inst. Adv. Energy, Kyoto Univ.

(5) February 15, 2023
T. Kojima
"Vectorial on-surface synthesis of polar 2D graphene nanoribbon crystals"
Inst. Adv. Energy, Kyoto Univ

6. INTEGRATED RESEARCH CENTER FOR CARBON NEGATIVE SCEINCE

2022 Activities

Introduction

The center was established on August 2022 to promote research on Carbon Negative Science to accelerate the Carbon Neutral Society in 2050. Until now, the balance between emissions and absorption of carbon dioxide has been maintained. But rapid human activity since the Industrial Revolution has led to an imbalance between emissions and absorption of carbon dioxide and carbon dioxide mission has become excessive that causes serious impact on our planet, climate change. To return to a balanced state, it will be difficult to achieve with "Zero Emission" technology alone. It is necessary to create a new energy system by introducing more aggressive carbon dioxide fixation processes. The Integrated Research Center for Carbon Negative Science will work to develop such new carbon dioxide fixation technologies in collaboration with the Graduate School of Engineering and the Graduate School of Energy Science at Kyoto University. Among several carbon dioxide fixation technologies, the center focuses on 1) Solar Energy Utilization for CO_2 Capture and Conversion, 2) Conversion of CO_2 into Useful Substances, and 3) Biological Utilization of CO_2.

The Center will also work on human resource development for “Carbon Negative Energy”, which is a new concept at this time.

In this line, we set up three research projects, 1) Solar Energy Utilization for CO_2 Capture and Conversion, 2) Conversion of CO_2 into Useful Substances, 3) Biological Utilization of CO_2, and preparation of the education system of “Carbon Negative Energy” in this year.

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. Upcoming research projects of this group include studies on thermo-photophysical properties of nanocarbons for solar energy applications, effective use of long wavelength light using MIR-FEL, application of laser/light to highly efficient hydrogen production, photonics and its energy applications based on nanoscience, vectorial on-surface synthesis of 2D polymer crystal as high-performance energy materials, and materials design of metal-doped catalysts for conversion of parabens and/or other compounds. All these diverse projects aim to realize new energy conversion systems using solar energy.

2. Conversion of CO_2 into Useful Substances

In this project group, we aim to convert CO_2 into useful substances. As a conversion method, we are particularly interested in electrochemical methods. For example, when molten salts are used as electrolytes, there is the potential to convert CO_2 into a variety of value-added carbon materials, such as diamonds, carbon nanotubes, and graphite. Also, when aqueous solutions, organic solvents, or ionic liquids are used as electrolytes, CO_2 can be converted into methane, ethylene, and other products. We are studying the optimal electrolyte composition, temperature, electrolysis conditions, etc. to produce the objective value-added materials more selectively, more efficiently, and faster. We also aim to elucidate the reaction mechanism to develop appropriate electrocatalysts and novel electrolysis methods.

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. The scope of the research is wide, and includes 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. Membranes, reactors and processes are being developed to enhance biomass utilization and develop efficient biorefineries. The identification of new microbial enzymes or metabolic pathways that can contribute to CO_2-fixation is also a major goal. Although the individual groups may specialize in diverse areas of research, they share common goals, and collaborative research is ongoing to contribute towards developing a bio-based society.

4. Education Activity

This group reformed the existing undergraduate class, “Advanced Energy Science” to adopt the Carbon Negative Energy concept. The new lecture series will start in the 2nd semester of 2023. As the graduate level lecture course, the Graduate School of Energy Science prepared the “Socio-Environmental Energy Science I and II” to include “Carbon Negative Energy” in this year. We also advertise the concept of “Carbon Negative Energy” to the visitors to the institute.

5. Other activities

The center secured the collaborative research rooms, etc. and started maintaining the research infrastructures and equipment in the main building at Uji Campus. Specifically, they are Laboratory 1-5,

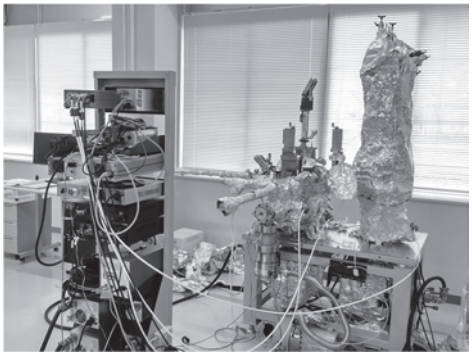


Fig. 1-1 STM

Fig. 1-2 GC-MS

Fig. 1-3 Waiting Room

Waiting Room 1-2, and Program-Specific Associate Professor's Room. The equipment includes STM, GC-MS, digital microscope, etc. as shown in Fig. 1-1, 1-2, 1-3.

ICaNS Events

June: Abbreviated name ICaNS and the logo was decided
September 28 1st Steering Committee meeting
October 1: Appointed to a full time and concurrent professors
October 1: Program-Specific Associate Professor was appointed.
October 8: Opening Ceremony
March 10, 2023: Annual Activity Report Meeting

7. PROJECT 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) Confinement improvement by hydrogen pellet injection, (3) relation between structure formation and plasma fluctuations in the core and peripheral region, (4) physics mechanism of hydrogen pellet ablation, (5) optimization of particle supply and heating scenario, (6) development of new technology in experiment and analysis.

Two results from this collaboration research in FY2022 are shortly reported below. The annual report for all the collaboration subjects in this program will be published by NIFS.

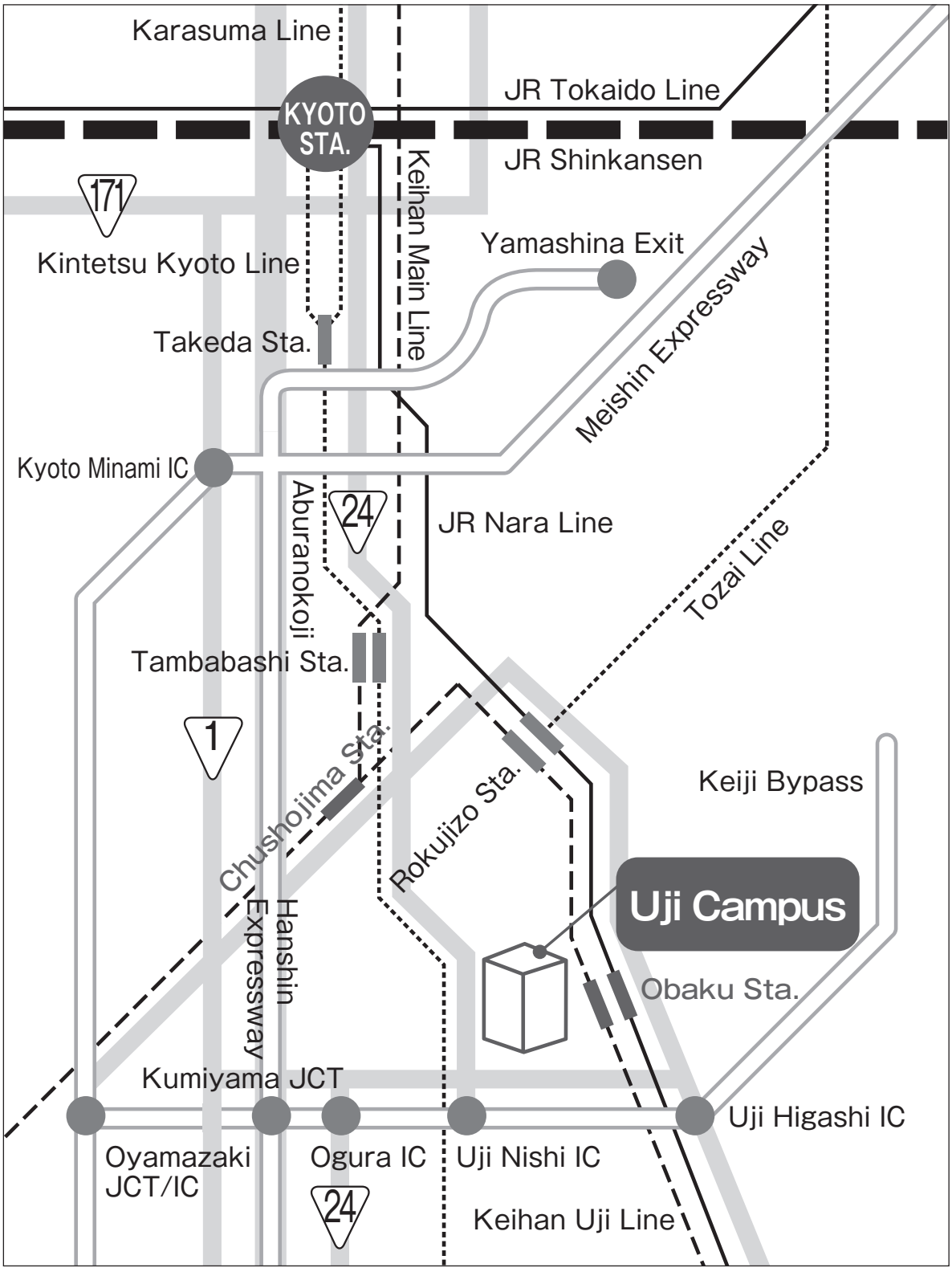
Magnetic configuration control for energy confinement: The energy confinement dependence on rotational conversion in Heliotron J shows a negative trend, which is inconsistent with the ISS04 scaling. As an indicator of neoclassical transport, the stored energy is studied against the effective helical ripple ε_{eff}. Although a negative dependence on ε_{eff} appears, such a dependence may be determined by a result at the lowest ε_{eff} configuration. If we exclude this configuration result, we obtain a weak regression with a evaluation coefficient of R^2~0.2, which means that the data for most of the configurations cannot be explained by ε_{eff}. The contribution of turbulent transport is under evaluation.

Control of the rotational transformation can change the position and width of magnetic islands produced at the rational surface. The period of the magnetic island structure (m/n=7/4, 8/4, 9/4) can also be controlled by the rotational transform. When the magnetic island is shifted from the periphery to the core region, the confinement degradation is clearly visible in a certain range. A ultra-high-resolution ECE measured with a recently introduced ultra-fast oscilloscope in the GHz band enable us to observe the response to modulated ECH in the magnetic island configuration. Probe measurements of the fluctuations at the magnetic island and electric field measurements using a Doppler reflectometer are also in progress.

In the magnetic configuration control experiments, a principal component analysis has been applied to study the relation among the parameters that characterize the confinement. The bumpiness scan experiment can be summarized as follows: the first component (PC1) is the plasma volume, the second one (PC2) is the rotational transform, and the third one (PC3) is a parameter related to bumpiness. This means that the rotational transform scan experiments can be controlled independently of the bumpiness and aspect ratio. This method will be a useful tool for analyzing the results of configuration control experiments in which many configuration parameters are interdependent.

Physics mechanism during hydrogen pellet ablation: The density of pellet ablation cloud can be measured from the Stark broadening of the emission lines of the Balmer series, which is the emission of hydrogen. In the near-infrared region, the Zeeman effect on the Doppler broadening and the Stark broadening are relatively large compared to the visible region, and this can be a particularly useful tool for medium-sized devices such as Heliotron J. The polarization separation measurement of helium atoms by Zeeman spectroscopy has been proved to be a useful tool. For Stark broadening, in addition to the conventional emission of H_β lines in the visible region, the Pa-α lines of the Paschen series in the near-infrared region have been used. The Stark broadening of the emission from the dissolved cloud passing through the line of sight has been measured using a small, simple near-infrared spectrometer, and is found to be slightly above the lower limit of the spectrometer ($< 4\times10^{21}$ m^{-3}), which is about two orders of magnitude smaller than a reported value (~10^{23} m^{-3}) in LHD. This means that measurements using multiple bandpass filters with different transparent bands are not applicable, suggesting the need for a different approach. Currently, we are developing i) a fast spectroscopy system to spatially track the density of the dissolved cloud through fast spectroscopy of the Stark broadening of the visible H_β line with increased resolution and using a high-speed camera, ii) a high-dispersion near-infrared spectroscopic diagnostic to simultaneously determine the Zeeman splitting, Stark broadening, and Doppler broadening, and iii) a near-infrared emission line intensity ratios to estimate the electron temperature of the ablation cloud.

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
http: //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