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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

2020

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CONTENTS

FOREWORD

The Institute of Advanced Energy was established in May 1996 for the purpose of exploring the next-generation energy by probing into the laws and basic principles of nature, and of developing the state-of-the-art technologies to utilize them for practical applications. For this purpose, 14 sections of research areas are organized as three divisions, each dedicated to one of the three basic kinds of energy processes: generation, conversion, and utilization of energy. On top of this, we set up the Laboratory for Complex Energy Processes which also includes 3 sections of research areas. This laboratory organically integrates all the disciplines to enable us to tackle complex energy related issues. Furthermore, we actively promote the internationalization of research and return the fruits of our research back into society incorporating with industry–academia–government collaboration. The institute is also in charge of the Graduate School of Energy Science's Cooperating Chair, which conducts student education and trains researchers in a leading-edge research environment.

The Institute of Advanced Energy focuses on two core research areas: "Plasma and Quantum Energy Science" and "Soft Energy Science". The first topic deals with the generation of energy by nuclear fusion on Earth, which is equivalent to that created in the Sun. The second topic addresses the development of methods for highly efficient energy based on the principles of biology and materials science, which has created the biosphere in the Earth's environment.

The Institute has coordinated these phenomena in the wide energy range to create a new energy philosophy incorporated with that referred to as "Zero-Emission Energy". We collaborate with researchers across a broad range of academic fields in Joint Usage/Research Center programs. We hope to develop the breakthrough of energy that will lead the 21st century through the active merging of research in the wide energy range, like the creation of beautiful patterns of fabric interwoven from threads of various forms and shapes.

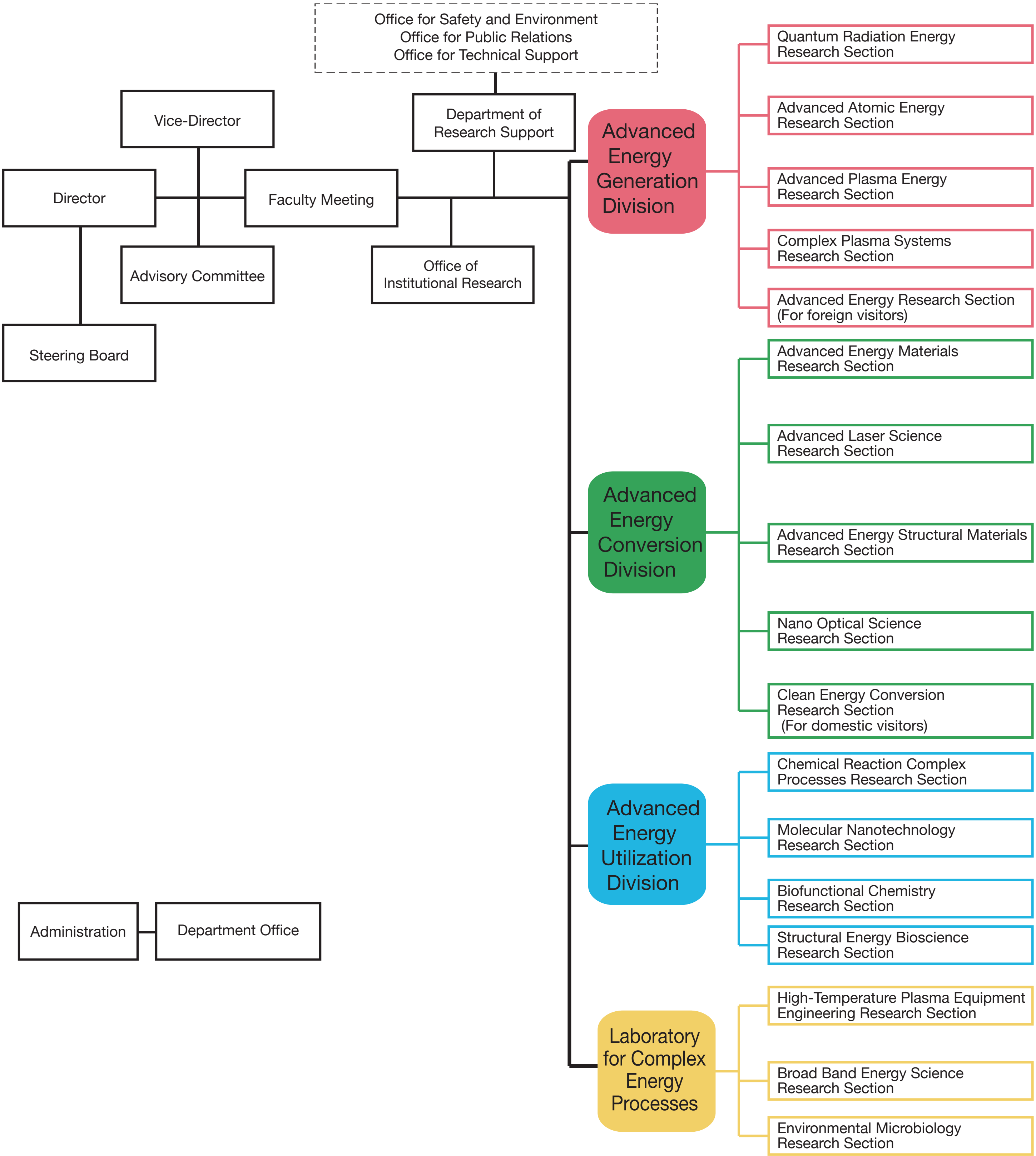
This annual report summarizes the IAE's research findings for FY2020 (April 2020-March 2021). Due to the space limitation, only key results including publication and presentation performed in the year in each division and research section, and also in Laboratory for Complex Energy Processes are edited. Please contact to each researcher for more detail information.

This year, the spread of COVID-19 has caused confusion in society and severely restricted research activities at the university. However, in spite of this tough situation, we have achieved many results. I would like to thank all of you for your cooperation and support. We hope that we will overcome COVID-19 next year and greatly promote exchanges with everyone.

March 2021

Yasuaki KISHIMOTO
Director
Institute of Advanced Energy
Kyoto University

2. ORGANIZATION CHART



3. RESEARCH ACTIVITIES

3-1. RESEARCH ACTIVITIES IN 2020

Quantum Radiation Energy Research Section

H. Ohgaki, Professor
T. Kii, Associate Professor
H. Zen, Assistant Professor
J. 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 a 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. A 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 turn-ability 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 40 mJ in a 2-μs macro-pulse at the wavelength of 4.9 μm. The FEL is routinely operated and opened for internal and external users.

Another topic of KU-FEL development is introduction of photo-cathode RF gun, which enables to generate higher peak power and wider tunable range MIR-FEL. Development of a UV-laser system for illuminating photo-cathode has been completed under collaboration with Dr. R. Kuroda, Researcher of AIST. In FY2014, we have achieved FEL lasing with photo-electron beam generated from LaB_6 cathode. In FY2018, the laser system has been upgraded under the Q-LEAP project organized by MEXT. This upgrade increases the macro-pulse duration of the photocathode operation. Under the photocathode operation, the world highest extraction efficiency of the oscillator-type FEL has been achieved.

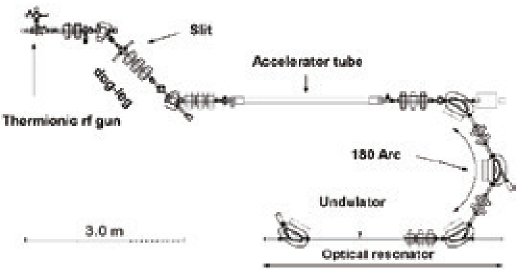


Fig. 1 Schematic drawing of the KU-FEL

2.2 THz Coherent Undulator Radiation Source

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

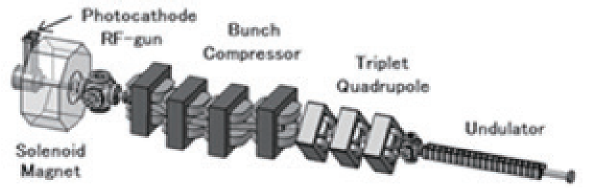


Fig. 2 3D image of THz coherent undulator radiation source.

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 space charge effect can be successfully 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 has been performed under the Joint Usage/Research Center for Zero Emission Energy Research of our Institute. In JFY2020, 14 external user groups used KU-FEL.

3. Bulk HTSC 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. Magnetic performance of bulk MgB_2 sample was measured using a new solenoid and a magnetic field scanner as shown in fig. 3.

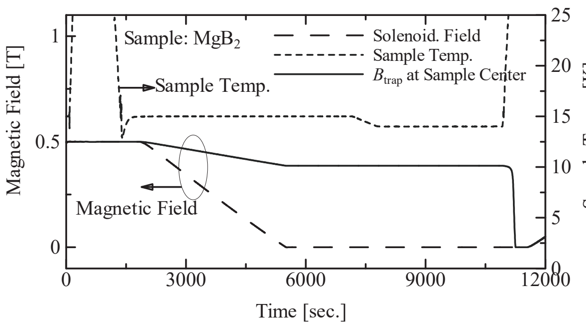


Fig. 3 Trapped magnetic field of MgB_2 sample.

4. Isotope Imaging for Nuclear Security

A Nuclear Resonance Fluorescence (NRF) method is a powerful tool for an isotope selective imaging. In 2020, we tried to obtain a 3D image of the CT target, which consists of two enriched isotope targets, ^{206}Pb (>93.3%) and ^{208}Pb (>97.8%), with an aluminum target holder. The LCS gamma-ray beam with a maximum energy of 5.528 MeV and a 10 photon$\cdot s^{-1}\cdot eV^{-1}$ flux density was developed

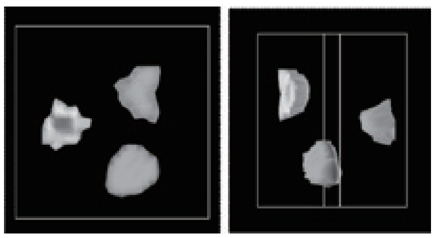


Fig. 4 3D NRF-CT image.

in UVSOR. The NRF transmission technique was employed. The transmission gamma-rays have also been measured to give a density distribution of the sample target at the same time. After suppressing the non-resonant absorption process, the NRF-CT images, which indicate the distributions of ^{208}Pb, were obtained as shown in Fig. 4.

5. Study on Social Aspect of Renewable Energy

Electrification projects using renewables in rural settings are essential to achieve SDG7. These projects can positively influence several other aspects of community development. Our group investigates the effects of electrification in rural contexts of ASEAN region comparing the process and outcomes of different electrification systems.

Fig. 5 Case studies since 2016

Our group has conceived a novel method to evaluate the social impact of electrification in SEA using quality of life (QoL) measures. With this approach, we assessed the conditions prior and after electrification in communities in Malaysia, Cambodia, Myanmar, Indonesia and The Philippines (Fig. 5). We also study on the relation between energy services and human well-beings in Japanese and Mexican communities.

Acknowledgment

These works were partially supported by the KAKENHI, Q-LEAP(MEXT), JASTIP(JST), UVSOR Collaboration Research, Heiwa Nakajima Foundation, Hitachi Zaidan, DASUnit, Kyoto University, and the Laboratory for Complex Energy Processes Collaboration Research, IAE.

Collaboration Works

大垣英明，University of Malaya（マレーシア），倉田奨励基金：「Before and After 手法による東南アジアにおける非電化地区への再生可能エネルギー導入の住民生活に与える影響に関する研究」

大垣英明，NSTDA（タイ），JASTIP，WP2

大垣英明，University of Malaya（マレーシア），JASTIP-net

大垣英明，Jordi Cravioto，NSTDA（タイ），JAPAN-ASEAN Science and Technology Innovation Platform, Energy and Environment field

大垣英明，Jordi Cravioto，University of Malaya（マレーシア），Theoretical and Experimental Investigation of Battery Dimensioning for Rural Electrification based on Segmented Quality of Life Progressions of Rural Communities in Malaysia

大垣英明，森井孝，片平正人，野平俊之，モンゴル国立大学，インドネシア大学，フィリピン大学ディリマン校，ベトナム国家大学ハノイ校，ラオス国立大学，王立プノンペン大学，アジア新興国産天然資源を由来とする機能性物質創生のための高度分析研究拠点の形成

大垣英明，分子科学研究所共同利用研究，UVSOR-BL1U からの LCS ガンマ線を用いた NRF 同位体 3D イメージング法の高分解能化

大垣英明分子科学研究所共同利用研究，UVSOR-BL1U からの LCS ガンマ線を用いた NRF 同位体 3D イメージング法の高分解能化

Financial Support

1. Grant-in-Aid for Scientific Research

大垣英明，基盤研究(A)，直線偏光ガンマ線のデルブリュック散乱（分担金）

大垣英明，基盤研究(B)，LCS-NRF による同位体 3D イメージング法の基盤確立

紀井俊輝，基盤研究(A)，新材料ＭｇＢ２と超伝導電流流体解析による新型アンジュレータ精密磁場制御法の確立

全炳俊，基盤研究(A)，直線偏光ガンマ線のデルブリュック散乱（分担金）

クラビオット ジョルディ，若手研究，Comparative studies of culturally-based characterisation of energy services

2. Others

大垣英明，国立大学改革強化推進補助金，ICT を利用したハイブリッド型による国内外フィールドワーク・実習教材の開発

大垣英明，東京大学，「先端レーザーイノベーション拠点「次世代アト秒レーザー光源と先端計測技術の開発」部門」「自由電子レーザーで駆動する高繰り返しアト秒光源のための基礎基盤技術の研究」

大垣英明，科学技術振興機構，サトウキビ収穫廃棄物の統合バイオリファイナリー

大垣英明，科学技術振興機構，日ＡＳＥＡＮ科学技術イノベーション共同研究拠点－持続可能開発研究の推進－

大垣英明，研究拠点形成事業（B)，アジア新興国産天然資源を由来とする機能性物質創生のための高度分析研究拠点の形成

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Advanced Atomic Energy Research Section

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J. Yagi, Junior Associate Professor
K. Mukai, Assistant Professor
M. Bakr, Program-Specific 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 cycle 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 2020.

-Experimental evaluation of tritium by DD neutron using a diamond detector

-Calculation of tritium generation and radioactivity of activation foils to be performed by DT neutron source

-Development of liquid lithium lead droplet system for efficient recovery of hydrogen isotope and electrochemical purification system

-Direct quantification of nitrogen in Fe-Ti alloy which trapped nitrogen in liquid lithium

-Development of DD neutron source using 3D printed electrode

2. Blanket mock-up neutronics study

Neutron distribution monitoring in fusion blanket mock up is a key to ensure the self-sufficiency of the tritium fuel. Developing a method of measuring tritium production rate and neutron flux distribution are required. Tritium production rate was experimentally evaluated by using a single-crystal diamond detector and a compact DD fusion neutron source as shown in Fig. 1. By using Monte-Carlo simulation code, MCNP-6, transport of deuterium-tritium (DT) fusion reaction neutrons were simulated by MCNP6 and activation calculations were performed by DCHAIN as shown in Fig. 2. The results of activation calculations indicate each activity of activation foils inside the blanket, which proposes the exposure conditions for measurements using imaging plate.

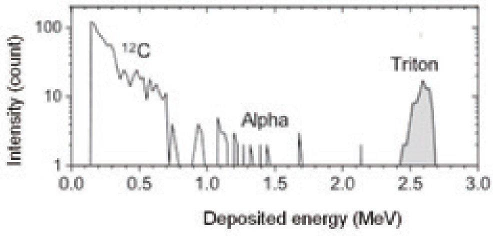

Fig. 1 Energy spectrum measured by single-crystal diamond detector with ^{6}LiF converter.

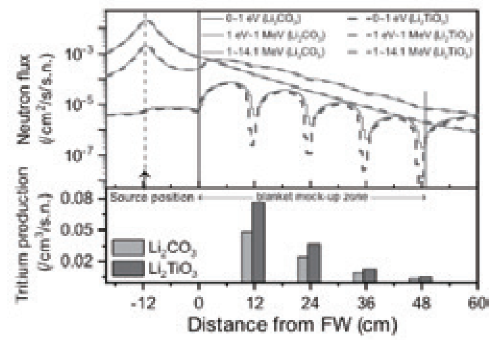

Fig. 2 Neutron fluxes and tritium production rate within a blanket mock-up irradiated with a DT neutron source

3. Development of liquid lithium purification 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

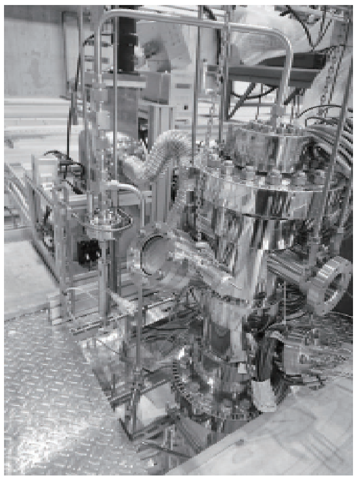

Fig.3: The VST system on Oroshhi-2 Pb-Li loop at NIFS.

blanket system with minimal tritium loss. The vacuum sieve tray (VST) method, tritium recovery from the liquid droplet surface falling in vacuum, is a candidate developed in this section. This fiscal year, on a collaboration work with National Institute for Fusion Science (NIFS) the operation of VST test device shown in Fig. 3 integrated to Oroshhi-2 (Liquid metal test loop) at NIFS has been started.

Oxygen impurity in Pb-Li is also important from the view point of material compatibility. Oxygen removal by an electrochemical method using LiCl-KCl molten salt developed in this section has also been investigated in this fiscal year, and oxygen in Pb-Li is confirmed to be removed as CO_2 when oxygen impurity transferred into the molten salt reacted with the glass-like carbon electrochemically.

4. Nitrogen hot trapping for liquid lithium

Liquid lithium which is also a hopeful candidate as a liquid breeding material, is to be used as a flowing target in an intense neutron source such as A-FNS or IFMIF those are indispensable for fusion reactor development. Nitrogen impurity in liquid lithium is known to degrade the compatibility of structure material against lithium as well as the surface contamination of yttrium which is used for tritium trapping in lithium. For the removal of nitrogen, hot trapping using Fe-Ti alloy has been investigated though the detail transport behavior of nitrogen in the alloy has not been clarified. In this fiscal year, using SXES (soft X-ray energy spectroscopy), nitrogen distribution and diffusion in the alloy has been investigated. Most of the nitrogen in the alloy is concentrated in the grain boundary where titanium is also concentrated and the effective diffusivity of nitrogen in the alloy at 823 K is shown to be in the order of 10^{-16} m^2/s. The nitrogen distribution in the alloy is shown in the figure 4. The X-axis of the figure is the depth from the surface of

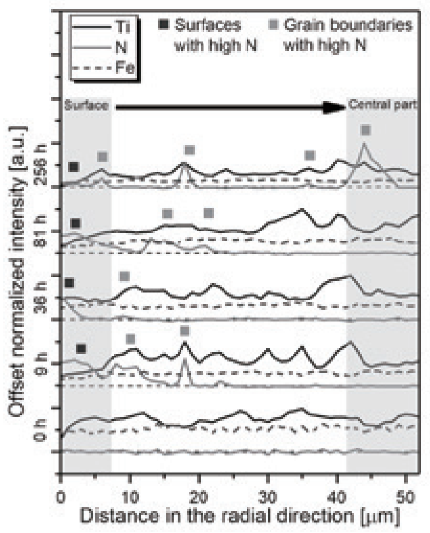

Fig.4: The nitrogen penetration into the Fe-Ti alloy quantified by SXES. Nitrogen is detected in deep region when the heating time is long (256h)

the alloy pebble, which was kept in N-containing Li (~1000wppm) at 823 K followed by the embedding into a resin and polish to show its equatorial plane.

From the practical view point, nitrogen trapping behavior in flowing lithium condition is also important. A small liquid lithium loop has been constructed in this fiscal year and the experiment using the device has also been started.

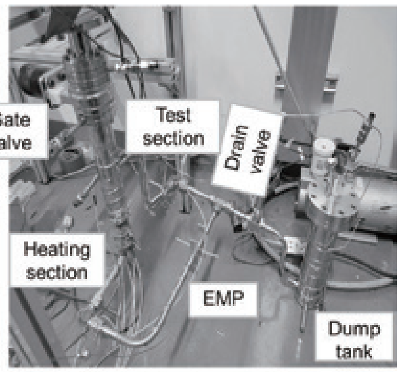

Fig.5: Major components of the lithium loop. The thermal insulator, a glove box connected to the gate valve, a casing with magnets of EMP etc. are not included.

5. Development of compact fusion neutron source with 3D-printed cathode

Development of a compact neutron source with a higher neutron production rate is of great importance for a wide range of its application, including radiography and boron neutron capture therapy (BNCT). Concentric spherical transparent cathodes made of stainless-steel and titanium were fabricated by a metal 3D printer (Figure 6). The measured neutron production rate using the Ti cathode is higher than that of the SS cathode by factors of 1.36–1.64 across the 20–70 kV range. Moreover, fusion on the Ti cathode surface enhances the total neutron yield significantly compared to the SS cathode under the same conditions. The Ti's considerable ability to accumulate D ions and molecules compared with that of SS explains the difference of measured NPR results.

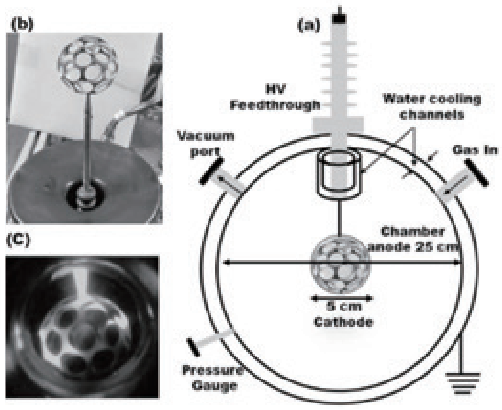

Fig.6 (a) a compact fusion neutron source. (b) buckyball-shaped grid cathode. (c) stainless-steel cathode during discharge

Collaboration Works

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Financial Support

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Advanced Plasma Energy Research Section

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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 the optimization of the helical-axis heliotron configuration are in progress under the collaboration with other groups of the international/national institutes and also groups of other universities under the auspices of the Collaboration Program of the Lab. Complex Energy Processes, IAE and the Collaborative Research Program of NIFS (National Institute for Fusion Science).

In this report, a remarkable result obtained in the Heliotron J experimental study in FY2020 is reported focusing on (1) O-X mode conversion analysis for the electron Bernstein wave heating and diagnostic, (2) development of interferometer system for the electron density measurement and (3) X-ray spectrum measurement in non-resonant microwave heated plasmas.

2. O-X mode conversion analysis using finite element method for EBW heating and diagnostics

Electron cyclotron wave (ECW) is used as one of the methods for heating and diagnostics in magnetic confinement fusion devices. The propagation modes, ordinary (O)-mode and extraordinary (X)-mode, are reflected when the plasma density reaches the cutoff density, resulting that we are not able to access the core region. To solve this problem, O-X-B (from O-mode to X-mode and then electron Bernstein wave (EBW)) mode conversion is proposed. In this study, we have analyzed the optimal conditions for O-X conversion and its conversion efficiency by the finite element method based on the wave equation using COMSOL Multiphysics and compared them with ray-tracing calculations.

We have used a two-dimensional model with a uniform magnetic field and a density gradient in the x-axis direction. we have analyzed the injection condition for maximal O-X conversion efficiency for three parameters, that is, the beam size, the focusing diameter of the injection port, and the angle of incidence, and we have obtained more than 80 % con-version efficiency for the entire injection beam. The conversion from O-mode to X-mode can be seen near the optimum incident angle in Fig. 1(b). In comparison with ray-tracing, there is no significant difference in the optimal angle, and the trajectories of both were consistent as shown in Fig. 1 (d). This suggests that the ray-tracing calculation is useful for finding the optimal incidence angle. In the finite element analysis, the beam width is seen to expand after conversion to X-mode, and the trajectory of the finite width EC beam can be traced.

3. Development of 320 GHz interferometer system in Heliotron J

Measurement of the density profile with high time resolution is required to understand the particle transport in fusion plasma experiments. A new multi-channel heterodyne Michelson interferometer with 320 GHz solid-state sources has been designed and is being constructed in Heliotron J for high-density

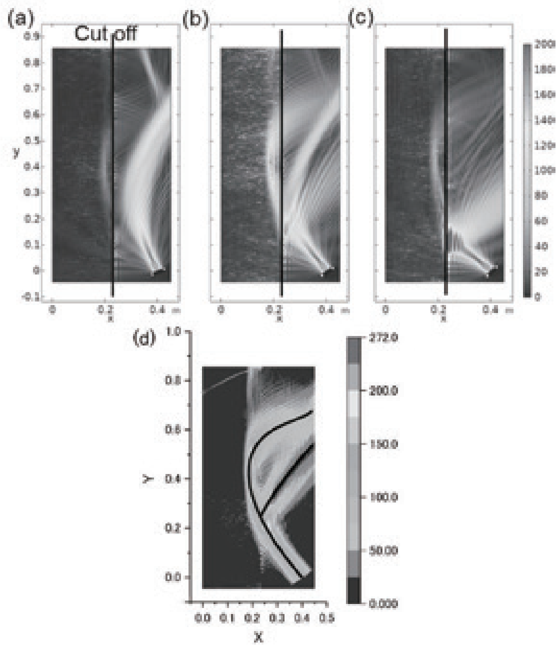

Fig. 1. The electric field norm of O-mode injection (42 GHz). The incidence angle is (a) 25 deg, (b) 35.7 deg and (c) 45deg to the magnetic field (1.8 T), and (d) Trajectory of ECW at optimal incidence conditions. COMSOL (color), ray-tracing (black line).

plasma operation.

To reduce the influence of the plasma refraction effect and ensure that the injected beam returns back in the original direction after reflection, an array of retroreflectors was mounted on the facing wall of the vacuum chamber. To make sure the influence on the beam profile with the retroreflector, an optical test experiment has been done to compare the reflection effects between the metal mirror and the retroreflector.

Figure 2 shows the experimental setup in the optical test experiment. The beam profile was measured by moving a detector in the horizontal and vertical directions. Figure 3 shows the measured beam profiles in the metal mirror and the retroreflector. The beam profile in the retroreflector is more peaked than that in the flat metal mirror, and the signal intensity is high even at large scanning angles, indicating that the retroreflector works for beam transmission. The retroreflector was installed on the inner wall of the vacuum chamber with the angle of less than 40 deg.

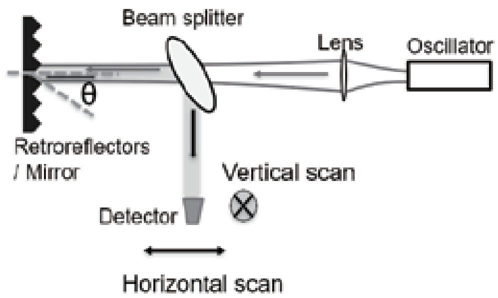

Fig. 2. The schematic view of the test bench experiment for 320 GHz interferometer system

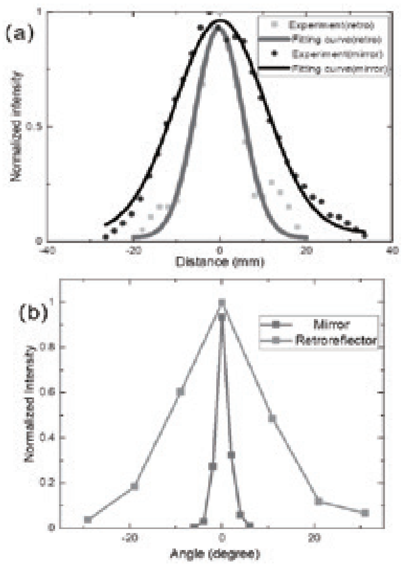

Fig. 3. (a) Beam profile in the horizontal direction and (b) dependence on the scanning angle obtained by the test experiment.

4. Behavior of high-energy electrons in non-resonant microwave heated plasma in Heliotron J

High-energy electrons have been generated by non-resonant 2.45 GHz microwaves in a magnetic field configuration of Heliotron J. To study the production mechanism, we measured the X-ray energy spectrum produced by Bremsstrahlung processes of the high energy electrons. Three sets of $LaBr_3$(Ce) scintillator covered with shields for stray radiation and magnetic field) have been installed to obtain the X-ray spectrum emitted in three (clockwise, perpendicular and counter-clockwise) directions to the magnetic field line. Each scintillator signal is measured with a multichannel analyzer (MCA) through a pre-amplifier and a shaping amplifier.

Even though the shielding effect by the vacuum vessel was not negligible, we confirmed the existence of MeV-class high energy electrons by the scintillator signal when the detector observes the X-ray flux in the perpendicular direction (see Fig. 4). The peak of the X-ray spectrum around 0.3 MeV may be due to the shielding effect by the Stainless-steel vacuum vessel whose thickness of 20 mm. The strong signal below than 0.1 MeV is attributed to the noise produced by the magnetic coil for the plasma confinement. We also found that the microwave power had a threshold to produce the high energy electrons and that the spectrum weakly depends on the microwave power once the high energy electrons were produced. These results indicate that (1) the observed high energy X-ray flux might be produced by the reactions when the high energy electrons hit the vacuum vessel and (2) the feature is consistent to the production mechanism that the high-energy electrons are produced by the stochastic acceleration.

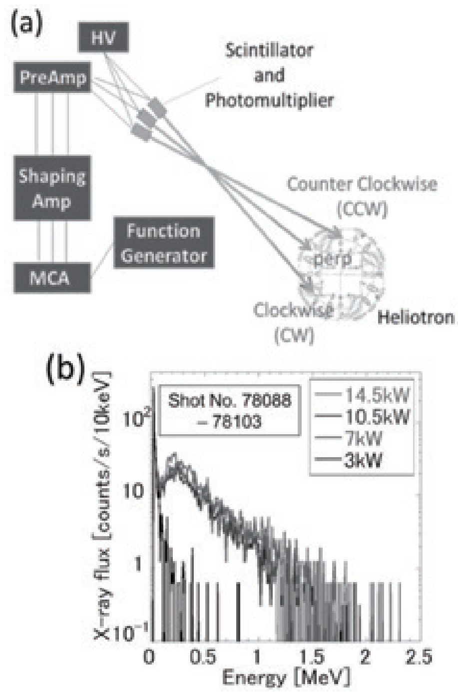

Fig. 4. (a) Schematic view of X-ray measurement system using $LaBr_3$ scintillator and (b) X-ray energy spectrum obtained in non-resonant microwave heated plasmas.

Collaboration Works

長崎百伸, 西南物理研究所（中華人民共和国）, IPP, Greifswald（ドイツ），University of Wisconsin（アメリカ），反射計を用いた電子密度分布・揺動解析

長崎百伸，IPP，Greifswald（ドイツ），電子サイクロトロン電流駆動の理論解析

長崎百伸, 岡田浩之, 小林進二, 南貴司, 大島慎介, Univ. Wisconsin（アメリカ），Oak Ridge National Laboratory（アメリカ）, Max Plank Institute（ドイツ）, Stuttgart Univ（ドイツ），CIEMAT（スペイン）, Australian National Univ.，（オーストラリア）, Kharkov Institute（ウクライナ）, Southwest Institute of Physics（中華人民共和国），ヘリカル型装置における SOL/ダイバータプラズマに関する研究

長崎百伸, 大島慎介, 岡田浩之, 南貴司, 小林進二, Stuttgart Univ.，CIEMAT，先進閉じ込め配位

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Financial Support

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Complex Plasma Systems Research Section

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

1. Introduction

Magnetic nuclear fusion energy has some attractive features as a future option for the base-load electrical power source: (1) inherent safety features, (2) no long-life nuclear waste emission, (3) no greenhouse gas emission during the energy production, (4) huge energy density stored in the fuel source(~90 MWh/g for D-T fuel), (5) abundant source availability spreading all over the Earth, and (6) high nuclear proliferation resistance, in terms of both resources and weapons technologies.

Among various issues to be overcome in physics and engineering fields, we have focused on the problems related to the plasma transport and magneto-hydrodynamics. Specifically, determination of a magnetic configuration that can efficiently confine high-density plasma at high temperature with a sufficiently long confinement time and developing diagnostics and control schemes for the high-temperature plasmas in such magnetic fields are regarded as crucial. In these respects, our research section investigates about heating and fueling, confinement and diffusion mechanisms and their diagnostics in a magnetic plasma confinement device, named Heliotron J.

Results in FY2020 featured in this report are about the comparison between the experiments and theory/simulation in turbulent and MHD phenomena.

2. Study of Turbulence Properties against Isotope Ratio and Zonal Flow Activity in Heliotron J

Confinement improvement in deuterium (D) plasmas, compared to the hydrogen (H) plasmas, called “isotope effect”, has been a long-standing issue in the study of magnetic confinement fusion. The isotope effect contradicts a fundamental model of transport, in which an increase of characteristic scale (ion Larmor radius or turbulence scale size here) simply gives the increase of transport, in other words, D plasmas should exhibit poorer performance than the H plasmas do, although experimental observations show the opposite result. A possible mechanism to explain the isotope effect is a favourable impact of a zonal flow, a type of coherent structure induced by turbulence itself, on the plasma transport. Several theoretical and experimental works also support the hypothesis. However, turbulence responses behind the isotope dependence of zonal flows, have not yet been studied in detail so far.

The frequency spectra of floating potential and ion saturation current indicate that the turbulence level gradually increases against the H/D ratio, as hydrogen is more dominated, as shown in Fig. 1(a) and (b). Interestingly, the small different characteristics can be seen by comparing two spectra; higher frequency components of > 100 kHz emerge in the case of floating potential, and fluctuation level in all the frequency range increases in ion saturation current, as hydrogen

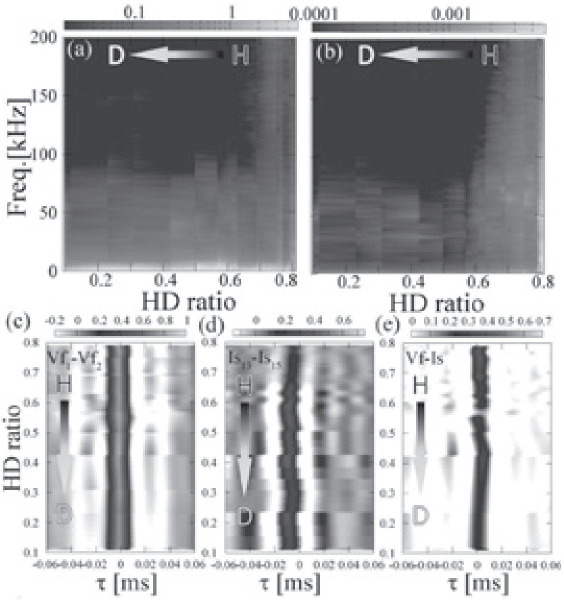

Fig. 1 (a)Dependence of frequency spectra on hydrogen/deuterium(H/D) ratio (~$n_H/(n_D+n_H)$) for potential fluctuation and (b) density fluctuation. (c)Isotope dependence of two-point correlation between adjacent probe signals with the distance of 5mm for floating potential (d)density fluctuations, and (e)between potential and density fluctuations. and double-path measurement using two forward backward scattered lights (chain line).

becomes dominant. This observation suggests that turbulence-induced transport increases in H plasmas.

Furthermore, the decorrelation of density and potential is also demonstrated from a statistical viewpoint using a joint probability density function(joint-PDF) technique. The observed decoupling of fluctuation has been revealed to be attributed to the enhancement of the zonal flow observed in this experiment.

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3. Simulation Study of Energetic Particle-driven MHD Modes and Energetic Particle Redistribution in Heliotron J

Sufficiently long energetic particle (EP) confinement time is important for realizing self-sustainable plasma; however, these EPs can resonate with the shear Alfvén waves (SAW) through fundamental and sideband resonances in the magnetic confinement fusion devices (e.g. tokamak and stellarator/heliotron).

The interaction between energetic particles (EPs) and EP-driven magnetohydrodynamic (MHD) instabilities in Heliotron J has been investigated by MEGA[1-2], a hybrid MHD-EP simulation code.

The three-dimensional magnetic field of Heliotron J is mainly composed of the helicity, toroidicity, and bumpy Fourier components. This creates additional interactions between EP and SAW[3].

It has been shown in Ref.4) that the free MHD boundary condition can have a significant impact on the stability of the low-n mode in the strongly shaped plasma. Then, we have recently made a success in improving the application of the MEGA simulation to free-boundary condition on the last closed flux surface (LCFS).

In this study, we analyzed the stability of the EP-driven MHD instabilities and their effects on the EPs confinement in Heliotron J. Both the fixed and free MHD boundary conditions are utilized. The simulation is conducted on the low (ϵ_{01}=0.01) bumpiness configurations.

The fixed boundary simulation results show that the n/m=2/4 mode is dominant while the n/m=1/2 mode is observed as a recessive component (Fig.2a). The time evolution of the n/m=1/2 mode is obscured due to the large difference in the amplitude between n/m=1/2 and n/m=2/4 modes. This contradicts with the experiments where the n/m=1/2 mode is dominant.

In the free boundary simulation, much higher linear growth rates are predicted for both the n/m=1/2 and 2/4 modes (Fig.2a). The change is much higher for the n/m=1/2 mode such that the n/m=1/2 mode emerges as the dominant mode, although both the

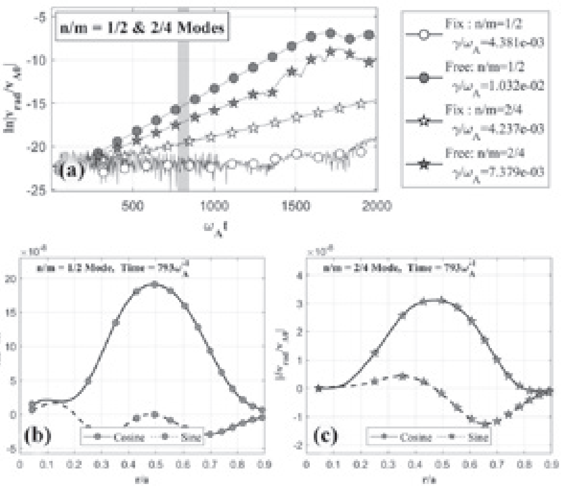

Fig.2 (a) The comparison of the logarithmic time evolution of the radial MHD velocity for n/m=1/2 and 2/4 modes between the fixed and free boundary simulations. The spatial profile of the n/m=1/2 and 2/4 modes at $793\omega_A^{-1}$ are shown in panels (b-c), respectively. $793\omega_A^{-1}$ is indicated by the vertical transparent gray bar in panel (a).

n/m=1/2 and 2/4 modes are located at the same radial location. The spatial profiles of the n/m=1/2 and 2/4 modes are shown in Figs.2b-c, respectively. In contrast to the fixed boundary case[2], the mode profiles are broadened and radially shift toward the edge. By analyzing the changes in the EP driving rate (γ_h) and MHD dissipation rate (γ_d), it shows γ_h is higher in the free boundary simulation while γ_d remains the same. The stronger EP-SAW interactions are brought about by the broadening of the mode profile. From the analysis of the EP redistribution in velocity space, the majority of the interactions are brought about by the high velocity co-passing EPs interact with the SAWs through high velocity toroidicity-induced resonance. These EPs have large orbit widths such that they can interact with the mode in the edge region.

This study shows that the boundary condition has a significant role in Heliotron J, a low shear helical-axis stellarator/heliotron. The boundary condition at the LCFS can significantly affect the linear properties of the low-n EP-driven mode, even if the mode's radial location is at r/a≈0.5. The prospective cause is the low magnetic shear of Heliotron J. This shall be verified in other low shear stellarators.

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Collaboration Works

大島慎介，西南物理研究所（中国），非線形結合同定のための新しい揺動解析手法に関する共同研究

大島慎介，長﨑百伸，岡田浩之，南貴司，小林進二，Wisconsin University（アメリカ），CIEMAT（スペイン），Max-Plank Institute（ドイツ），ヘリカル磁場配位における周辺揺動研究

長﨑百伸，岡田浩之，小林進二，南貴司，大島慎介，Univ. Wisconsin（アメリカ），Oak Ridge National Laboratory（アメリカ），Max Plank Institute（ドイツ），Stuttgart Univ（ドイツ），CIEMAT（スペイン），Australian National Univ.，（オーストラリア），Kharkov Institute（ウクライナ），Southwest Institute of Physics（中華人民共和国），ヘリカル型装置における SOL/ダイバータプラズマに関する研究

長﨑百伸，大島慎介，岡田浩之，南貴司，小林進二，Stuttgart Univ.，CIEMAT，先進閉じ込め配位

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），低磁気シアヘリカル装置における高速イオン励起 MHD 不安定性に関する研究

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1. Grant-in-Aid for Scientific Research

南貴司，基盤研究(C)，電磁場制御による核融合プラズマの内部輸送障壁形成手法の新展開

大島慎介，基盤研究(C)，乱流の非線形性を介在した同位体効果発現機構の実験的検証

大島慎介，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（分担金）

大島慎介，基盤研究(C)，非接触核融合プラズマモデリングを目指した周辺プラズマ・中性粒子輸送コード開発（分担金）

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Advanced Energy Materials Research Section

T. Hinoki, Associate Professor

1. Introduction

The research activity puts emphases on R&D of the advanced energy materials like SiC composites reinforced with SiC fibers with 10 μm diameter and tungsten composites reinforced with SiC fibers for aerospace, nuclear advanced fission and fusion application utilizing nano-technique. The R&D include development of novel materials, surface modification, and environmental effects including high temperature oxidation and irradiation effects from basic science through engineering. Many collaborative researches are ongoing with domestic and international institutions in US, EU and OECD.

2. Development of Particle Dispersion Silicon Carbide Composites by Liquid Phase Sintering

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

Silicon carbide composites were fabricated by liquid phase sintering (LPS) method. Silicon carbide with BN matrix was formed by mixture of SiC powder and BN powder in LPS composites. The prepreg technique was developed for industrial application under collaboration with industry. Mechanical properties were characterized by various methods including tensile test and fatigue test in air up to 1400 C. Microstructures and fracture surfaces were characterized by FE-SEM and FE-TEM.

The BN particle dispersion composites showed excellent high temperature oxidation resistance. Oxidation was limited to near surface. The BN particle dispersion composites don't require fiber/matrix interphase. It decreases material cost significantly. Productivity is also excellent compared to conventional SiC composites. The BN particle dispersion composites didn't break applying 190 MPa following 100,000 cycles at 1400 C of fatigue tests in air without any coating. Machinability of BN particle dispersion composites is good. Stress-strain curves of the material fabricated by LPS seems brittle. However it has reliable matrix cracking stress and lower notch sensitivity like pseudo-ductile composites. Figs. 1 show silicon carbide fibers, prepreg and BN particle dispersion SiC composites.

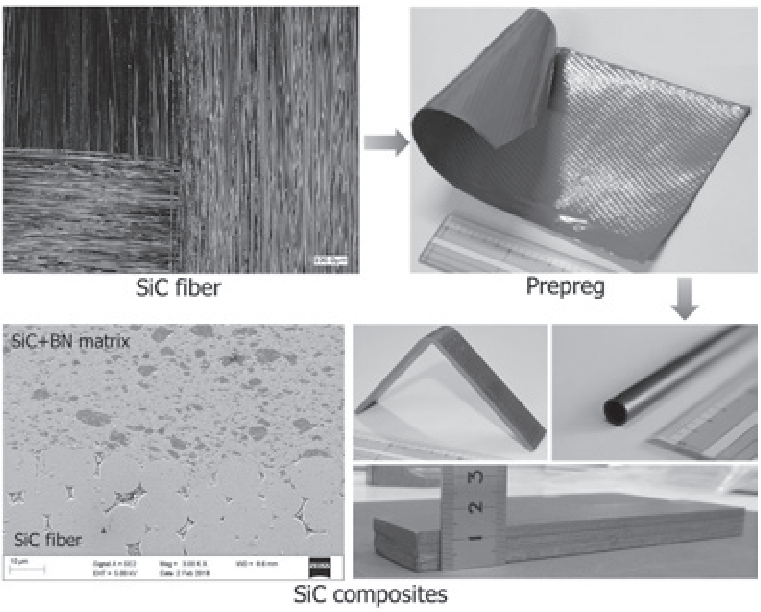

Fig. 1 Silicon carbide fibers, prepreg and BN particle dispersion SiC composites.

3. Ion Irradiation Effect on SiC Composites

Silicon carbide composites are expected to apply for nuclear fission and fusion environments due to stable properties under neutron irradiation. Dimensional change of high purity SiC saturated at around 1dpa in most of temperature range. Microstructure and mechanical properties didn't change above around 1 dpa. Silicon carbide composites consist of SiC fiber, fiber/matrix interphase and matrix. Carbon interphase is a candidate for nuclear application.

It was found that C was unstable at high fluence in particular at relatively low temperature. One of highly crystalline SiC fiber, Hi-Nicalon type-S has small amount of C. Disorder and elimination of C interphase happened following 100 dpa ion irradiation by DuET. Shrinkage of Hi-Nicalon type-S was observed by AFM following 100 dpa ion irradiation as shown in Fig. 2, where high purity SiC matrix swelled. Carbon ribbons observed by FE-TEM for non-irradiated Hi-Nicalon type-S disappeared following 100 dpa irradiation. It is considered that C ribbons were dissolved in SiC grains. The issues of C interphase and C in Hi-Nicalon type-S were discussed under steering committee of Generation IV International Forum (GIF) –Gas Cooled Fast (GFR) Reactor System-, OECD NEA. Evaluation of high dose irradiation using ion irradiation and development of high dose irradiation tolerant SiC composites will be carried out under PROJECT ARRANGEMENT ON FUEL AND CORE MATERIALS under GIF GFR framework.

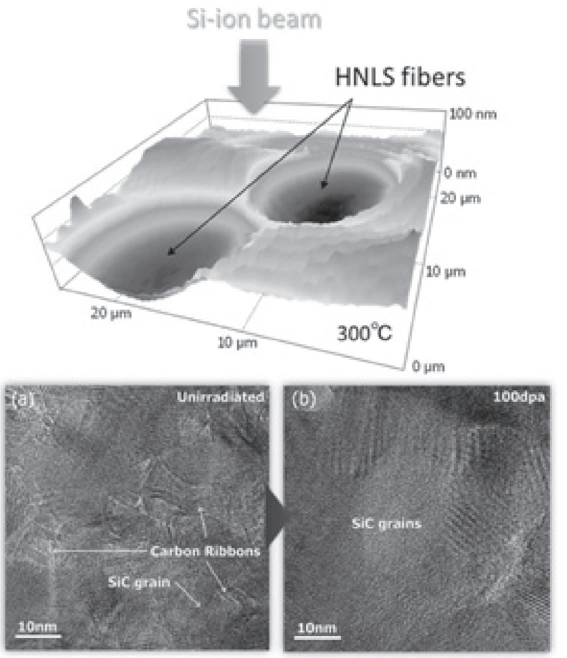

Fig. 2 Irradiation effect on irradiation induced swelling and microstructure of SiC composites.

4. Development of Silicon Carbide Fiber Reinforced Tungsten Composites

Tungsten is a primary candidate material for divertor and first wall. A tungsten material is expected to be used at high temperature due to its extremely high melting point. However mechanical properties of tungsten degrade at high temperature due to recrystallization of pure tungsten above 1000°C. Neutron irradiation also affects mechanical properties significantly. Silicon carbide has very close coefficient of thermal expansion with tungsten. Silicon carbide fibers can be used at above 1000°C under neutron irradiation without significant degradation of mechanical properties. The objective of this work is to develop the tungsten material with ductile behavior under high temperature neutron irradiation environment by reinforcement of silicon carbide fibers.

Tungsten foils or tungsten powders were sintered with silicon carbide fibers by various conditions at 1000~1800°C and ~20MPa. Carbon coated fibers and non-coated fibers were used. Mechanical properties were characterized by tensile test. Microstructure was evaluated by FE-SEM.

Very dense composites were fabricated in case of composites sintered with relatively small tungsten powders less than 1 um and reinforced with non-coated silicon carbide fibers, however pseudo-ductile fracture wasn't observed. The composites showed pseudo-ductile fracture behavior by fiber pull-out attributed to weak fiber/matrix interfacial strength in case of composites sintered with relatively large tungsten powders or tungsten foils, or composites reinforced with carbon coated silicon carbide fibers as shown in Fig. 3. The pseudo-ductile fracture behavior is independent of embrittlement of tungsten above recrystallization temperature or under neutron irradiation. The magnitude of tungsten can be reduced by replacing with silicon carbide fibers. It can contribute to safety in case of severe accident.

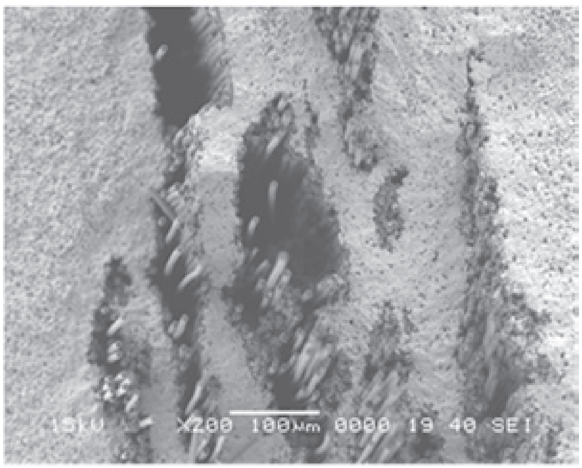

Fig. 3 Fracture Surface of SiC Fiber Reinforced W Composites.

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Advanced Laser Science Research Section

T. Nakajima, Associate Professor

1. Introduction

Laser is a very powerful tool to synthesize/modify the target materials and also remotely probe the various dynamics. This year we have studied the properties of metal-polymer nanocomposites with a focus on its molecular weight, and developed a simple but efficient technique to detect and also size nanoparticles in bulk water.

2. Probing the concentration profile of dissolved gas in proximity to the electrode during hydrogen gas evolution

Hydrogen evolution reaction (HER) through water electrolysis is considered to be one of the promising methods to store renewable energy. While water electrolysis is a well-known process, it does not mean that realization of high efficiency for the practical use is a trivial task. From the material science viewpoint, developing efficient and durable electrocatalysts is obviously an important issue. From the physical chemistry and chemical physics viewpoint, HER involves important bubble dynamics such as nucleation, detachment, and transport of bubbles. The concentration of the dissolved gas in close proximity to the electrode increases and reaches supersaturation during electrolysis, and depending on the supersaturation level a tiny local fluctuation triggers the nucleation of gas bubbles. Needless to say, the concentration of dissolved hydrogen gas in proximity to the electrode shows a gradient, and up to what distance and size the bubbles can grow with what rates depends on the electrolysis conditions. Clearly, such information is crucial toward the efficient HER. Traditionally, electrochemical methods with micro/nanoelectrodes are used to study nucleation on the electrode. However, such methods cannot be applied under the presence of bubbles, since it hinders the accurate monitoring of nucleation dynamics.

Knowing the above we have developed a new technique to probe the concentration profile of the dissolved gas during HER, which itself is useful not only to understand the bubble nucleation dynamics but also to optimize the electrolysis conditions. The setup of our detection system is shown in Fig. 1. We employ an Ni wire and Pt mesh as a working and counter electrodes, respectively. Both electrodes are fixed on a squared PTFE frame, and immersed in the 60 mL KOH solution at 0.1 M in an acrylic cuvette (Fig. 1(a)). The working electrode is at the lower position than the

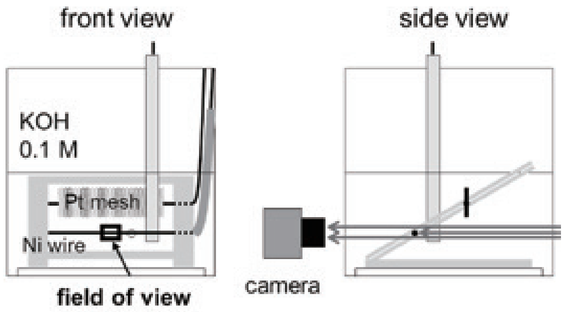

Fig. 1 Experimental setup to optically detect the electrolysis bubble. (a) front view and (b) side view. As shown in (b) bubbles are illuminated from behind the wire electrode by LED.

counter electrode (Fig. 1(b)) to secure a clear view of hydrogen bubbles without the presence of oxygen bubbles. To observe bubbles we take the shadowgraphic images of bubbles in proximity to the Ni wire electrode with a fast camera under the LED illumination through a telecentric lens.

Fig. 2(a) shows an example of hydrogen bubbles in proximity to the Ni wire electrode under the constant current mode of −8 mA (equivalent to the current density of -85 mA/cm^2). There are a few big bubbles which hinder the image analysis, and hence we focus on the area, defined by the two dashed vertical lines of Fig. 2(a), to analyze the bubble dynamics. To evaluate the radii and growth rates of individual bubbles we have developed a home-made software. Once these quantities have been obtained from the image analysis of bubbles, we can use the diffusion model to extract the concentration of dissolved gas as a function of distance from the electrode, and the corresponding results are shown in Fig. 2(b). When the bubbles are too close to the wire electrode it is not easy to isolate tiny bubbles from the electrode through the image analysis described above. Under the current experimental conditions, the closest distance for the image analysis of bubbles is about 15 μm from the electrode. Therefore, we perform the linear fittings to the concentration (left axis of Fig. 2(b)) and extrapolate the fitted line to distance zero to obtain the concentrations of dissolved hydrogen gas on the electrode to be 30.9±1.8 mM for the current density of −85 mA/cm^2. We point out that

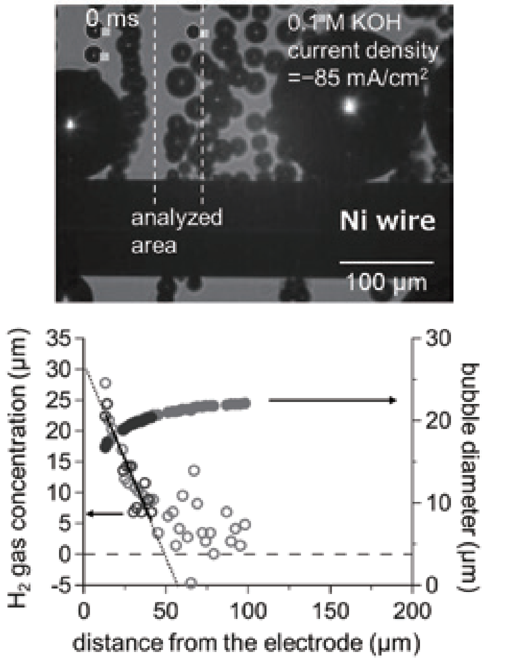

Fig. 2 Analysis of H_2 gas concentration in proximity to the Ni wire electrode. (a) Optical image and (b) H_2 gas concentration obtained from the bubble growth rate at the different distances from the electrode.

this concentration is much lower than the one expected for the classical bubble nucleation with a nanoelectrode, and hence it suggests that the bubble nucleation mechanism with a macroscopic electrode like our case is not classical. A further study is necessary to clarify this point.

3. First observation of the formation of nanoparticles inside the ablation by laser scattering

Use of laser ablation in liquid is one of the flexible techniques to produce various kinds of nanoparticles. However, the physical mechanism of nanoparticle formation upon laser ablation in liquid is not yet well understood. One powerful technique to tackle this problem is small-angle x-ray scattering. Application of the laser-scattering technique in a similar context faces some difficulties, since the curved bubble surface does not allow a probe laser to go into the bubble, and even if it goes into the bubble the extremely weak

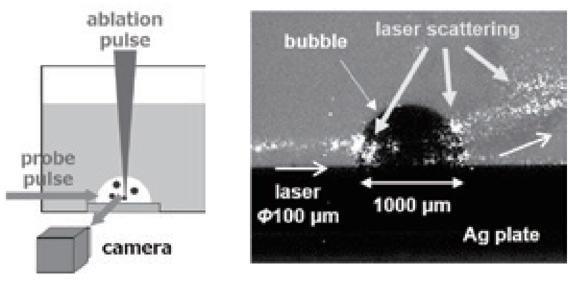

Fig. 3 Experimental setup for the time-resolved optical detection of single nanoparticles by laser scattering.

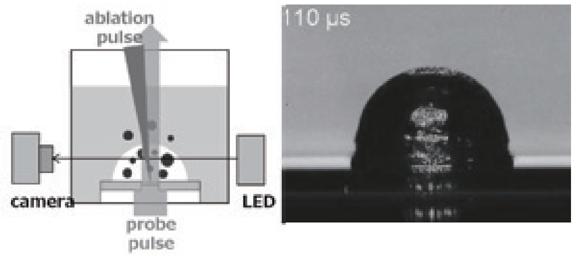

Fig. 4 Our setup to optically observe the inside of ablation bubble by laser scattering. A probe pulse is introduced into the bubble through a flat transparent window produced by laser ablation of thin metallic film on a glass substrate.

scattering signal from inside the bubble is overwhelmed by the very strong reflection at the bubble surface (Fig. 3). We have solved those problems by sending the probe laser into the bubble through a laser-induced flat transparent window, and demonstrate the clean observation of laser-scattering signals from the inside of the ablation bubble (Fig. 4). We have found the signature of nanoparticle formation around the two areas inside the bubble, that is, around the central area and apex inside the bubble (Fig. 4(b)). By changing the delay time between the ablation and probe pulses until the bubble collapses (<150 μs after the ablation pulse) we have found that the scattering signals originating from the central area of the bubble persistently stay throughout the entire growth and shrinkage stages of the bubble. More interestingly, the scattering signals originating from the apex inside the bubble gradually emerges after the bubble size becomes maximum, and they become brighter during the shrinkage stage. Those findings are consistent with the scenario of nanoparticle formation obtained by small-angle x-ray scattering experiments.

To better understand where in the bubble the scattering light comes from, we consider the inverse light scattering problem (Fig. 5), and find that the scattering signal from point P1 comes from the scatterers located at point Q in the right panel of Fig. 5. The scattering signal from point P2 can be understood as scattering light that has reached the camera directly from point Q without refraction. This is the first clear observation of nanoparticle formation insider the ablation bubble by laser scattering, which allows us to track the nanoparticle formation process.

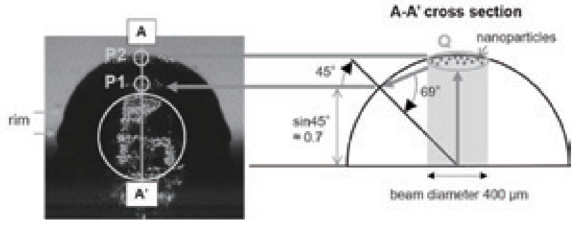

Fig. 5 (Left) Laser scattering image superimposed on the shadowgraph image. (Right) Optical path of the scattering light cut at A-A' cross section.

Financial Support

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Advanced Energy Structural Materials Research Section

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P. Song, Researcher
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1. Introduction

Materials development and maintenance management is essential for establishment of the safety and efficient operation of advanced nuclear energy systems. This section addresses the mission of establishing a maintenance management methodology as well as material R & D for advanced nuclear energy systems such as fusion and fission reactors. Current main researches are as follows:

(1) Plant integrity analysis: The structural integrity of a reactor pressure vessel (RPV) is important for reactor safety and was investigated using three-dimensional computational fluid dynamics (3D-CFD) and the finite element method (FEM). Pressurized thermal shock (PTS) during emergency water cooling, the most severe situation, was focused in the present study. Through this investigation, the magnitude of the risk of the RPV function loss was evaluated and proposed as an indicator available for optimizing the maintenance strategy.

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

(3) Irradiation effects on microstructure evolution and properties 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. Hence, 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. PKA energy dependence of defect production in collision cascades

Since there are no fusion reactors at present, it is necessary to understand material behavior in a fusion reactor for a realistic design of fusion DEMO reactor. The production of primary defects in collision cascades in a material is a phenomenon that occurs in a very short time; therefore, it should be analyzed by computational simulation technique based on molecular dynamics (MD) method. In the MD simulation, behavior of collision cascades can much depend on some variable parameters such as PKA energy and the incident direction of a PKA (primary knock-on atom). The objective of this study is to systematically investigate the parameter dependence of the collision cascade behavior with a statistical analysis.

In this study, by means of MD method, we examined the relationship between the PKA energy and the number of non-equilibrium produced defects, in which Mendelev potential was applied to evaluate the cascade damage process in α-Fe. In the MD simulations, the number of produced defects was evaluated as a function of PKA energies ranging from 0.02 to 10 keV, with 1000 case calculations for each of the PKA energies. In this analysis, when PKA energy is lower than 0.1 keV, the number of surviving defects increases in proportion to PKA energy, leading to a good agreement with the NRT model. In contrast, when PKA energy is higher than 0.1 keV, the number of surviving defects nonlinearly increases with PKA energy,

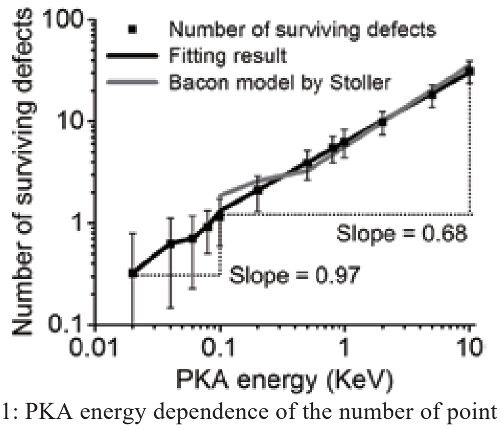

Fig. 1: PKA energy dependence of the number of point defects produced by displacement cascades.

resulting in a similar trend to Bacon' model.

3. **Structural integrity assessment of reactor pressure vessels: A probabilistic risk evaluation**

Reactor pressure vessels (RPVs) are an important component in nuclear power plants and function to keep nuclear fuel and radioactive materials confined. The structural integrity of RPVs has been verified by regulation through periodic and special inspections, where judgments are made as to whether regulations are satisfied. Unfortunately, however, the judgments are only deterministic, and the degree of satisfaction is beyond their scope. In the present study, to clarify the degree of satisfaction, uncertainties in the structural integrity are quantified. Using the probability density distribution function of the stress intensity factor and that of the fracture toughness, the probability of the occurrence of the irradiation-induced brittle fracture of RPVs during pressurized thermal shock (PTS) events is evaluated and defined as an indicator representing fracture risks. The characteristics of the indicator are found to show that it increases significantly with the reactor operating time and therefore indicates a more appropriate quantified parameter of aging phenomena than the conventional $\Delta DBTT$ (ductile-to-brittle transition temperature shift). The indicator is finally proposed to be employed for the optimization of the inspection and maintenance of RPVs.

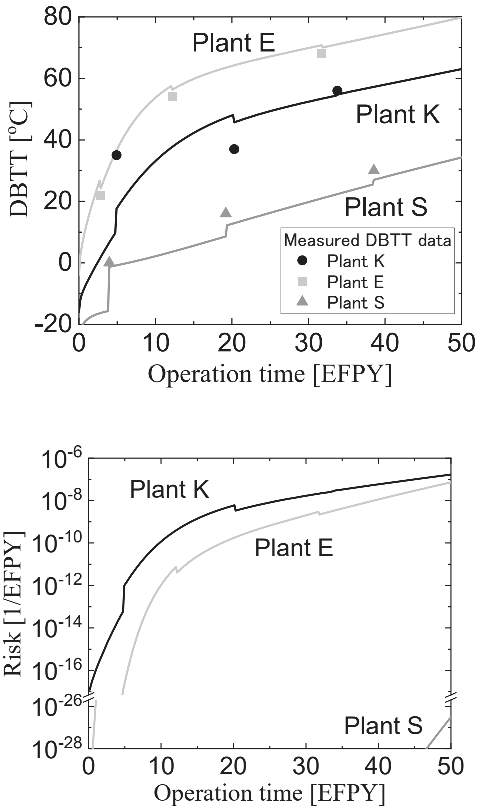

Fig. 2: The time evolutions of the predicted and corrected DBTT values and embrittlement risks for the three plants.

4. **Irradiation effects on microstructure evolution and properties of materials**

Tungsten (W) is considered to be the primary choice for the plasma facing materials (PFM) in fusion reactors due to its attractive combination of properties such as high melting point, good thermal conductivity, high creep resistance, good high-temperature strength and low vapor pressure. We has investigatd the irradiaton effect of tungsten (W), which is a candidate material for fusion divertar, using an ion accerelator (DuET: Fig. 3). We found that the microstructure evolusion under ion irradiation depends on the crystal orientation using W single crystals with {001} and {011} surafcace orientation for ion-irradiation (Fig. 4). Defect zone depth is deeper in {001} crystal than in {011} crystal. The mechanism has been discussed with DFT, MD, and so on. The knowledge obtained in this study is fruitful for fusion diverter design and integrity. Moreover, we performed a systematic theoretical study of the interactions between transition metals (TM) elements and point defects in bcc W using density functional theory (DFT) calculations. The effects of transition metals elements on the microstructure evolution was discussed.

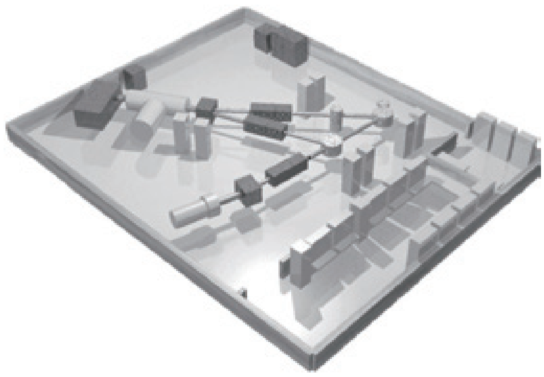

Fig. 3: Ion-accelerator (DuET)

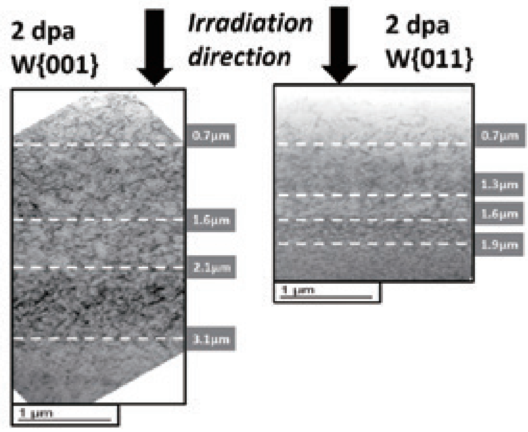

Fig. 4: TEM micrographs of W single crystals after 6.4 MeV Fe^{3+} ions.

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藪内聖皓，基盤研究(B)，超微小試験技術による照射脆化のミッシングリンク解明（分担金）

藪内聖皓，若手研究，格子欠陥の熱拡散に及ぼす磁壁の影響

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Nano Optical Science Research Section

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K. Shinokita, Assistant Professor
T. Nishihara, Program-Specific Assistant Professor

1. Introduction

We are working on basic and applied research of nano-materials from a viewpoint of optics and material science. Our research aims at exploring new physical and chemical phenomena leading to applications of novel nano-materials including carbon nanotubes, layered transition metal dichalcogenides, perovskite for efficient utilization of light energy and development of future optoelectronic devices with ultra-low energy consumption. Followings are main research achievements in the year of 2020.

1. Magnetic proximity effect and charge transfer in monolayer semiconductor and double-layered perovskite manganese oxide van der Waals heterostructure

Recently, monolayer transition metal dichalcogenides (MX_2: M=Mo, W, X=S, Se, Te) have gained increased attention, owing to their novel physical properties and potential applications. The strong confinement and reduced dielectric screening of optically generated electrons and holes in semiconducting monolayer MX_2 enhance Coulomb interaction. Consequently, this imparts an extraordinarily large binding energy to a neutral exciton as a bound electron-hole pair, and to negatively (positively) charged excitons or trions as a bound two electron-hole pair (or an electron and two holes). The excitons and trions in monolayer MX_2 exhibit valley degrees of freedom because the electrons and holes comprising the band-edge located excitons and trions are located at the energy degenerate valleys (K, −K), which are situated at the corners of the hexagonal Brillouin zone. The valley degrees of freedom coupled with the spin degrees of freedom (spin-valley locking), which originate from strong spin-orbit interactions and the breaking of inversion symmetry, enable the selective photogeneration of excitons and trions at the K or −K valleys by shining circularly polarized light; this leads to the formation of valley-polarized excitons and trions (valley polarization) in monolayer MX_2.

The optically generated excitons and trions are highly sensitive to the physical properties of substrate materials, owing to the proximity effect. The monolayer MX_2 on the insulating ferromagnetic materials provides a platform for investigating the exchange interactions between the valley spin-polarized excitons (trions) and ferromagnetic spins via proximity magnetic-exchange effects, which leads to tunable valley spin polarization and large valley splitting. The strongly correlated electron system of perovskite manganese oxide has been extensively studied as a model ferromagnetic system for the double-exchange interactions of *d*-orbital electrons in Mn sites through O 2*p*-orbitals. Numerous novel physical phenomena such as colossal magnetoresistance and charge ordering have emerged in perovskite manganese oxides. The e_g electrons in perovskite Mn oxide trigger the electronic and magnetic phase transition via double-exchange interactions from the paramagnetic insulator phase to the ferromagnetic metal phase at Curie temperature. Even though electronic and magnetic phase transition materials are ideal platforms for creating van der Waals (vdW) heterostructures together with semiconducting 1L-MX_2, studies regarding the optical physics of these types of vdW heterostructures have not been reported thus far.

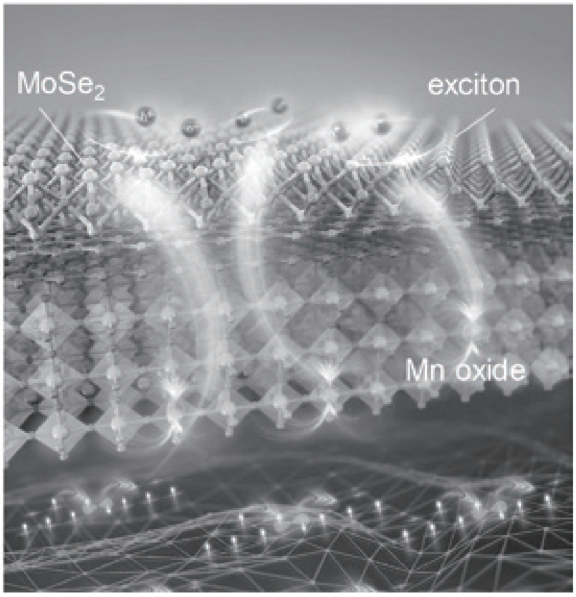

Fig. 1 Schematic of magnetic proximity effect and charge transfer in monolayer $MoSe_2$ and perovskite manganese oxide in the hetero-structure.

Here, we showed the charge transfer and magnetic proximity effect of vdW heterostructures, which are composed of monolayer $MoSe_2$ (1L-$MoSe_2$), few-layer *h*-BN, and double-layered perovskite Mn oxide ($(La_{0.8}Nd_{0.2})_{1.2}Sr_{1.8}Mn_2O_7$). This vdW heterostructure enabled us to systematically study the interface interactions between the excitonic states (excitons and trions) and magnetic spins as well as charge carriers. We found that the photoluminescence properties of 1L-$MoSe_2$ strongly depend on the electronic and magnetic properties of the substrate; the charges are transferred from metallic Mn oxide to 1L-$MoSe_2$, and the valley splitting and polarization are significantly enhanced by introducing a ferromagnetic substrate (Mn oxide), as shown in Figure 1. Moreover, these interactions between 1L-$MoSe_2$ and Mn oxide can be modulated and controlled by varying the thickness of the few-layer *h*-BN. The vdW structures using electronic and magnetic phase transition materials demonstrated here can provide new opportunities for the modulation and controllability of excitonic states via dielectric screening, charge carriers, and magnetic spins.

2. Inter-valley trion relaxation dynamics in monolayer two-dimensional semiconductor under magnetic field

Novel science and application of valley degree of freedom for information transmission and storage have emerged as valleytronics, which is a new platform for future electronic applications. Monolayer transition metal dichalcogenides 1L-MX_2 as novel two-dimensional (2D) semiconducting materials have attracted tremendous attention for developing valleytronics with coupled spin and valley degrees of freedom. The breaking of Krammers degeneracy due to strong spin-orbit coupling and broken spatial inversion symmetry in 1L-MX_2 produces K or -K valleys at the corner of the hexagonal Brillouin zone that is inequivalent but energy-degenerate. This enables the valley-dependent optical selection rule, in which electrons and holes in a specific valley and spin can be selectively excited by circularly polarized light. The σ+ and σ− circularly polarized light can selectively excite the valley-spin polarized excitons (trions) at K and -K valleys. The valley degree of freedom (valley polarization) of excitons (trions) defined as their population difference between K and -K valleys can be monitored through the difference of circularly polarized emission intensity with σ+ and σ− component.

The valley polarization of 1L-MX_2 under external field such as electric and magnetic field has been extensively studied from the viewpoints of fundamental valley physics. The breaking of valley degeneracy under the magnetic field because of the broken time-reversal symmetry leads to the photoluminescence (PL) peak splitting of excitons (trions) with σ+ and σ− circularly polarized component by Zeeman splitting in 1L-MX_2. Moreover, the valley polarization could be

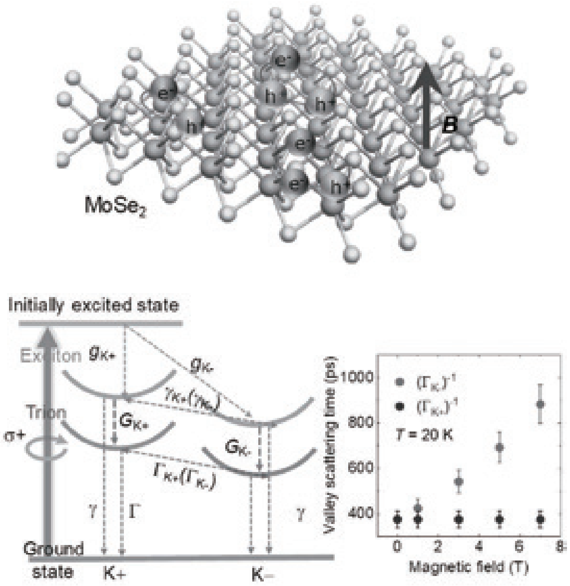

Fig. 2 Schematic of exciton and trion under the magnetic field. Magnetic field induced exciton and trion relaxation dynamics and valley relaxation time under the magnetic field.

modulated by applying magnetic field due to breaking valley degeneracy, where the excitonic valley polarization is dominated by its dynamics: the generation of valley-polarized excitons (trions) and intra-valley and inter-valley relaxation of excitons (trions). The excitonic valley polarization under zero magnetic field in the degenerated valley conditions has been revealed. However, no systematic studies on the dynamics of excitonic valley polarization under magnetic field have been performed. The new insights for the dynamics of excitonic valley polarization show the guides toward long-time keeping and easily controlling of valley polarization, which is strongly required for future valleytronics applications.

In this study, we systematically studied the dynamics of excitonic valley polarization in hexagonal boron nitride (*h*-BN) encapsulated monolayer $MoSe_2$ (1L-$MoSe_2$) by polarization- and time-resolved PL spectroscopy under magnetic field. The valley Zeeman splitting induced by an external magnetic field results in the asymmetric valley scattering of trions (excitons) from K to -K valley and vice versa, generating the valley polarization at a finite magnetic field, as shown in Figure 2. To understand the valley dynamics under magnetic field, we build a relaxation model of an exciton and trion including an asymmetric valley scattering rate between K and -K valleys. By solving rate equations obtained from the relaxation model, we described the magnetic field and temperature dependence of the trion valley polarization in 1L-$MoSe_2$. Our work shows new physical insights for the valley polarization dynamics of excitonic states under magnetic field, which would give a guide to manipulate the valley degree of freedom in valleytronics.

Collaboration Works

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

Financial Support

1. Grant-in-Aid for Scientific Research

松田一成，基盤研究(S)，原子層物質におけるバレースピンフォトトニクスの創生と応用

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，挑戦的研究（萌芽），高次データー科学による原子層物質のバレースピン制御

宮内雄平，基盤研究(B)，量子物質を用いた非従来型赤外光電変換学理の開拓

篠北啓介，若手研究，二次元遷移金属ダイカルコゲナイドにおけるバレースピン分極の緩和モデルの構築と制御

西原大志，若手研究，熱光エネルギーの高度利用に向けたカーボンナノチューブの熱放射特性の完全解明

2. Others

宮内雄平，科学技術振興機構，原子層ヘテロ構造の光物性・機能開拓

宮内雄平，科学技術振興機構，ナノ物質科学を基盤とするサーモエキシトニクスの創成

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Clean Energy Conversion Research Section

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1. Aim of research

In Heliotron-J, a large amount of time series data has been obtained by the progress of simultaneous multi-point plasma measurements for many years. It is necessary to coarse-grain and visualize this large amount of data to extract deep correlation and hidden causarity. In order to coarse-grain the data under the assumption that "physics is simple", it is necessary to define some kind of simplified model and to quantify and minimize the statistical distance between the observation and the model [1]. Following this approach, we focus on time series data in particular, and extract some temporal patterns inherent in the data. This method can represent the non-stationarity, intermittence, and non-linearity of the plasma with fewer degrees of freedom than the Fourier analysis, which has been the main tool for time series data analysis so far. In this study, we develop such a new analysis tool using Heliotron-J time series data, and discuss the non-stationarity, suddenness, and non-linearity of Heliotron-J plasma. Heliotron-J has accumulated a large amount of time series data as described above, and in addition, it has large-scale data such as digital ECE using ultrafast oscilloscopes, which has been conducted in previous collaborative research. There are few projects in Japan where such data sets are available. Therefore, it is necessary to conduct this project as a collaborative research at Heliotron J.

2. Application of ARMA model to turbulent time series data

In this study, we develop a method for extracting characteristic patterns from time series data. We are not interested in patterns that appear on very short time-scales, but rather those that have relatively long time-scales. For this reason, we consider extracting the longest time-scale from the time series data. However, it is difficult to determine the time scale with high accuracy because the peaks of periodogram of time series data with weak periodicity, such as turbulent flow, are wide. Therefore, we adopted one of the statistical modeling of time series, the ARMA (autoregressive moving average model) [2], which is a model to predict the current value from past time series data and can be written as follows,

$$X(t) = \epsilon(t) + \sum_{i=1}^{p} \varphi_i X(t-i) + \sum_{i=1}^{q} \theta_i \epsilon(t-i),$$

where $X(t)$ is the discrete time series data, $\epsilon(t)$ is the Gaussian noise, φ_i and θ_i are the coefficients, and p and q are the maximum degrees of freedom of the model. In order to obtain the long-term time scale from this model, the maximum degree of freedom of the model becomes large and the computational cost increases accordingly. In this study, we tested how long time-scales can be extracted from the ARMA model by using turbulent time series data obtained from the fundamental plasma experiment. The target time series data are shown in Fig. 1. The ARMA model is a stationary model, so it is applied to the stationary part of the data, which is indicated by the red line in the figure. The extended Dickey-Feller test rejects the non-stationarity of the data with a probability of 1-2 × 10^{-9} [3]. To reduce the computational cost, a Bessel-type anti-aliasing filter is applied and the sampling frequency is set to 1/20 (50 kHz).

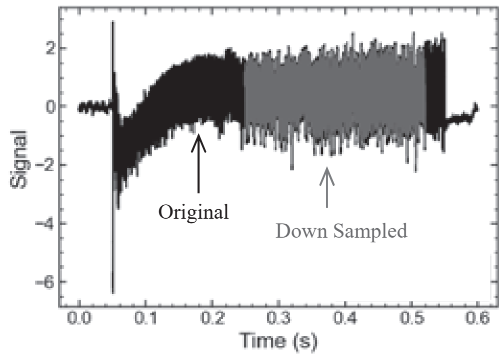

Fig.1: Target time series data. Red line indicates down-sampled data.

3. Detecting long time-scale with the ARMA model

Although there is no general method to determine p and q in the ARMA model, information about p can be obtained from the partial correlation function. The cross-correlation function and the partial cross-correlation function are shown in Fig. 2. The partial correlation function has significantly large values for the first 10 lags. For this reason, 27 models were obtained in a brute force fashion with $1 \leq p \leq 10$, $0 \leq q \leq 2$, and the difference from the predicted values was calculated. The best model was determined as the condition that minimizes the Akaike's information criterion [4], and (p, q) = (9, 2) was obtained. The best model is given as $X(t) =$ 0.603+3.30 $X(t-1)$-5.47 $X(t-2)$+ 6.08 $X(t-$ 3) - 5.16 $X(t-4)+$ 3.69 $X(t-5)$ - 2.33 $X(t-$

6) + 1.27 $X(t-7)$ - 0.563 $X(t-8)$ + 0.156 $X(t-9)$ - $1.06\epsilon(t-1)$ + $0.613\epsilon(t-2)$.

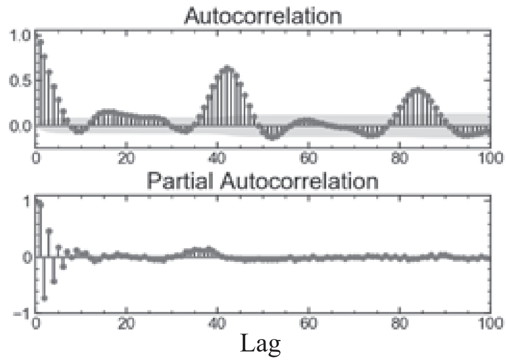

Fig.2: Auto correlation function and partial auto correlation function.

The in-sample prediction (fitting) is shown in Fig. 3. Here initial 2000 points are used as training data. For the in-sample prediction, the ARMA model shows a good agreement. The longest lag obtained is 9×50=450 μs. Although evidence of the in-sample predictability is found, the model shows very poor prediction accuracy for the out-of-sample prediction as shown in Fig. 4.

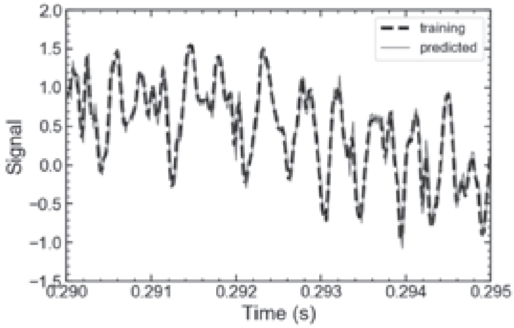

Fig.3: Result of the in-sample prediction.

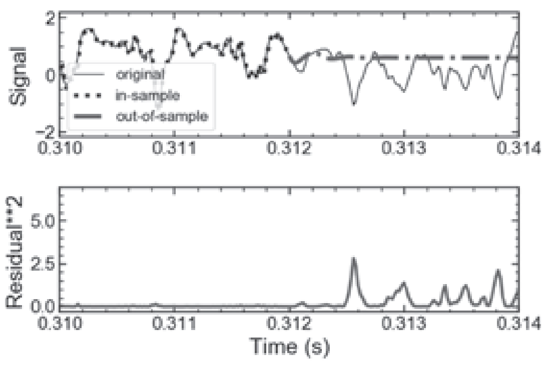

Fig.4: Result of the out-sample prediction and squared residual between model and data.

Why does the ARMA model have poor predictive performance? Figure 5 compares the Fourier spectrum estimated by the ARMA model with the Fourier spectrum of the training data. It can be seen that the ARMA model cannot reproduce the low frequency components. To detect longer periods, we need to explore a larger (p,q) space, which is difficult with the current computational resources. The good predictable capability of the ARMA model does not guarantee the out-of-sample predictability. In order to detect long time-scales at the sacrifice of short time-scales, it is necessary to introduce sparsity into the ARMA model so that the computational cost does not increase even for large (p,q) spaces.

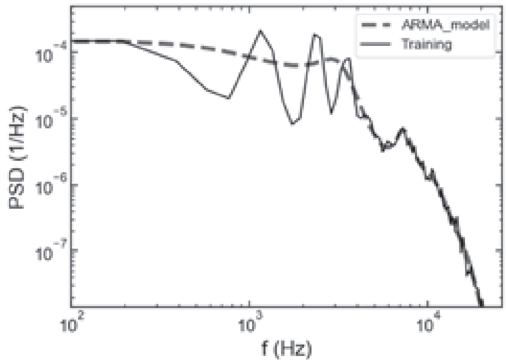

Fig.5: Comparison of the Fourier power spectrum.

4. Discussion and Summary

The performance improvement of out-of-sample prediction for turbulent flow data can be greatly improved by applying deep learning with RNN (Recurrent Neural Network) instead of the ARMA model [5]. However, the RNN is not able to extract the time scale. On the other hand, the ARMA model is good in terms of mapping to physical mechanics, and it can be easily extended to multi-channel data. In the future, we aim to improve the prediction performance by increasing the number of channels to be analyzed and increasing the input information.

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Clean Energy Conversion Research Section

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1. Introduction

For conventional photovoltaic solar cells, a PN junction is essential for generating a photocurrent via the dissociation of photo-generated electron-hole pairs. However, there is a maximum theoretical power conversion efficiency of PN photovoltaic solar cells, known as the Shockley-Queisser (SQ) limit [1]. A PN junction is not strictly required for photocurrent generation, and an alternative mechanism called the bulk photovoltaic effect (BPVE) [2] has been known. The BPVE generates a steady photocurrent in single-phase homogeneous materials without inversion symmetry. In contrast to the PN photovoltaic effect, the BPVE can generate a photo-voltage above the band gap [3], which makes it possible to overcome the SQ limit [4]and thus surpass the conversion efficiency of conventional solar cells. A primary mechanism in the BPVE is the shift current effect [5,6], a nonlinear optical response where the center of mass of the electron wave function changes in the intracell during photo-excitation [5,7]. First-principles calculations of the shift current have reproduced experimental observations of the BPVE in ferroelectric $BaTiO_3$ [6]. The topological aspects of the shift current have been previously studied [7], and the relation between the shift current and the polarization has been clarified. For a deeper understanding of the BPVE, it is crucial to elucidate the mechanisms that determine the magnitude and direction of the shift current. Recent studies on topological materials found that topologically nontrivial electronic structures give rise to a large shift current response [8]. On the other hand, many-body effects are also important factors that determine the magnitude of the shift current. Morimoto and Nagaosa [9] studied nonlinear excitonic processes and found that the dc current flow is caused by excitons below the band gap without the dissociation of excitons into free electrons and holes. First-principles calculations using the GW and Bethe-Salpeter equation [10] and the time-dependent GW approximation [11] have been conducted to investigate quasiparticle and exciton effects on the shift current. The former demonstrated that excitons reduce the shift current in bulk $BaTiO_3$, but have little influence on the shift current in monolayer SnSe. The latter found that excitons enhance the shift current in monolayer GeS. Importantly, many-body effects become quite noticeable in the optical response, especially that of one-dimensional materials, because almost all the optical intensity is transferred to the lowest exciton state [12,13]. They are thus anticipated to have a crucial influence on the shift current. A recent experiment demonstrated that quasi-one-dimensional transition-metal dichalcogenide nanotubes exhibit an extraordinarily large shift current [14]. However, the exciton effect on the shift current in such one-dimensional materials is still unclear. In the present study, we aim to clarify properties of the shift current in single-walled boron-nitride nanotubes (SW-BNNTs) as a representative one-dimensional material with broken inversion symmetry [15].

2. Shift Current

The shift current is generated to second order in an electric field. For a monochromatic electric field $E_b(t) = E_b(\omega)e^{i\omega t} + E_b(-\omega)e^{-i\omega t}$, the shift current is generally expressed by a response function σ_{sc}^{abc}.

$$J^a = 2\sum_{bc} \sigma_{sc}^{abc}\,(0,\omega,-\omega)E_b(\omega)E_c(\omega)$$

For the one-dimensional structure considered in the present study, we only consider the component σ_{sc}^{zzz}, where the nanotube axis is parallel to the z direction. Below, we denote σ_{sc}^{zzz} as σ_{sc} for simplicity. By using the equation of motion for the density matrix, the expression for the shift current response function that includes the exciton effect can be obtained as

$$\sigma_{sc}(\omega) = \frac{\hbar e^3}{8\pi V}\sum_{mn}\sum_{kk'k''}\frac{v_{vc,k}v_{cv,k''}^{*}}{E_m E_n(E_n - \hbar\omega)} \times \psi_k^m \psi_{k'}^{m*}\psi_{k'}^n \psi_{k''}^{n}{}^{*}\left(-\frac{d\log\psi_k^n}{dk'} + i\Omega_{cv,k'}\right) \quad (1)$$

where ψ_k^m is the wave function of nth exciton state at the wavevector of k, E_n is the nth exciton energy, V is the volume of a SW-BNNT, $v_{vc,k}$ is the matrix element between the conduction and valence bands of the velocity operator v, and $\Omega_{cv,k} \equiv \Omega_{cc,k} - \Omega_{vv,k}$, with $\Omega_{mn,k}$ being the Berry connection.

3. Results and Discussion

Figure 1 plots the response function for the shift current calculated using Eq. (1) for the chirality of (10,0) and (11,0) SW-BNNTs. Here, the chiral index (n_1, n_2) uniquely determines the structure of SW-BNNTs. We set the amount of broadening to 0.02 eV. The shift current response in the presence of the exciton effect exhibits symmetric peaks. A comparison with the absorption spectrum indicates that each peak corresponds to the exciton states. For the non-interacting case, the shift current response shows a single asymmetric peak structure starting at the energy of the band gap. A key factor that determines the intensity of the shift current response is the joint density of states (JDOS). For one-

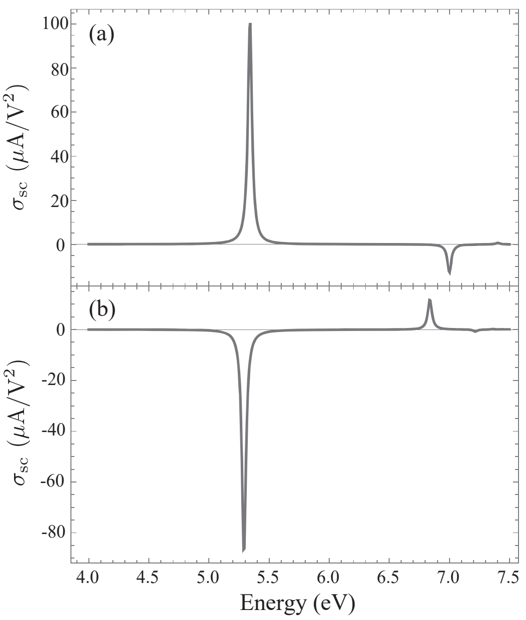

Fig.1 Shift current response for (a) (10,0) and (b) (11,0) SW-BNNT.

dimensional materials like SW- BNNTs, the JDOS is divergently large around the band edge because of the van Hove singularity. In fact, the absorption spectrum becomes largest at the band edge. When the Coulomb interaction effect is included, however, almost all the oscillator strength, which is the largest at the van Hove singularity with the divergently large JDOS for the free electron-hole pairs, is transferred to the lowest exciton state due to exciton formation in one-dimensional materials. As a result, the response of the exciton shift current in a nanotube structure is larger than that of the normal shift current without the exciton effect.

It is important to note that, in Fig. 1, the sign of the response function between (10,0) and (11,0) is opposite for responses with and without the exciton effect. This feature indicates that the direction of the shift current depends on the chiral index of SW-BNNTs. To elucidate the chiral index dependence of the direction of the shift current in SW-BNNTs, we derive an approximate analytical expression for σ_{sc}. Under the assumption that $v_{cv,k}$ is independent of k, Eq. (1) becomes

$$\sigma_{sc} \cong i\frac{e^3\gamma^2 A}{4\pi^3\hbar V}\frac{\Delta}{\kappa_\nu\sqrt{\Delta^2+\gamma^2\kappa_\nu^2}}\sum_n \frac{|\psi^n(z=0)|^2}{E_n^2(E_n-\hbar\omega)} \quad (2)$$

where we have used the relation $\psi^n(z=0) = \frac{1}{\sqrt{A}}\sum_k \psi_k^n$. Because the excitons in SW-BNNTs are Frenkel-type, as determined from ab initio calculations, Eq. (2), whose derivation is justified for Wannier-type excitons where electron and hole pairs are well limited in momentum space to a small neighborhood of $k = 0$, is not expected to quantitatively reproduce the numerical results. However, we can discuss some qualitative features of the exciton shift current in SW-BNNTs. Equation (2) is an odd function of $\kappa_\nu = -2\pi\nu/3L$, where $\nu = \mathrm{mod}(n_1 - n_2, 3)$, and onsite potential Δ, and thus explicitly shows that the sign of the response function is determined by ν and Δ. The sign of the onsite potential is fixed such that $\Delta > 0$ for the B site and $\Delta < 0$ for the N site. We thus conclude that the direction of the exciton shift current is solely determined by ν of SW-BNNTs; the sign of the shift current is positive for (10,0) SW-BNNTs because $\nu = 1(> 0)$, and negative for (11,0) SW-BNNTs because $\nu = -1(< 0)$. Since the parameter ν is defined by the chiral index, the sign of the shift current is determined by the chiral index of SW-BNNTs.

5. Summary

We investigated the exciton effect on the shift current in SW-BNNTs and found that the shift current is enhanced by the exciton effect and that the direction of the shift current is determined by the nanotube chiral index. The present study clarifies remarkable many-body effects in the bulk photovoltaic effect and provides an essential theoretical basis for the control of the shift currents, which will be an important and useful knowledge for future photovoltaic applications.

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Chemical Reaction Complex Processes Research Section

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T. Kodaki, Associate Professor
T. Yamamoto, Assistant Professor

1. Introduction

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

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

2. Development of New Plating Processes of Titanium Using Molten Salt Electrolytes

Titanium metal has excellent properties such as high specific strength, high corrosion resistance, and biocompatibility. In addition to these properties, the amount of titanium present in the earth's crust is more than 40 times greater than the commonly used copper and nickel. However, titanium is not widely used due to two problems: high cost and poor workability. Therefore, there is a need for new smelting and processing methods. One way to solve these problems is to plate titanium metal on an inexpensive substrate. Electrodeposition of titanium is a promising plating method in terms of cost and flexibility of substrate shape. Therefore, electrodeposition of titanium metal using molten salt at high temperature has been studied for a long time [1-3].

We have already reported the electrodeposition of compact, smooth and well adherent titanium films using molten salts of KF–KCl and LiF–LiCl containing Ti(III) ions at 923 K [4,5]. However, as the titanium film thickness increases, the crystal grains become larger and the surface becomes rougher. It is expected that the titanium film has a smoother surface at lower electrodeposition temperature. In the present study, we investigated the effect of temperature on the morphology and smoothness of titanium films electrodeposited in LiF–LiCl eutectic melt at 823-973 K.

Galvanostatic electrolysis was carried out at 823, 873, 923 and 973 K. The cathode current density was 100 mA cm^{-2} and the electrolysis time was 10 min. Figure 1 shows the optical and surface SEM images of the samples. All the samples have metallic luster; the 823K sample has the highest brightness and metallic luster. SEM observation of the surface shows that the grain size

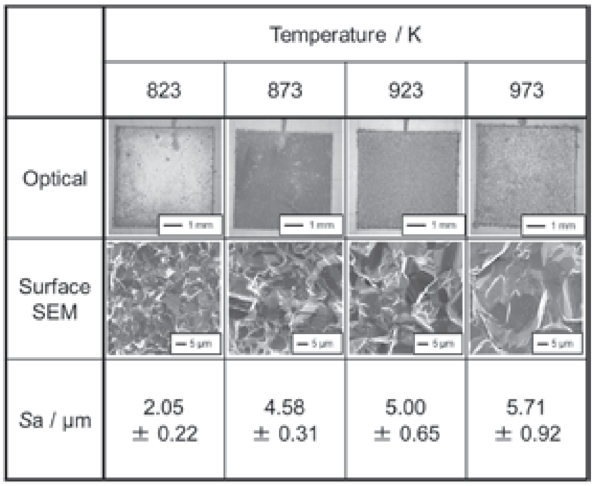

Fig. 1. Optical and surface SEM images of the samples obtained by galvanostatic electrolysis of Ni plates in molten LiF–LiCl after the addition of Li_2TiF_6 (2.0 mol%) and Ti sponge (1.3 mol%) at 823, 873, 923, and 973 K. Cathodic current density and time: 100 mA cm^{-2} and 10 min. Arithmetic mean heights (*S*a) are also listed.

increases with increasing temperature. This trend can be reasonably explained by previous studies on temperature-dependent grain growth of Ti [6]; the value of Arithmetic mean height (*S*a) also increases with increasing temperature. These results conclude that at lower temperatures, smoother surface Ti films can be electrodeposited by suppressing the grain growth of Ti.

3. Development of Potassium Secondary Batteries Using Ionic Liquid Electrolytes

Widespread installation of large-scaled energy storage devices is essentially required to establish the sustainable society based on renewable energy resources such as solar and wind power. Lithium-ion batteries (LIBs), which has been applied for portable electronic devices, could be candidates of large-scaled energy storage devices. However, scarce lithium resources and flammable organic solvents are used as main components of LIBs, which might be a major barrier to the further distribution. Our group has focused on potassium secondary batteries using ionic liquid electrolytes because potassium resources are abundant in the Earth's crust and ionic liquids possess high safety such as negligible volatility and nonflammability [7].

In this fiscal year, we developed several ionic liquid electrolytes for potassium secondary batteries. K[FSA]–[C_2C_1im][FSA] ionic liquid (FSA = bis(fluorosulfonul)amide, C_2C_1im = 1-ethyl-3-methylimidazolium; K[FSA] molar fraction: x(K[FSA]) = 0.20) exhibited an ionic conductivity of 10.1 mS cm^{-1} at 298 K, which was twice as high as that of K[FSA]–[C_3C_1pyrr][FSA] counterpart (C_3C_1pyrr = *N*-methyl-*N*-propylpyrrolidinium) [7]. We also explored new ionic liquids with an asymmetric anion, FTA^- (FTA = (fluorosulfonyl)(trifluoromethylsulfonyl)amide). K[FTA]–[C_4C_1pyrr][FTA] ionic liquid (C_4C_1pyrr = *N*-butyl-*N*-methylpyrrolidinium; x(K[FTA]) = 0.20) showed a moderate ionic conductivity of 2.2 mS cm^{-1} at 298 K. Lastly, charge–discharge behaviors of graphite negative electrodes were investigated using the K[FTA]–[C_4C_1pyrr][FTA] ionic liquid at 313 K. As shown in Fig. 2, the graphite electrode exhibited reversible capacities of ca. 230 mAh $(g\text{-}C)^{-1}$, corresponding to 80–85% of the theoretical capacity (279 mAh $(g\text{-}C)^{-1}$).

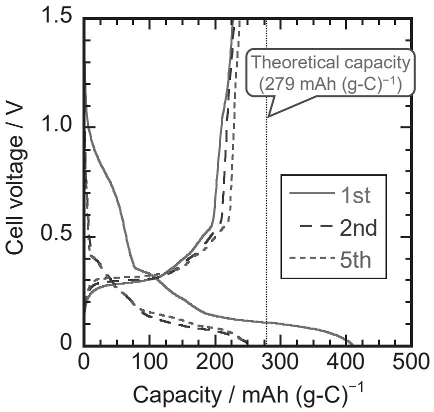

Fig. 2. Charge–discharge curves of a K/graphite cell using K[FTA]–[C_4C_1pyrr][FTA] electrolyte at 313 K. Current density: 27.9 mA $(g\text{-}C)^{-1}$.

4. Efficient Bioethanol Production from Lignocellulosic Biomass Using Ionic Liquid

Recently, pretreatment with ionic liquid was found to be improved yields of sugars from lignocellulosic biomass. On the other hand, ionic liquid was deleterious for growth of microorganisms including yeast.

In this fiscal year, several mutant strains of a recombinant xylose fermenting yeast with increased tolerance to ionic liquid were isolated in order to improve fermentation efficiency in the presence of ionic liquid. Ionic liquid tolerant yeast strains were selected by culturing in the presence of 150 mM of a ionic liquid, 1-butyl-3-methylimidazolium chloride ([Bmim]Cl) after UV irradiation mutation. As shown in Fig. 3, a representative mutant strain was grown even in the presence of 300 mM [Bmim]Cl. Furthermore, this strain metabolized both glucose and xylose, and fermented ethanol efficiently in the presence of 300 mM [Bmim]Cl (Fig. 4).

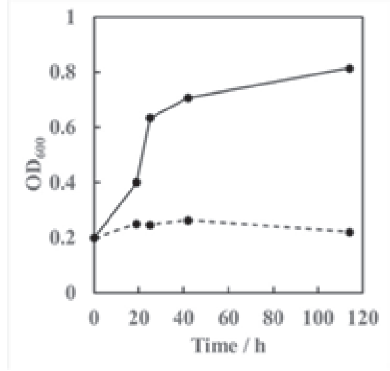

Fig. 3. Growth in the presence of 300 mM [Bmim]Cl. ionic liquid tolerant strain: solid line, wild type strain: dashed line.

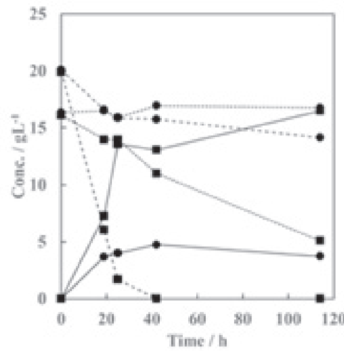

Fig. 4. Glucose and xylose consumption and ethanol fermentation in the presence of 300 mM [Bmim]Cl. ionic liquid tolerant strain: square, wild type strain: circle, ethanol: solid line, glucose: dashed line, xylose: dotted line.

Acknowledgement

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Collaboration Works

大垣英明，森井孝，片平正人，野平俊之，モンゴル国立大学，インドネシア大学，フィリピン大学ディリマン校，ベトナム国家大学ハノイ校，ラオス国立大学，王立プノンペン大学，アジア新興国産天然資源を由来とする機能性物質創生のための高度分析研究拠点の形成

Financial Support

1. Grant-in-Aid for Scientific Research

野平俊之，基盤研究(A)，シリカ直接電解還元と液体合金カソードを用いた高生産性太陽電池用シリコン製造法

山本貴之，若手研究，カリウムイオンを電荷担体とする新規イオン液体電解質の開発

法川勇太郎，特別研究員奨励費，金属チタンのより広範な利用を目的とした新規電解めっき法に関する研究

華航，特別研究員奨励費，溶融フッ化物電解と合金隔膜を用いた希土類金属の高精度・高速分離プロセスの構築

2. Others

野平俊之，新エネルギー・産業技術総合開発機構，高効率な資源循環システムを構築するためのリサイクル技術の研究開発事業

野平俊之，（独）国際協力機構，JICA 研修員受入

野平俊之，住友電気工業（株），200℃以下の融点を有する溶融塩を用いた高付加価値材料のめっき技術に関する共同研究

野平俊之，住友電気工業（株），溶融塩を用いた高付加価値材料の電解技術に関する共同研究

小瀧努，科学技術振興機構，サトウキビ収穫廃棄物の統合バイオリファイナリー

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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 2020 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 are required for desired properties. Bottom-up synthesis of GNRs is a one of suitable method to satisfy these requirements because of definition of their edge structures and widths by the shape of precursors. Atomically precise synthesis of armchair-edged GNRs have already been achieved under ultra-high vacuum (UHV) condition. However, given GNRs in this method were low yield and density was still low. Therefore, it was difficult to develop organic electronic devices with them. To develop devices, high-yield fabrication of assembled GNR films, isolation, and device fabrication are required.

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

On the other hand, fully π-conjugated 2D structure attract much attention since they can provide conducting carbon-based nanostructures with holey structure suitable for various electronic applications. Utilization of large fully π-conjugated building blocks such as GNRs, which are 1D carbon-based nanowires, is becoming a promising approach to produce extended 2D π-conjugated systems via surface assisted lateral fusion of GNR chains.

However, it was difficult to efficiently create such sophisticated GNR-linkage structures, since their formation is based on a stochastic surface reaction that requires closed proximity between the precursors on the surface.

We have already successfully produced carbon-based 2D materials, named 2D-Graphene Nanoribbon Networks (GNNs) via lateral fusion of well-organized acene-type GNRs.

Acene- and armchair-type 2D-GNNs were fabricated on the surface of Au(111) through the thermally induced interchain reactions of densely packed self-assembled GNRs (5-CGNR-1-1 and 7-AGNR), which is the new concept of transforming 1D chains into a 2D network.

The thermal conductivity of 2D-GNNs generated from 5-CGNR-1-1 shows a value of 0.11 $Wm^{-1}K^{-1}$, which is one of the lowest values among carbon-based materials as well as inorganic semiconductor materials, while maintaining the electrical conductivity of 188 Sm^{-1}. These findings will open new perspectives in the field of research on the utilization of GNRs for TE applications.[3]

Additionally, introduction of functional group into GNR is of interest because of creating electronical asymmetry. However, it was difficult with on-surface synthesis because of decomposition of functional group at high temperature during dehydrogenation reaction to form GNR from precursor polymer. Now we focused on this great challenge with new concept.

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 nanoribbon (GNR) with tunable electronic and optical properties. Asymmetrically edge-functionalized GNR have attracted a great deal of interest in view of the relationship between the unique structure and properties. Several theoretical predictions have been made to change the properties of these systems through edge modifications. Introduction of different functional groups to the edges of GNR backbone would offer a promising strategy to exhibit new properties. Although the solution-phase syntheses of GNRs having symmetric substitutions have already 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 from Z-shaped precursor by Pd-catalyzed cyclization followed by oxidative dehydrogenation reactions. The spectroscopic and

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 side of the edges. The relationship between the functionalization of edge structures and their properties will be explored.

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信末俊平，中江隆博，坂口浩司，生物原理を用いる新ナノ炭素の気相表面合成，高分子，印刷中.

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信末俊平，中江隆博，坂口浩司，生物原理を用いる新ナノ炭素の気相表面合成，高分子

Biofunctional Chemistry Research Section

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S. Nakano, Assistant Professor
H. Dinh, Program-Specific Assistant Professor

1. Introduction

A transition to renewable energy technologies requires new chemistry to learn from nature. Nature has developed fantastic solutions to convert the solar energy to the chemical energy and to utilize them in the exceptionally efficient manners for almost 3 billion years. It is our challenge to understand the efficient bioenergetic processes of nature and to construct bio-inspired energy utilization systems. The research interests in our group focus on the design of biomacromolecules and their assemblies for molecular recognition, catalysis and signal transduction in water, the solvent of life. We take synthetic, organic chemical, biochemical and biophysical approaches to understand the biological molecular recognition and chemical reactions. Proteins and protein/nucleic acids assemblies are explored to realize biomimetic function of biological systems, such as visualization of cellular signals by fluorescent biosensors, directed self-assembly of peptides and proteins to build up nanobiomaterials, tailoring artificial receptors and enzymes based on the complex of RNA and a peptide or a protein, and reconstitution of the functional assemblies of receptors and enzymes on the nanoarchitectures. Followings are main research achievements in fiscal year 2020.

2. Enhanced enzymatic activity exerted by a packed assembly of a single type of enzyme

Enzymes are often spatially organized within the cell, either in close proximity on the cell membrane or confined inside a micro-compartment. Such environments are believed to play key roles in enabling the extraordinary efficiency and specificity of sequential metabolic enzymatic reactions. A typical example is the hetero oligomeric assembly of enzymes. Compartmentalization also regulates the spatial organization of enzymes. In spite of being crucial for cellular functions, enzymatic reactions in such highly packed states have not been fully addressed.

In this work, we apply a protein adaptor to assemble a single type of monomeric enzyme, carbonic anhydrase, on a DNA scaffold in a packed state with less than a few nanometers inter-enzyme distance or dispersed state and show that the esterase reaction proceeds faster in the packed than in the dispersed state (Figure 1).

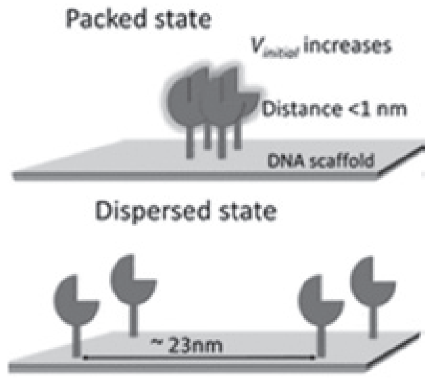

Fig. 1 Schematic representations of four ZS-CAs in the packed (upper image) and dispersed (lower image) states.

In the packed assembly, the reaction is accelerated more prominently for substrates with higher hydrophobicity and is more tolerant of inhibitors (Figure 2).

When another enzyme xylose reductase was assembled in the packed state, a similar acceleration of the reaction in the packed state over the dispersed state was also observed (Figure 3). We propose that the entropic force of water increases local substrate concentration within the domain confined between enzyme surfaces, thus accelerating the reaction. Our finding offers a new insight on the efficiency of reaction by single type of enzyme in the packed state. The water-entropy effect increases as the enzyme structure becomes less flexible in the packed assembly. Therefore, a greater effect is expected within the spatially more constrained cellular compartments. Our system provides a reasonable model of enzymes in packed state; this would help in engineering artificial metabolic systems.

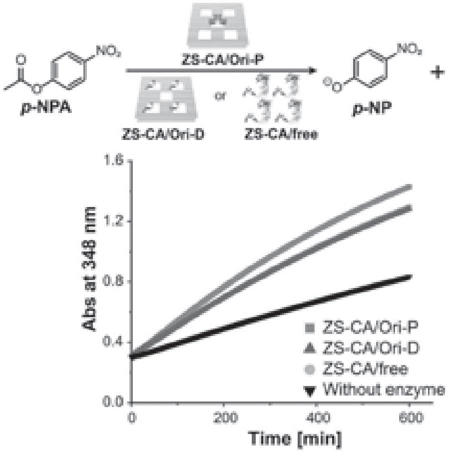

Fig. 2 Time-course profiles of the esterase reactions of ZS-CA (4 nM) on DNA scaffold with *p*-NPA was monitored at 348 nm.

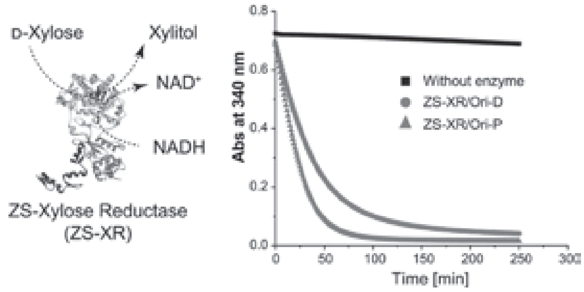

Fig. 3 Time course profiles for the reaction of ZS-XR on DNA scaffold monitored by the oxidation of NADH at 340 nm.

3. Evaluation of the role of the DNA surface for enhancing the activity of scaffolded enzymes

Enzymes have been widely applied in the chemical, medical and food industries. Immobilizing enzymes of interest on the surface of a carrier provides the simplest yet useful method for practical enzyme applications. Immobilized enzymes often display higher activity and stability than their free form; however, the exact mechanism for enhanced activity is still under debate. The catalytic enhancements of enzymes loaded on DNA nanostructures have been attributed to the characteristics provided by highly negative charges on the surface of the DNA scaffold, such as the modulation of the local pH near enzymes.

In this study, two enzymes with different pH preferences, xylose reductase (XR) and xylitol dehydrogenase (XDH), were individually assembled on a DNA scaffold through a modular adaptor. Catalytic enhancements were observed for both the scaffolded XR and XDH over the respective free enzyme. The different optimal pH profiles of XR (pH 6.0) and XDH (pH 8.0), the neutral or net negative charge of their substrates and cofactors indicated that neither the local pH change nor the surface–substrate or –cofactor electrostatic attractive interactions accounted for the increase in the activities of the assembled enzymes. We also suggest that the improved stability or reduced adsorption of scaffolded enzymes alone is not the determining factor for enhancing the activity of enzymes on the DNA scaffold.

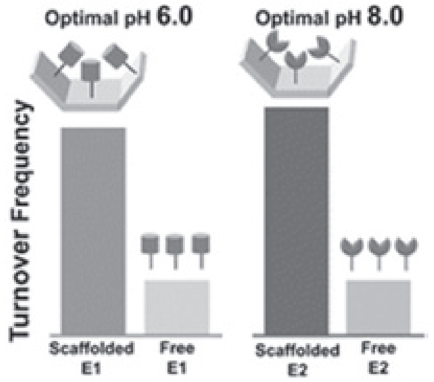

Fig. 4 Schematic representations and comparison of the activity of the free and scaffoled XR (left) and XDH (right).

4. RNA-Peptide Conjugation through an Efficient Covalent Bond Formation

RNA-peptide (RNP) complex is a good scaffold for construction of the receptor-based fluorescent sensors. We have reported the method for construction of RNP sensors that show the fluorescent intensity change upon binding the targeted molecule. We also have developed the method for formation of covalent linkage between RNA and peptide in order to improve the stability of RNP sensor. A representative method was applied for the formation of Schiff base or dihydroxymorpholino linkage between a dialdehyde group at the 3'-end of sugar-oxidized RNA and a hydrazide group introduced at the C-terminal of peptide subunit through a flexible peptide linker. In this study, we investigated effects of the solution pH and contribution of the RNA and peptide subunits to the conjugation reaction by using RNA and peptide mutants. The reaction yield reached 90% at a wide range of solution pH with reaction within 3 hours. The efficient reaction was mainly supported by the electrostatic interaction between the RNA subunit and the cationic peptide subunit of RNP scaffold.

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Collaboration Works

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

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森井孝，中田栄司，Seoul National University（韓国），特定空間に配置された酵素複合体の構築

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

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大垣英明，森井孝，片平正人，野平俊之，モンゴル国立大学，インドネシア大学，フィリピン大学ディリマン校，ベトナム国家大学ハノイ校，ラオス国立大学，王立プノンペン大学，アジア新興国産天然資源を由来とする機能性物質創生のための高度分析研究拠点の形成

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1. Grant-in-Aid for Scientific Research

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

中田栄司，基盤研究(B)，DNA ナノ構造体の階層的自己組織化による高効率な酵素連続反応場の構築

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Structural Energy Bioscience Research Section

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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 2020.

2. Activity analysis of *Pe*GE on the cleavage of ester-linkage in natural woody biomass

The major components of woody biomass, cellulose, hemicellulose, and lignin, are promising carbon-neutral resources to produce biofuels and various materials. These components form the rigid complex so-called lignin-carbohydrate complex (LCC) in natural biomass. One of the direct linkage contributing to LCC formation is ester-linkage between lignin and glucuronic acid residue in hemicellulose. Fungal glucuronoyl esterases (FGEs) catalyze the cleavage of the ester linkage and thereby facilitate the isolation of woody biomass components. Our previous study revealed that FGE from *Pleurotus eryngii* (*Pe*GE) has the highest activity toward a model substrate, benzyl glucuronic acid. This year, we have investigated the activity of *Pe*GE on the cleavage of the ester-linkage in natural LCC. NMR spectra of the LCC fraction that was extracted from natural woody biomass were recorded before and after the treatment by *Pe*GE. Change in the signal intensity of the ester-linked lignin and glucuronic acid residue proved that *Pe*GE can catalyze the cleavage of the ester-linkage in woody biomass.

3. Structural and functional analysis of lytic polysaccharide monooxygenase

Saccharification of cellulose by cellulolytic enzymes is a crucial process in the production of 2nd-generation biofuels. Lytic polysaccharide monooxygenases (LPMOs), which catalyze oxidative cleavage of glycosidic linkage, are known to have a synergistic effect on the activity of cellulases on the degradation of crystalline cellulose. Previously we had obtained a crystal of LPMO of a white-rot fungus and solved the crystal structure. We further refined the structure, which revealed that this LPMO has a canonical structure of AA9 family, having a copper ion at the catalytic center (Figure 1). Some polar amino acid and three tyrosine residues around the catalytic center apparently participate in the binding with cellulose. Furthermore, the synergy of LPMO

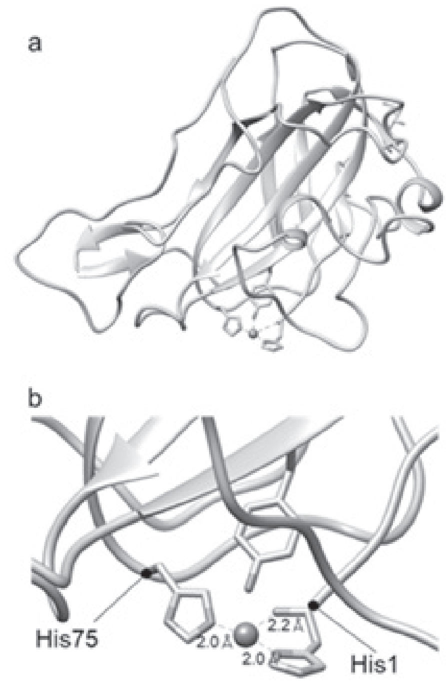

Figure 1. Over-all structure (a) and copper-coordination (b) of LPMO. The copper ion and its coordinating residues are connected with dashed lines and distances.

and cellulase cocktail was investigated. In our previous study, simultaneous use of LPMO and cellulase cocktail exerted a 1.3-fold higher glucose yield from crystalline cellulose than the individual use of LPMO and cellulase cocktail. This year we optimized the conditions for the cellulose degradation, by which a 4.7-fold higher glucose yield was recorded.

4. Aggregation of FUS induced by mechanistic shear stress on pipetting and its suppression by non-coding RNA

Fused in sarcoma (FUS) has been considered as a molecular link between apparently different neurodegenerative diseases such as amyotrophic lateral sclerosis (ALS). Although the neurodegenerative diseases have different manifestations, FUS aggregation is associated with all of them, which suggests a common pathway for their neuropathologies. We found that FUS transforms into the amorphous aggregation state as an instant response to the shear stress caused by usual pipetting, by means of fluorescence spectroscopy, fluorescence microscopy, and transmission electron microscopy (TEM) (Figure 2). The more the number of strokes of pipetting is, the more the number of aggregates is. It was also revealed that non-coding RNA can suppress the transformation of FUS into aggregates. There is the possibility that RNA bound to the C-terminal region of FUS masks the interface required for the formation of aggregates, resulting in the prevention of aggregate formation. It is also likely that RNA bound to the C-terminal region of FUS neutralizes the cations and reduces the cation-π interaction between the N- and C-terminal regions, resuktinh in the prevention of aggrergate formation. The suppressive effect of RNA on FUS aggregation is sequence-dependent. These results suggested that the non-coding RNA could be a prospective suppressor of FUS aggregation caused by mechanistic stress in cells. Our finding might serve for the development of therapies for neurodegenerative diseases by using RNA as aggregation inhibitors.

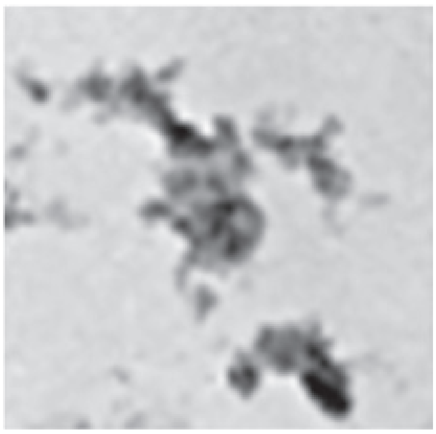

Figure 2. The TEM image showing FUS aggregates formed after 30 strokes of pipetting.

5. The detection of the DNA triplex structure in the living human cells

DNAs reportedly fold into not only a double-helix structure but also a triple-helix or triplex structure under *in vitro* conditions. However, the formation of the triplex structure of DNA in living human cells has not been proven. Here, the oligodeoxynucleotide (triplex ODN) that forms a triplex structure under *in vitro* conditions was introduced into HeLa cells by cell-resealing system utilizing a pore-forming toxin. The NMR spectrum of this sample was recorded, in which the imino proton signals of the triplex ODN inside the living cells were clearly detected. Most importantly in the living cells, all the imino proton signals that correspond to the triplex structure of the triplex ODN formed under *in vitro* conditions were commonly observed. This result indicates that the triplex ODN forms the triplex structure that is similar, if not the same, to that formed in *in vitro* even in the living human cells.

6. Interaction of human origin recognition complex subunit 1 with human G-quadruplex DNAs

DNA replication initiates from particular loci in genomes called replication origins. Origin recognition complex (ORC) binds to a replication origin and recruits other replication factors. ORC in some organisms reportedly bind to a replication origin sequence-specifically. However, the manners by which human ORC (hORC) recognizes a replication origin is ellusive. Genome-wide studies revealed previously that guanine (G)-rich sequences are present in most replication origins in human genome. Our previous study implied that the amino acid region 413-511 of the first subunit of hORC, hORC1(413-511), binds preferentially to G-rich DNAs that form a G-quadruplex (G4) structure. Here, we investigated the interaction of hORC1(413-511) with various G-rich DNAs derived from human c-myc promoter and telomere regions. Fluorescence anisotropy revealed that hORC1(413-511) binds preferentially to DNAs that formed G4 structures over ones having double-stranded structures. CD and NMR clearly showed that the G4 structures of those G-rich DNAs were retained even after complex formation. Importantly, NMR chemical shift perturbation analyses revealed that hORC1(413-511) primarily binds to the external G-tetrad planes of the G4 structures. Our study propose that human ORC1 may recognize replication origins through the G4 structure.

Collaboration Works

片平正人，Gyeongsang National University（韓国），プリオン蛋白質の悪性化を阻害する RNA アプタマーに関する構造機能相関

片平正人，University of Naples "Federico II"（イタリア），プリオン蛋白質の悪性化を阻害する RNA アプタマーへの化学修飾の導入による高性能化

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

片平正人，永田崇，BIOTEC，NSTDA（タイ），LIPI（インドネシア），NUOL（ラオス），サトウキビ収穫廃棄物の統合バイオリファイナリー

大垣英明，森井孝，片平正人，野平俊之，モンゴル国立大学，インドネシア大学，フィリピン大学ディリマン校，ベトナム国家大学ハノイ校，ラオス国立大学，王立プノンペン大学，アジア新興国産天然資源を由来とする機能性物質創生のための高度分析研究拠点の形成

永田崇，Institute of Biophysical Chemistry，Goethe-University，Frankfurt am Main，（ドイツ），深層学習の技術を取り入れた多次元 NMR 解析とタンパク質立体構造解析のシステム開発

永田崇，Institute of Biophysical Chemistry，Goethe-University，Frankfurt am Main（ドイツ），有糸分裂から減数分裂への切り替えを担う因子 YTHDC2 の立体構造解析

永田崇，State University of New York at Albany，Albany, NY，United States（アメリカ），核酸の in-cell NMR 測定方法の開発

Financial Support

1. Grant-in-Aid for Scientific Research

片平正人，基盤研究(B)，神経変性疾患に関連した反復配列 RNA 分子の反復回数に依存した液液相分離の構造基盤

片平正人，挑戦的研究（萌芽），同一 RNA 分子によるプリオン蛋白質と Aβ 蛋白質の無毒化及び三者間のクロストーク（期間延長）

片平正人，挑戦的研究（萌芽），Aβ 受容体であるプリオン蛋白質を RNA で阻害することによる抗アルツハイマー病効果

永田崇，基盤研究(C)，核酸とペプチドツールを用いたアルツハイマー病関連複合体の形成原理の解明

永田崇，基盤研究(C)，癌・幹細胞増殖性維持に関わる翻訳抑制複合体の形成原理と創薬に向けた分子基盤の構築（期間延長）

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2. Others

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片平正人，科学技術振興機構，サトウキビ収穫廃棄物の統合バイオリファイナリー

永田崇，日本医療研究開発機構，中分子アゴニスト創薬のロジカルデザイン～ＯＸ４０ アゴニスト開発を実施例として～

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Advanced Energy Utilization Division

A. Rajendran, Junior Associate Professor

1. Introduction

Topology-specific DNA structures, such as small loops,[1] supercoils,[2] knots,[3] and catenated mini and maxicircles,[4] occur in numerous instances in vivo. Polycatenanes can be found in the kinetoplast DNA, a part of the mitochondrial DNA of certain protozoa, consists of a network of thousands of minicircles with 0.5-10 kb and dozens of maxicircles with 20-40 kb.[4] Synthetic molecules with interlocked units were achieved in macromolecular chemistry decades ago,[5, 6] and is the current topic of interest in structural DNA nanotechnology. Interlocked-DNAs, such as DNA catenanes, are of special interest for the construction of molecular switches, motors,[7] and logical devices[8].

2. Synthesis of topologically-interlocked minicircle DNAs inside a DNA origami frame

By considering the potential of the minicircle and interlocked DNAs, we have designed and characterized the formation of DNA rotaxane and catenane inside a frame-shaped DNA origami (Figure 1).[9, 10] This origami frame contains four ss-loop connectors (denoted as A, B, C & D) that serve as attachment sites for the rotaxane linear duplex or functions as one of the two rings for the catenane when base-paired with complementary strand. The rotaxane linear duplex contains 67 bp with additional 32 bases long ss-overhangs at each end for attachment with the loop regions of the origami. The rotaxane and catenane rings were prepared by using six different ssDNAs (total length: 183 bp), all phosphorylated at the 5′-end. Intrinsically bent AT-tracts were used to induce the curvature of the ring.[11, 12] The formation of the interlocked structures was characterized by agarose gel electrophoresis (AGE) using fluorophore-labelled DNA, and also by atomic force microscopy (AFM). As designed, we have successfully prepared the top rotaxane and catenane inside the origami frame (Figure 1, AGE images). The average formation yields before and after ligation were respectively 14 and 31% for top rotaxane, and 42 and 62% for catenane. This indicated clearly that the ligation of the nicks in the rings is necessary to stabilize the interlocked structures. Next, the formed structures were directly visualized by AFM which clearly revealed the linear duplex and ring of the rotaxane, and their attachment between the connectors A-B. The catenane is also formed as designed, and the smaller (loop-A, 64 bp) and the larger (183 bp) rings are clearly observed. The formation yields estimated from the AFM images were 30 and 59% respectively for top rotaxane and catenane, being similar to the AGE results. The outer diameters of the top rotaxane and catenane rings estimated from the AFM images were 25 and 24 nm, respectively, which agree well with the theoretical value of ~24 nm. The rotaxane structure was also prepared at the bottom position between the connectors C-D (42% yield), and at both top and bottom positions (dual rotaxane, 60% yield).

3. Probing nucleosomal DNA topology and DNA-protein interactions

Besides their presence in vivo, DNA minicircles have been used to probe the topological features of

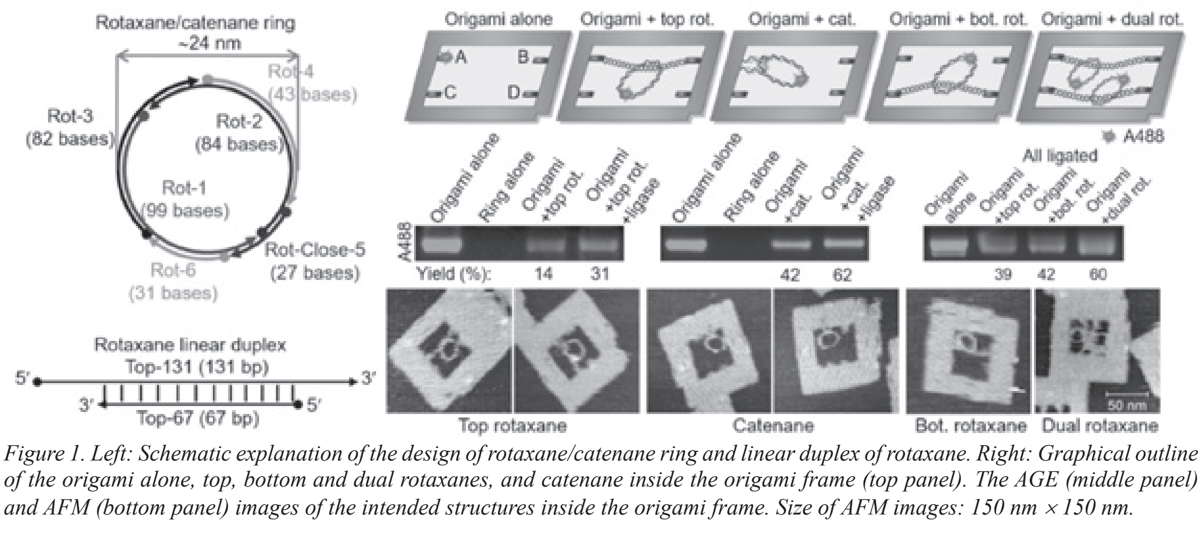
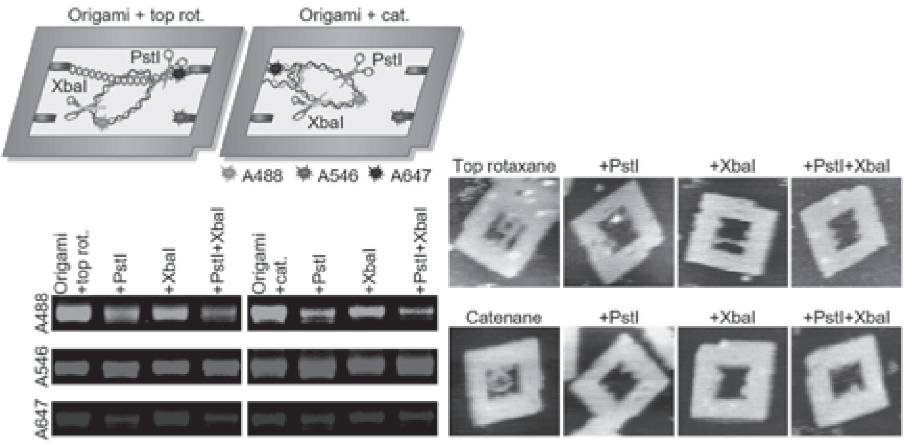


Figure 1. Left: Schematic explanation of the design of rotaxane/catenane ring and linear duplex of rotaxane. Right: Graphical outline of the origami alone, top, bottom and dual rotaxanes, and catenane inside the origami frame (top panel). The AGE (middle panel) and AFM (bottom panel) images of the intended structures inside the origami frame. Size of AFM images: 150 nm × 150 nm.



Structures inside origami + Enzymes	% Reaction AFM	% Reaction AGE
Cat.+PstI	41	52
Cat.+XbaI	57	49
Cat.+PstI+XbaI	63	65
Top rot.+PstI	53	48
Top rot.+XbaI	49	42
Top rot.+PstI+XbaI	71	65
Bot. rot.+PstI		50
Bot. rot.+XbaI		42
Bot. rot.+PstI+XbaI		60
Dual rot.+PstI		36
Dual rot.+XbaI		48
Dual rot.+PstI+XbaI		65
Top linear 131/67+PstI	48	
Top linear 141/77+PstI	56	
Top linear 151/87+PstI	62	

Figure 2. Left: Graphical representations (top) and AGE analyses (bottom) of the restriction enzymatic reactions on the interlocked structures. Middle: Representative AFM images of the singly and doubly digested structures. Right: List of the enzymatic reaction yields for all the structures inside the origami. Size of AFM images: 150 nm × 150 nm.

DNA and DNA-protein interactions.[13] The energetic and steric limits of DNA gyrase were probed using DNA minicircles and was shown to be capable of introducing two negative supercoils into a minicircle of length 174 bp.[14] Further, the minicircles with 75 and 86 bp were also used to mimic the nucleosome-induced DNA curvature in the absence of histones for the process of retroviral integration.[15] The HIV-1 integrase reaction was enhanced 5-10 and 15-20 fold respectively in the absence and presence of the LEDGF/p75 integration cofactor for the minicircles when compared to linear DNA of the same length and sequence. This indicated the importance of DNA topology such as curvature; additionally, the cofactor activates integration into nucleosome-like curved DNAs even in the absence of histones. Here, we have utilized the synthesized topologically-interlocked nano-assemblies to probe the DNA topology and DNA-protein interactions by the restriction reactions (Figure 2). For comparison, we have adapted the free-linear duplexes and the duplexes attached inside the origami with relatively less flexibility, and free- or topologically-interlocked minicircles inside the origami. Restriction enzymatic reactions were chosen as they were often used to probe the protein (e.g. transcription factors) accessibility to promoter DNA in chromatin in the methods such as “restriction enzyme protection assay” as proxies for transcription factors. The enzyme PstI has single scission site in the linear duplex of rotaxane and the ring of catenane, while XbaI has a single site in both the rotaxane and catenane rings. At first, the steady state reactions were probed on the interlocked structures inside origami. Though, the enzymatic reactions were proceeded, the estimated reaction yields were as low as 36% to as high as 57%. The double digestions yielded higher reactions of 60-71%, but the reactions never went completion. The time- and enzyme concentration-dependent digestion reactions were also carried out on the interlocked-structures. The reactions proceeded slowly and steadily, and the obtained maximum yields were ≤30%. Further, the analysis was also carried out on the linear duplex and rings in the absence of origami. Except the free-linear duplex, all tested structures were reluctant for the restriction digestion, indicating that the topological features of DNA, such as flexibility, curvature, and groove orientation, play a major role in DNA-protein interactions. Our results by using the histone-free artificial DNA structures are consistent with the investigations carried out on nucleosomal DNAs and revealed the critical influence of DNA topology, similar to the one in nucleosomal DNA, on the DNA-protein interactions.

4. References

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Collaboration Works

Rajendran Arivazhagan， Visvesvaraya Technological University（インド），Stabilization of DNA nanomaterials by enzymatic and chemical methods

Rajendran Arivazhagan，National Institute of Technology, Calicut（インド），DNA nanomaterials for the analysis of single molecular reactions

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

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

Financial Support

Rajendran Arivazhagan，（公財）京都大学教育研究振興財団，ＤＮＡオリガミを利用して構築するケミレジスタセンサーの開発

Presentations

Rajendran A., Park S., Nakata E., Kwon Y., Osheroff N., Morii T., Enzymatic reactions on topologically-interlocked DNA structures inside a DNA origami frame, The 100th CSJ Annual Meeting, Tokyo University of Science, Tokyo, 2020.3.22-25

Rajendran A., Single molecular analysis of chemical and biological processes using DNA origami, International Conference on Recent Advancement in Chemical Sciences, Online, 2020.8.10-14

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 resources consumption and environmental protection, becoming an important 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 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 utilisation efficiency in catabolism. Also, we are remarking on the sustainable methods of food production, which is the energy of life. We are globally working with academisms, biotechs and university start-ups to aim for networking of researches toward social implementation of our technologies.

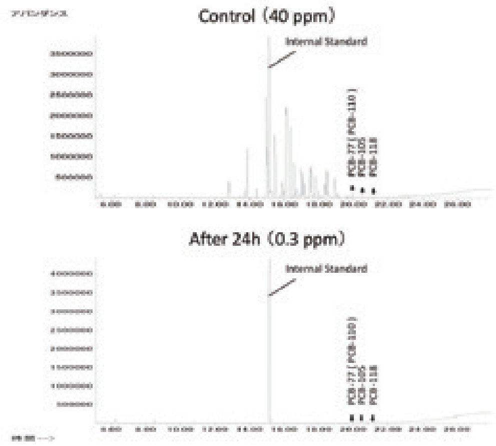

Figure 2. The data from the gas chromatography-quadrupole mass spectrometer showing the PCBs degradation by the composite BDOs-microbial catalyst.

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

Polychlorinated biphenyls (PCBs) are well known environmental pollutants and dispersed in all our living environments. Biphenyl dioxygenase (BDO) plays a crucial role in the degradation of PCBs. BDO catalyses the incorporation of two oxygen atoms into the aromatic ring of PCB, which induces the aromatic ring cleavage. Importantly, we developed the composite type of catalytic enzyme that consists of the two BDOs with different substrate specificities; moreover, we developed the bioreactor for generating oxygen microbubbles that enhances the enzymatic activities of 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 of Japan.

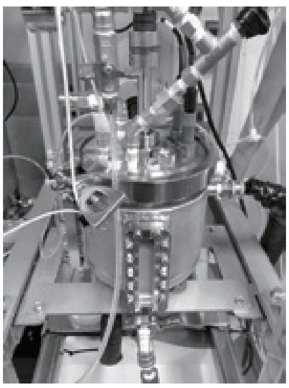

Figure 1. The composite BDOs-microbial catalyst was evaluated in the dedicated experimental bioreactor with the device of oxygen microbubble generation.

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

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 *Dehalobacter* sp. and *Desulfitobacterium* sp. by 16S rRNA gene phylogenetic analysis. Wang and He (*Environ Sci Technol*, 2013) reported that '*Dehalobacter*' dechlorinates penta-/hexa-chlorinated 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 so far. Besides, we also observed that these two bacterial species reduce PCBs in the artificial model of the polluted environmental. Even today, repeated long-term observation is being made to confirm whether the result is correct.

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

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

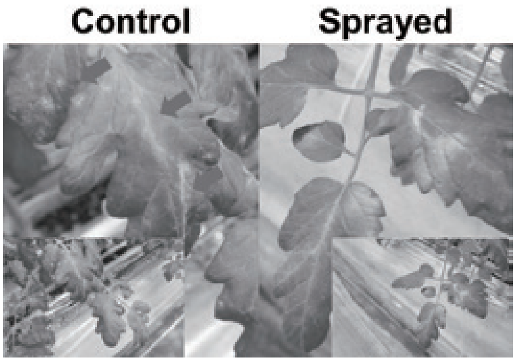

Figure 3. The glycosidase secreted type of the composite microbial catalyst inhibited tomato-*Pestalotia disease*.

fied into approximately 130 families, and their catalytic reactions are roughly divided into anomeric inversion and/or anomer retention and exoglycosidase or endoglycosidase. Given, the classification of glycosidase can be understood as diverse. We have considered that it is possible to efficiently digest fungi cell wall by compositely capably using these diversities of enzyme activities.

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

We investigated the fungicidal properties of glycosidases produced by a phytopathogenic filamentous strain belonging to basidiomycetes. This filamentous strain secretes enzymes when grown in a bran medium and exhibits various glycosidase activities. The crude enzyme fraction showing such composite glycosidase activities digested 3 out of 6 wet-rice-specific epidemically filamentous fungi (Figure 4). There are not so many enzymes showing high digesting activity against multiple strains of phytopathogenic filamentous fungi. Single glycosidase activity, however, digested only 2 strains. These results suggest that the compositive glucosidase has a highly fungicidal activity rather than the individual glycosidase. In fact, we try to purify the components of this crude enzyme.

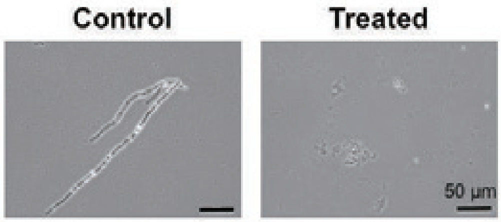

Figure 4. The crude enzyme fraction secreted from the phytopathogenic filamentous fungus digested a wet-rice specific epidemically filamentous fungal strain.

Soon, we will be able to clarify the effectively fungicidal mechanism of this crude enzyme by definite the type of the enzyme(s), the amounts of the secretion, and the specific activities.

4. Pigmented and non-pigmented *Bacillus* spores work together to improve growth, quality and health of shrimp.

The collaborative research with Vietnam National University found that two strains of *Bacillus* isolated from the intestinal tract of white-leg shrimp showed excellent health-improving effects (1). This *Bacillus* probiotic avoids using antibiotics and synthetic chemicals in feeding, enhances shrimp health and growth efficiency, and reduces the energy consumption in white-leg shrimp cultivation. This cultivates industry has been recently growing in Japan, but there is really almost no appropriate feed. To meet that market demand, we have begun considering the possibility of feed registration with the Ministry of Agriculture, Forestry and Fisheries of Japan in collaboration with the company in Vietnam and Japan.

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Collaboration Works

原富次郎，髙塚由美子，Lamont Doherty Earth Observatory-Clumbia University（アメリカ），ポリ塩化ビフェニル類を分解する微生物とその由来酵素

原富次郎，髙塚由美子，Department of Civil and Environmental Engineering-National University of Singapore（シンガポール），ポリ塩化ビフェニルを脱塩素化する細菌

Financial Support

1. Grant-in-Aid for Scientific Research

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

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

2. Others

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

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

原富次郎，（株）竹中工務店，環境微生物学研究部門

原富次郎，東洋ガラス（株），環境微生物学研究部門

原富次郎，とつかわ水産（株），環境微生物の調査研究のため

Publications

T.T. Nguyen, H.T. Nguyen, H.T.T. Pham, A.H. Nguyen, T.N. Phan, T. Hara, Y. Takatsuka, A.T.V. Nguyen, Cooperative improvement in growth rate, red-colour score and astaxanthin level of white-leg shrimp by Bacillus strains originating from shrimp gut, Journal of Applied Microbiology, 129, 1, 51-62, 2020

T. Jamnongkan, R. Mongkholrattanasit, A. Wattanakornsiri, P. Wachirawongsakorn, Y. Takatsuka, T. Hara, Green adsorbents for copper (II) biosorption from waste aqueous solution based on hydrogel-beads of biomaterials, South African Journal of Chemical Engineering, 35, 14-22, 2020

Presentations

原富次郎，微生物が生み出す小さなエネルギーの社会利用 ～五月雨を集めてはやし最上川～，第 36 回京都大学宇治キャンパス産学交流会，オンライン開催，2020.9.1

A.T.V. Nguyen, Y. Takatsuka, N.T.H Le, A.P. Bui, M.T. Tran, S.V. Chu, H.T.N. Vo, T.T. Nguyen, H.T.T. Pham, N.T. Phan, A.H. Nguyen, K. Yokota, T. Ohira, F. Yamane, T. Hara, Investigation of carotenoid synthesis and microbiome changes in shrimp gut upon feeding shrimp with combined pigmented and non-pigmented Bacillus spores, The 11th International Symposium of Advanced Energy Science, Online, 2020.9.15-16

A. Khankhuean, T. Hara, Y. Takatsuka, T. Jamnongkan, Preparation and characterization the enzyme immobilization by entrapment within a bio-polymer hydrogel network, The 11th International Symposium of Advanced Energy Science, Online, 2020.9.15-16

M. Ueno, Y. Gondo, S. Matsumoto, T. Hara, Y. Takatsuka, Developmental research on microbial community structure analysis and biopest applications in medicinal plant cultivation, The 11th International Symposium of Advanced Energy Science, Online, 2020.9.15-16

T. Tsurumi, T. Fujimaki, Y. Takatsuka, T. Hara, K. Yokota, Structural identification and biological activity of fengycin, cyclic lipopeptide, derived from Bacillus subtilis YAE51, The 11th International Symposium of Advanced Energy Science, Online, 2020.9.15-16

T. Jamnongkan, A. Yosta, B. Thanesthakul, M. Sugimoto, T. Hara, Y. Takatsuka, R. Mongkholrattanasit, Effect of ZnO nanoparticles on the physical properties of PLA/PBS biocomposite films, 2020 8th International Conference on Mechanical Engineering, Materials Science and Civil Engineering (ICMEMSCE2020), Bangkok, Thailand, 2020.11.23-24

3-2. AWARD

Young Scientist Award of the Physical Society of Japan

Quantum Radiation Energy Research Section
Heishun Zen (Assistant Professor)

Assistant Professor Heishun Zen was awarded Young Scientist Award of the Physical Society of Japan (JPS) on March 13th, 2021. The award has been established in order to encourage young researchers in their research work and further enliven the physics community. Recipients are selected from each division for their activities including lectures at academic meetings, publications, and degree theses. He was awarded this award on the achievements of "Research and Development of improving performance of a mid-infrared free electron laser".

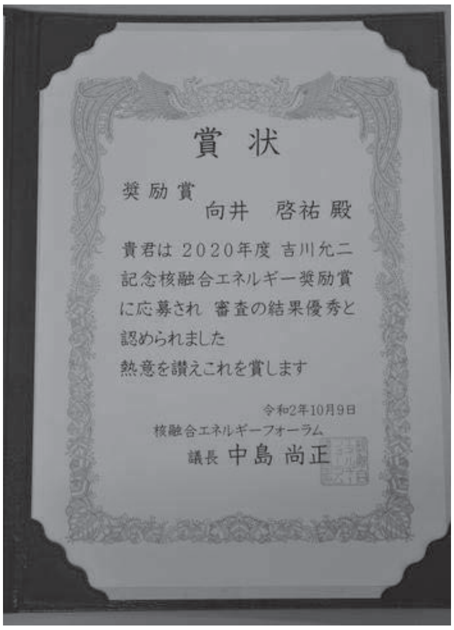
In his award lecture, which was held on March 13th, 2021 in the online conference, he presented two research works to improve the performance of midinfrared free electron laser in Kyoto University. One is a beam loading compensation method named "cavity detuning" for compensating the heavy transient beam loading effect in a thermionic RF gun used for driving a midinfrared free electron laser. He invented this method when he was a doctor course student of Graduate School of Energy Science, Kyoto University. The other is the high efficiency lasing enabled by dynamic cavity desynchronization. By this research he achieved the highest extraction efficiency of the oscillator-type free electron laser which driven by a normal conducting linear accelerator.

2020 Masaji Yoshikawa Memorial Prize for Fusion Energy Fusion Energy Forum of Japan

Advanced Atomic Energy Research Section
Keisuke Mukai (Assistant Professor)

Assistant Professor Keisuke Mukai was awarded 2020 Masaji Yoshikawa Memorial Prize for Fusion Energy from the Fusion Energy Forum of Japan (FEFJ). The FEFJ, chaired by Dr. Naomasa Nakajima, Emeritus Professor of the University of Tokyo and Headmaster of Kaiyo Academy, inaugurated the Masaji Yoshikawa Prize for Fusion Energy in 2007 to manifest outstanding dissertations and publications by young scientists and students who are expected to contribute to successful achievements in fusion research.

The research title is "Fundamental studies on structure, chemical properties, and fuel production of breeding blanket materials". Assistant Professor Keisuke Mukai received the prize in the online celemony in 13th FEFJ Plenary meeting on 9th March 2021.



17th Young Researcher Award in Fusion Engineering Division, Atomic Enrgy Society of Japan

Advanced Atomic Energy Research Section
Keisuke Mukai (Assistant Professor)

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

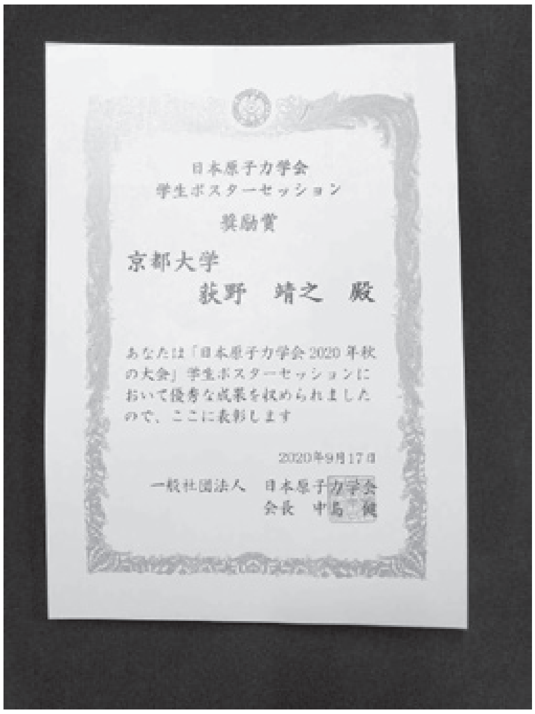
Assistant Professor Keisuke Mukai performed high temperature neutron diffraction study and showed ion diffusion pathways within the bulk of lithium metatitanate ceramic breeder. Vapor chemistry and its effect on corrosion of reduced activation ferritic martensitic steel were studied experimentally in his research. He was awarded 17th Young Re-searcher Award in Fusion Engineering Division, Atomic Energy Society of Japan in an online celemony on 27th October 2020.

Student Poster Award, Atomic Energy Society of Japan

Advanced Atomic Energy Research Section
Yasuyuki Ogino (D2)

Yasuyuki Ogino (D2) was awarded Student Poster Award from Atomic Energy Society of Japan (AESJ) on 17th September 2020. This poster session is hosted by the AESJ Student Network and the AESJ Diversity Promotion Committee. In the session, diverse presentations are made by students, who range from undergraduate to doctoral, and the Diversity Promotion Committee.

Yasuyuki Ogino conducted neutron transport simulations for measuring neutron spatial distribution in a fusion blanket mock-up. Combinations of activation foils were investigated in the study to measure fast, epi-thermal, and thermal neutrons separately.



Young Researcher Award in 37th Annual Meeting of JSPF

Advanced Atomic Energy Research Section
Yasuyuki Ogino (D2)

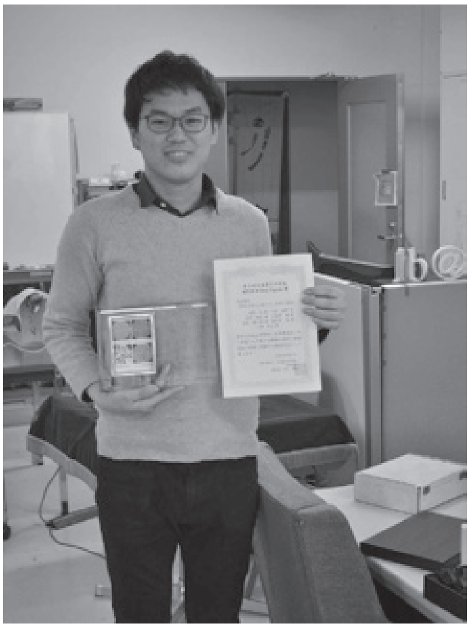
Japan Society Plasma Fusion (JSPF) gives the Best Presentation Awards at the JSPF Annual Meeting to the excellent oral/poster presentations by young researchers and/or students. Yasuyuki Ogino (D2) was awarded the best presentation award at the 37th JSPF annual meeting on 4th December 2020. He measured the γ-ray distribution in the Large Helical Device in National Institute for Fusion Science using a portable high-purity germanium detector. The activation of the vacuum vessel and armor materials were compared with photon transport calculations using Monte Carlo Simulation code.

3rd Best Figure Award in Material Science and Technology Division, Atomic Energy Society of Japan

Advanced Atomic Energy Research Section
Ryo Omura (M2)

Scientific figures by Ryo Omura (M2) were selected for 3rd Best Figure Award from Material Science and Technology Division, Atomic Energy Society of Japan on 17th March 2021. This award is given for beautiful figures which contribute to nu-clear material research and development. He was awarded this prize on cross-section images of aged Fe–Ti alloy taken by scanning electron microscope.

The analysis using energy dispersive X-ray (EDX) and electron back-scatter diffraction (EBSD) showed Ti segregation and N trap in the grain boundary of the Fe–Ti sample immersed in liquid Li.



Best Poster Presenter Award (COMSOL CONFERENCE 2020 TOKYO)

Advanced Plasma Energy Research Section
Yuki Oka (M2)

COMSOL Multiphysics is a Finite Element Method software for multiphysics analysis based general purpose physics simulation software developed by COMSOL AB, Sweden. It can simulate any physical phenomenon, regardless of the field. COMSOL Conference is held annually in the United States (Boston), Europe, and Asian cities including Tokyo, and is a forum for COMSOL users to present their case studies.

Yuki Oka (M2) attended the conference in the field of electromagnetism and optics, and made a poster presentation on the title of "Simulation of Electromagnetic Mode Conversion in Millimeter-Wave Frequency Band in Magnetically Confined Fusion Plasmas".

He received the Best Poster Presenter Award from the KEISOKU ENGINEERING SYSTEM CO., LTD. which is the exclusive distributor in Japan for COMSOL, Inc.

Student Presentation Award (2020 Autumn meeting of the Physical Society of Japan)

Advanced Plasma Energy Research Section
Ryota Matoike (D2)

The 2020 Autumn meeting of the Physical Society of Japan was held on the web from 8th-17th September, 2020. Ryota Matoike (D2) attended the meeting in the field of plasma (Category 2), and made an oral presentation on the title of "Peripheral plasma transport characteristics against 3D magnetic field structure in Heliotron J". He received the Student Presentation Award from the Physical Society of Japan. In this research, he analyzed the cause of the change in the heat load distribution in high-density plasmas using a three-dimensional tra

The Physical Society of Japan
日本物理学会学生優秀発表賞
領域2
的池 遼太 殿
あなたの2020年日本物理学会
秋季大会における講演
9pB2-2 Heliotron Jにおける三次元磁場構造を背景とした周辺プラズマ輸送特性
は、当学会の学生優秀発表賞を受賞されましたことをここに証します
2020年10月10日
一般社団法人日本物理学会
会長 永江知文

CERTIFICATE
Student Presentation Award
of the Physical Society of Japan
Division2
To
Matoike Ryota
Title of presentation
Peripheral plasma transport characteristics against 3D magnetic field structure in Heliotron J
At 2020 Autumn meeting of the Physical Society of Japan.
Presentation ID 9pB2-2.
October 10, 2020
President, The Physical Society of Japan
Tomofumi Nagae

Student Presentation Award (2020 Autumn meeting of the Physical Society of Japan)

Complex Plasma Systems Research Section
Panith Adulsiriswad (D2)

2020 Autumn meeting of the Physical Society of Japan was held on September 8-11, 2020, on-line. This meeting has a long history since 1946 and it has covered almost all fields of physics.

Panith Adulsiriswad (D2) attended in the meeting and made a presentation titled "Numerical Investigation of the Energetic Particle Redistribution and Interaction with Alfvén Eigenmode in Heliotron J".

He received the Student Presentation Awared of the Physical Society of Japan (division 2, or plasma physics).


The Physical Society of Japan
日本物理学会学生優秀発表賞
領域2
Adulsiriswad Panith
あなたの2020年日本物理学会秋季大会における講演
8pB2-4 Numerical Investigation of the Energetic Particle Redistribution and Interaction with Alfven Eigenmode in Heliotron J
は、当学会の学生優秀発表賞を受賞されましたことをここに証します
2020年10月10日
一般社団法人日本物理学会
会長 永江知文

CERTIFICATE
Student Presentation Award of the Physical Society of Japan
Division2
To
Adulsiriswad Panith
Title of presentation
Numerical Investigation of the Energetic Particle Redistribution and Interaction with Alfven Eigenmode in Heliotron J
At 2020 Autumn meeting of the Physical Society of Japan.
Presentation ID 8pB2-4.
October 10, 2020
President, The Physical Society of Japan
Tomofumi Nagae

4th Asia-Pacific Conference on Plasma Physics, AAPPS-DPP Poster Prize

Complex Plasma Systems Research Section
Panith Adulsiriswad (D2)

AAPPS-DPP2020, or 4th Asia Pacific Conference on Plasma Physics, Division of Plasma Physics, Association of Asia-Pacific Physical Societies was held on 26-31, October, 2020 on-line.

This conference, under the authority of AAPPS-DPP for scientific discussions on plasma physics, orients to physics and provides interdisciplinary and in-depth discussions among and in various fields of plasma physics and application.

Panith Adulsiriswad (D2) attended the meeting and made an on-line poster presentation titled "Simulation Study of Energetic Particle-driven MHD Modes and Energetic Particle Redistribution in Heliotron J".

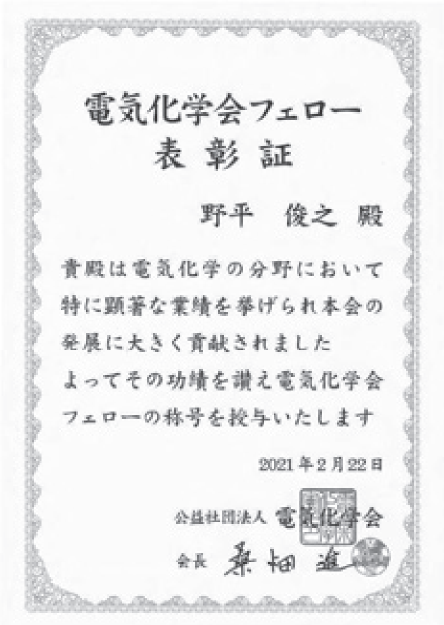
He received the Poster Prize for his presentation.


AAPPS DPP
AAPPS-DPP Poster Prize
Following poster presentation is selected as significant work.
Poster ID: MF- P17
Presenter: P. Adulsiriswad
Presentation Title:
"Simulation Study of Energetic Particle-driven MHD Modes and Energetic Particle Redistribution in Heliotron J"
Members : Y. Todo, S. Kado, S. Yamamoto, S. Kobayashi, S. Ohsima, T. Minami, H. Okada, A. Ishizawa, Y. Nakamura, S. Konoshima, T. Mizuuchi, K. Nagasaki
Selection committee Chair
Abhijit Sen
4th Asia-Pacific Conference on Plasma Physics
October 26 (Monday) -31(Friday), 2020
On-line Remote Conference
AAPPS

The Fellow of The Electrochemical Society of Japan

Chemical Reaction Complex Processes Research Section
Toshiyuki Nohira (Professor)

Professor Toshiyuki Nohira was awarded the Fellow of The Electrochemical Society of Japan on February 22nd, 2021. The title of Fellow is awarded to those who are under 65 years of age and who have made particularly notable academic or practical achievements, or who have made particularly notable contributions to the management of the Society.


電気化学会フェロー
表彰証

野平 俊之 殿

貴殿は電気化学の分野において
特に顕著な業績を挙げられ本会の
発展に大きく貢献されました
よってその功績を讃え電気化学会
フェローの称号を授与いたします

2021年2月22日

公益社団法人 電気化学会
会長 桑畑 進

Research Encouragement Award at The 52nd Symposium on Molten Salt Chemstry

Chemical Reaction Complex Processes Research Section
Xianduo Meng (M2)

The 52nd Molten Salt Symposium, which was sponsored by the Molten Salt Committee of the Electrochemical Society of Japan, was held on 26th November, 2020. This event provides young researchers and students in the field of molten salt chemistry and its surrounding area an opportunity to present their works.

Xianduo Meng (M2) attended and made an oral presentation on the topic of "The Effect of Temperature on Smoothness and Crystal Phase of Tungsten Films Electrodeposited in Molten CsF–CsCl–WO_3".

He received the Research Encouragement Award from the Molten Salt Committee of the Electrochemical Society of Japan.

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

Chemical Reaction Complex Processes Research Section
Makoto Unoki (M2)

The 3rd Kansai Electrochemistry Workshop was held on 28st November 2020 on Webinar, which was held by the Kansai Branch of the Electrochemical Society of Japan. This event provides young researchers and students in the field of electrochemistry and its surrounding area an opportunity to present their works.

In the meeting, Mr. Makoto Unoki (M2) attended and made a poster presentation on the topic of "Optimization of electrolysis conditions for Ti film electrodeposition from LiF–LiCl eutectic molten salt", and received the Young Researcher's Award. He investigated the optimum conditions for electrodepositing compact, smooth, and adherent Ti films in LiF–LiCl–Li_3TiF_6 at 823 K. The Li_3TiF_6 was formed in-situ in the melt via comproportionation reaction between Li_2TiF_6 and Ti powder. The solubility of Li_3TiF_6 was confirmed to be higher than 7.1 mol% by cyclic voltammetry and ICP-AES measurement. Galvanostatic electrolysis was conducted on Ni plate substrates at various concentrations of Li_3TiF_6 (0.55, 2.6, 7.1 mol%) and cathodic current density (50–1200 mA cm^{-2}). In this study, Ti films having the smoothest surface were obtained at 7.1 mol% of Li_3TiF_6 and 50 mA cm^{-2}.

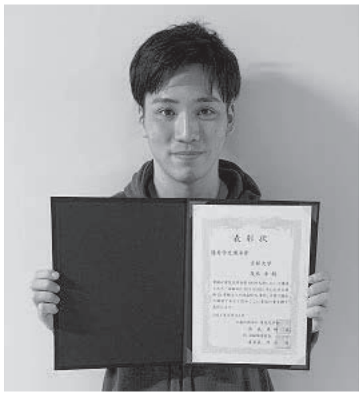
Research Encouragement Award at The 88th ECSJ Spring Meeting

Chemical Reaction Complex Processes Research Section
Wataru Moteki (M1)

The 88th ECSJ Spring Meeting, which was sponsored by the Electrochemical Society of Japan, was held on 22–24th March, 2021. This event provides young researchers and students in the field of molten salt chemistry and its surrounding area an opportunity to present their works.

Wataru Moteki (M1) attended and made an oral presentation on the topic of "Crystalline Si electrodeposition of molten KF–KCl–K_2SiF_6 on liquid Zn electrode".

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. 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.

Poster of the 10th International Symposium

Many researchers have participated in this program. In FY2020 Joint Usage/Research collaborations of total 116 subjects (including two workshop) on Zero Emission Energy were performed with more than 263 visiting participants from 51 all-Japan Universities and Institutions including graduate/undergraduate students. Researchers from 9 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 2020". The meeting to present some of remarkable results obtained in FY2020 was planned to be held online on March 9, 2021. If you have interest to this collection, please contact to the Office of Zero Emission Energy Research.

In addition to the Joint Usage/Research collaborations, we organized "The 11th International Symposium of Advanced Energy Science -Research Activities on Zero-Emission Energy during the COVID-19 Peril-" on September 15–16, 2020. This symposium was held online due to the COVID-19. This symposium consists of oral and poster sessions, and satellite meeting. 234 scientists and students including 5 foreign and 6 domestic invited speakers participated in the symposium. (http://www.iae.kyoto-u.ac.jp/zero_emission_e/ZEcalendar/)

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

In FY2018, the intermediate evaluation by MEXT was conducted for all the Joint Usage/Research Center Programs. Our program was given "A" evaluation. Since then, we had been continuing the effort to keep this high evaluation with the researchers of the related communities. At the end of FY2020, we submitted the documents for the evaluation of all of the second term to MEXT, hoping the high evaluation again.

List of Zero Emission Energy Joint Usage/Research Subjects in FY 2020

(Subject, Principal Researcher, IAE Key Person)

Photoinduced electron-transfer reactions of metal complexes as photosensitizers bound to the active site of enzyme, H. Takashima, E. Nakata

Influence of Alloying Elements on Radiation Damage Formation and Hydrogen Isotope Trapping in Tungsten, Y. Hatano, T. Hinoki

Elucidation of the energy production system in mitochondria by intracellular thermosensors, R. Sakaguchi, T. Morii

Feasibility study and development of novel technique of measuring tranverse velocity field using optical vortex emitted from photonic crystal laser, H. Himura, S. Kado

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

Effects of Metal Nanoparticles and Magnetic Field on Photoproperties of Dye-Metal Nanoparticle Composite Films, H. Yonemura, H. Sakaguchi

Preparation of low molecular weight glucose-glucosamine copolymer and its characterization, M. Takeda, M. Katahira

Hydrogen and helium mixed plasma irradiation effects on tungsten materials with rhenium, Y. Ueda, T. Hinoki

Protonic Function Search by Novel Synthesis of Ammonium Solvate Ionic Liquid, A. Kitada, M. Katahira

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

Study on optimization of alloying elements of tungsten alloys for improved irradiation tolerance, S. Nogami, K. Yabuuchi

Development of thermal diffusivity evaluation method using miniature specimens at elevated temperature, M. Akiyoshi, T. Hinoki

Chemical state analysis of borocarbides, R. Kasada, K. Yabuuchi

NMR analysis on conformational alteration of RNA-binding protein with inhibitor for phase separation, R. Kurokawa, M. Katahira

Study of formation process of solute clusters in stainless steel with ion irradiation, K. Fukumoto, K. Yabuuchi

High-Fluence Irradiation Behavior of Reduced Activation Fusion Reactor Materials, H. Tanigawa, T. Hinoki

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

Development of anode/electrolyte interface for advanced Na-ion battery, H. Sakaguchi, T. Nohira

Photocarrier dynamics of Kankyo semiconductor magnesium silicide single crystals revealed using plasma reflection in mid-infrared region, M. Kitaura, H. Zen

Development of hyper-efficient degradation method of baiomass-related compounds by using mid-infrared free electron laser, T. Kawasaki, H. Zen

Investigation of carotenoid synthesis and microbiome changes in shrimp gut upon feeding shrimp with combined pigmented and non-pigmented Bacillus spores, N. Anh, Y. Takatsuka

Analysis of transition from axisymmetric torus to helical axis toroidal plasma, A. Sanpei, K. Nagasaki

Combined effect of high-temperature irradiation with heavy ion and helium on hydrogen permeation behavior in functional coating for fusion reactor blanket, T. Chikada, K. Yabuuchi

Effect of high energy He ion implantation on hydrogen isotope behavior in tungsten, Y. Oya, T. Hinoki

Solvate structure analysis of fluoride ion by NMR spectroscopy, K. Matsumoto, M. Katahira

The effects of dangling-bond on anodic dissolution of ceramics, S. Kondo, T. Hinoki

Irradiation effect of oxide particles in oxide dispersion strengthened (ODS) alloys, N. Oono, K. Yabuuchi

Development of High Temperature Ductile ODS Steels for Advanced Nuclear System, N. Iwata, K. Yabuuchi

Development and applications of functional organic materials for energy conservation-directed light-emitting devices, M. Shimizu, H. Sakaguchi

High-speed polarization switching using super radiant THz undulator radiation, S. Kashiwagi, H. Zen

Thermal control of phase change material using graphite powder, M. Shibahara, T. Hinoki

Mode-selective phonon excitation in semiconductors of energy functionality with mid-infrared free-electron laser, K. Hachiya, H. Ohgaki

Elucidation of change in element density distribution in solid lithium electrolyte during electrodialysis by rf-GD-OES analysis, K. Sasaki, K. Mukai

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

Clarification of hydrogen retention behavior for beryllium and beryllides, K. Jaehwan, K. Mukai

Study on development of compound-based anode for K-ion battery and on compatibility with molten salt electrolyte, Y. Domi, T. Yamamoto

Evaluation of the stability of irradiation induced point defect clusters during annealing, S. Jitsukawa, T. Hinoki

Development of a high peak power and quasi-monochromatic compact THz laser and its applications, K. Sakaue, H. Zen

Analysis of the binding of human replication initiation protein ORC to guanine quadruplex DNA, S. Waga, M. Katahira

Photoenergy Conversion System Utilizing Organic-Inorganic Hybrid Nanomaterials Assembled on DNA, K. Yamana, T. Morii

Improvement of the small-scale biogas plant for a household in a rural village, V. Vai, H. Ohgaki

Design of physical property and functionality of atomi layered materials, S. Okada, K. Matsuda

NMR analysis for the development of peptides and RNAs to control biomolecular functions, T. Sakamoto, T. Nagata

The study of mechanism evaluation of material degradation in irradiation damage microstructure of tungsten for divertor, K. Tougou, K. Yabuuchi

Observation of temporal evolution of coherent edge radiation during free-electron laser oscillations, N. Sei, H. Ohgaki

High spacial resolution near-field imaging of exciton in atomically thin layered materials, M. Sakai, K. Matsuda

Research and development of enzymatic activity control using VHH antibody, A. Takaori, T. Nagata

Elucidation of correlation between quadruplex-based gene expression regulation and their structure. , Y. Tanaka, T. Nagata

Spatially resolved measurement of atomic emission line spectra using NIR Zeeman spectroscopy, T. Shikama, S. Kado

Quanitative relationship between plasma-produced reactive radical amount and biological/chemical reaction promotion, H. Matsuura, S. Kado

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

Electrochemical Surface Finishing of SiC electrode by controlling the lattice defects: Comparison in the effect of defect formation between DuET and FEL, K. Fukami, H. Zen

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

Effect of irradiation on Coated Materials for Tritium Barrier, S. Ohnuki, K. Yabuuchi

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, T. Imai, T. Nagata

Nondestructive evaluation of residual elastic strain distribution around the interface between non-irradiated areas and ion irradiated area, T. Shibayama, T. Hinoki

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

Analysis of the mechanism of ultrasound-enhanced cellular internalization of bioactive molecules, T. Ohtsuki, E. Nakata

Development of a new scheme concerning shock acceleration of ions and experiment utilizing a structured medium, R. Matsui, K. Matsuda

Development of reduced activation high entropy materials for high energy reactor, N. Hashimoto, K. Yabuuchi

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

Time-series data analysis of Heliotron-J plasma by statistical modeling, S. Inagaki, K. Nagasaki

Study on impurity behaviors and materials corrosion in liquid metals for advanced nuclear systems, T. Oda, J. Yagi

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

Clarification on retention processes of He and H in ion irradiated pyrochlore oxides, B. Tsuchiya, T. Hinoki

Strengthening and improvement of ductility by precipitation control for low-activation vanadium alloy for fusion reactors, T. Nagasaka, K. Yabuuchi

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

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

A study of irradiation-induced precipitation on tungsten-rhenium alloys, T. Miyazawa, K. Yabuuchi

Irradiation field dependence of microstructural evolution of feriritc steel during irradiation, Y. Watanabe, K. Morishita

Analysis of radiation induced nano-clustesr in RPV steels, H. Watanabe, K. Yabuuchi

Study of periodic nanostructures on semiconductors produced by mid-infrared free electron lasers, M. Hashida, H. Zen

Preparation and characterization the enzyme immobilization by entrapment within a bio-polymer hydogel network, T. Jamnongkan, T. Hara

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

Control of electric current and heat flux using single particle diodes toward energy harvesting, N. Yonekura, Y. Miyauchi

Study of Hydrogen Isotope Separation Technology by Molten Salt, H. Matsushima, T. Nohira

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

Developmental research on microbial community structure analysis and biopest applications in medicinal plant cultivation, M. Ueno, T. Hara

Study of the suitability of different types of battery for rural electrification and its impact to the quality of life of the communities, N. Rahim, H. Ohgaki

Study for electron-hole plasma on semiconductor surface at mid-infrared region, K. Kawase, H. Zen

Development of high-speed camera image analysis method using magnetic field information, N. Nishino, H. Okada

Enhancement of High Temperature Mechanical Protperties on the ODS Ferritic Steels for Next generation Nuclear and Thermal Power Systems, S. Noh, K. Yabuuchi

R&D of BN/CNTs heat dissipation sheets as heat transfer Ⅱ, K. Shimoda, T. Hinoki

Feasibility and lithium analysis on the anion doped oxide - organic nano composite for energy utilization and lithium, S. Takayama, J. Yagi

Transport analysis for neutral beam heated plasmas in advanced heliotron configuration, M. Yoshikawa, S. Kobayashi

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

Development of RNA editing technology for gene regulation involved in an intracellular energy production and utilization, M. Fukuda, T. Morii

Processing of organic-inorganic hybrid materials by infrared free electron laser, J. Fuzioka, H. Zen

On-site, rapid, qualitative DNA/RNA detection in resource-poor settings, M. Hagihara, T. Morii

Investigation of current-induced electronic phase in devices based on strongly correlated electron systems, H. Narita, T. Hinoki

Behavior of hydrogen on the surface of fusion reactor materials by computer simulations, H. Iwakiri, K. Morishita

Formation and crystalline characterization of periodic nanostructures on semiconductor substrates irradiated by intense mid-infrared laser pulses, N. Ozaki, H. Zen

Development of valleytronic devices using the layered material and nitride semiconductor, S. Mouri, K. Matsuda

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

Development of a short nucleic acid that regulate transient protein interactions, Y. Katsuda, T. Morii

Identification and characterization of novel antimicrobial cyclic lipopeptides derived from Bacillus sp, K. Yokota, T. Hara

Study of basic properties of fine bubbles in the liquid, Y. Ueda, T. Morii

Novel synthesis process of ammonia at ambient condition, T. Ogawa, M. Katahira

High-Temperature Raman Spectroscopic Analysis of Silicon Coordination in Molten Salts for the Production of Solar-Grade Silicon, K. Yasuda, T. Nohira

Electrochemical preparation of Si-based energy materials in molten salt and their characterization, X. Yang, T. Nohira

Control of inner structure of apatite microcapsules fabricated by biomimetic method, T. Yabutsuka, T. Hinoki

Determination of the free energy of the late-blooming phase (2), Y. Matsukawa, K. Yabuuchi

The effect of ion beam irradiation on the properties of heavily doped nanocrystals, M. Sakamoto, T. Hinoki

Study on neutron imaging techniques for inspection of fusion blanket modules with DD neutron source, T. Tanaka, K. Mukai

Analysis of electroretinograms from the crayfish's compound eyes stimulated by mid-infrared of KU-FEL, F. Shishikura, H. Ohgaki

Quantification of cell-surface markers using enzyme-antibody conjugates, I. Takashima, E. Nakata

Mechanism of Cycle Performance Improvement for Mechanochemically Activated $LiMn_2O_4$, S. Takai, T. Morii

Study on emission process of scintillation material using the one electron beam and evaluation of scintillation properties for darkmater search, S. Kurosawa, H. Ohgaki

Study of experiment and simulation for the synergisitic effect of displacement damage and helium on irradiation hardening behavior, E. Wakai, K. Yabuuchi

Deuterium desorption from heavy ion irradiated tungsten using isothermal desorption method, N. Ashikawa, T. Hinoki

Depth profile measurements of hydrogen isotopes of damaged tungsten, M. Yajima, T. Hinoki

Development of laer nanoprocessing technique by using short-range surface plasmons excited with few-cycle laser pulses, G. Miyaji, K. Matsuda

Carbon dioxide gas fixation by laser irradiation response to calculus forming bacteria, T. Kono, H. Ohgaki

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

Workshop on "Physics and control of non-linear and non-equlibrium plasma based on the concept of broad band energy science", Y. Kishimoto, K. Matsuda

Safety enhancement of nuclear power system by advanced ICT technology, H. Yoshikawa, K. 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 2020, the actual implementation of the collaborative activity, the Pandemic of COVID-19 had a significant impact because the traffic and actual meeting were strictly avoided.

However despite the difficulty in organizing the cooperative research program, 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 usually supported, however in this fiscal year, to reduce the risk of the infection was given the highest priority, and no meetings or exchange was planned.

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

A brief summary of the cooperative research subjects carried out in FY2020 are shown next pages, which were proposed by young researchers of IAE and selected by the program committee of the Laboratory through each division to promote the project with strong leadership.

The framework of the cooperative researches in the section A2 and A3 have been changed in 2018, and some of the programs are continued in the second year, while programs were selected as a single year project. The financial resource is focused to a small number of project proposals under the leadership of the chairs of three divisions who review the proposals from IAE researchers and arrange the accepted ones.

The research program was focused into 5 topics. The number of research subjects is listed in Table 1 according to the project categories.

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

The whole sum 5

Category			Total
A1	A2	A3	
0	2	3	5

The individual research subjects are as follows

<u>A2</u>

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

- S. Kobayashi, K. Nagasaki, H. Ohgaki, T. Kii, H. Zen, H. Okada, K. Tokuhara, T. Minami, S. Kado, S. Ohshima, S. Torsten, H. Laqua (Max-Planck Institute for Plasma physics)
- , T. Mizuuchi, S. Konoshima (Inst. Adv. Energy, Kyoto Univ.)
- S. Torsten, H. Laqua (Max-Planck Institute for Plasma physics)

"Influences of three dimensional magnetic field on a diverter plasma in a torus device"

- S. Ohshima, T. Minami, S. Kado, S. Kobayashi, H. Okada, K. Nagasaki, T. Mizuuchi, S. Konoshima, K. Mukai (Inst. Adv. Energy, Kyoto Univ.)
- R. Matoike, A. Miyashita (Grad. Sch. Energy Sci., Kyoto Univ.)

<u>A3</u>

"Development of time-resolved detection system for measuring kinetic process of recognition and its application"

- E. Nakata, T. Morii, K. Matsuda (Inst. Adv. Energy, Kyoto Univ.)
- Z. Zhengxiao (Grad. Sch. Energy Sci., Kyoto Univ.)
-

"Macroscopic alignment control of carbon nanotubes using biopolymer"

- Y. Miyauchi, E. Nakata, T. Morii, K. Matsuda, A. Takakura, H. Wu, T. Nishihara (Inst. Adv. Energy, Kyoto Univ.), K. Tanaka (Grad. Sch. Energy Sci., Kyoto Univ.)

"Development of Irradiation Apparatus for Novel Material Synthesis by Mid-Infrared Free Electron Laser"

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

THE LABORATORY SEMINARS

Laboratory Seminars

The Laboratory promotes topical academic seminars in order to strengthen the research activities in each research section and to enhance the mutual cooperation among a lot of academic fields. The Laboratory also planned a symposium on April 2, 2021 for discussions of the cooperative research results in FY2020.

In FY2020, in order to prevent possible infection, very few meetings were planned and one seminar was held with the following theme.

1. Topical Seminars

(1) November 27, 2020

M. Hide

"反応閾値と数理的拡散モデルから解く慢性蕁麻疹の病態と治療"
Graduate School of Biomedical and Health Sciences(Medicine), Hiroshima University

6. PROJECTS WITH OTHER UNIVERSITIES AND ORGANIZATIONS

NIFS Bilateral Collaboration Research Program on Heliotron J

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

The main objective of the research in our Heliotron J group under this joint research program is to investigate experimentally/theoretically the transport and stability of fusion plasma in advanced helical-field, and to improve the plasma performance through advanced helical-field control in Heliotron J. Picked up in FY2020 are the following seven key-topics; (1) transport study concerning field configuration control and relating plasma structure formation control, (2) control of plasma profile, plasma flows, plasma current for confinement improvement, (3) investigation of structure formation of plasma fluctuations in core and peripheral region, (4) understanding of MHD instabilities of energetic particle modes and its control, (5) enhancement of operation region of high density plasmas, (6) optimization of particle supply and heating scenario, (7) development of new technology in experiment and analysis.

Two results from this collaboration research in FY2020 are shortly reported below. Annual report for all the collaboration subjects in this program will be published by NIFS.

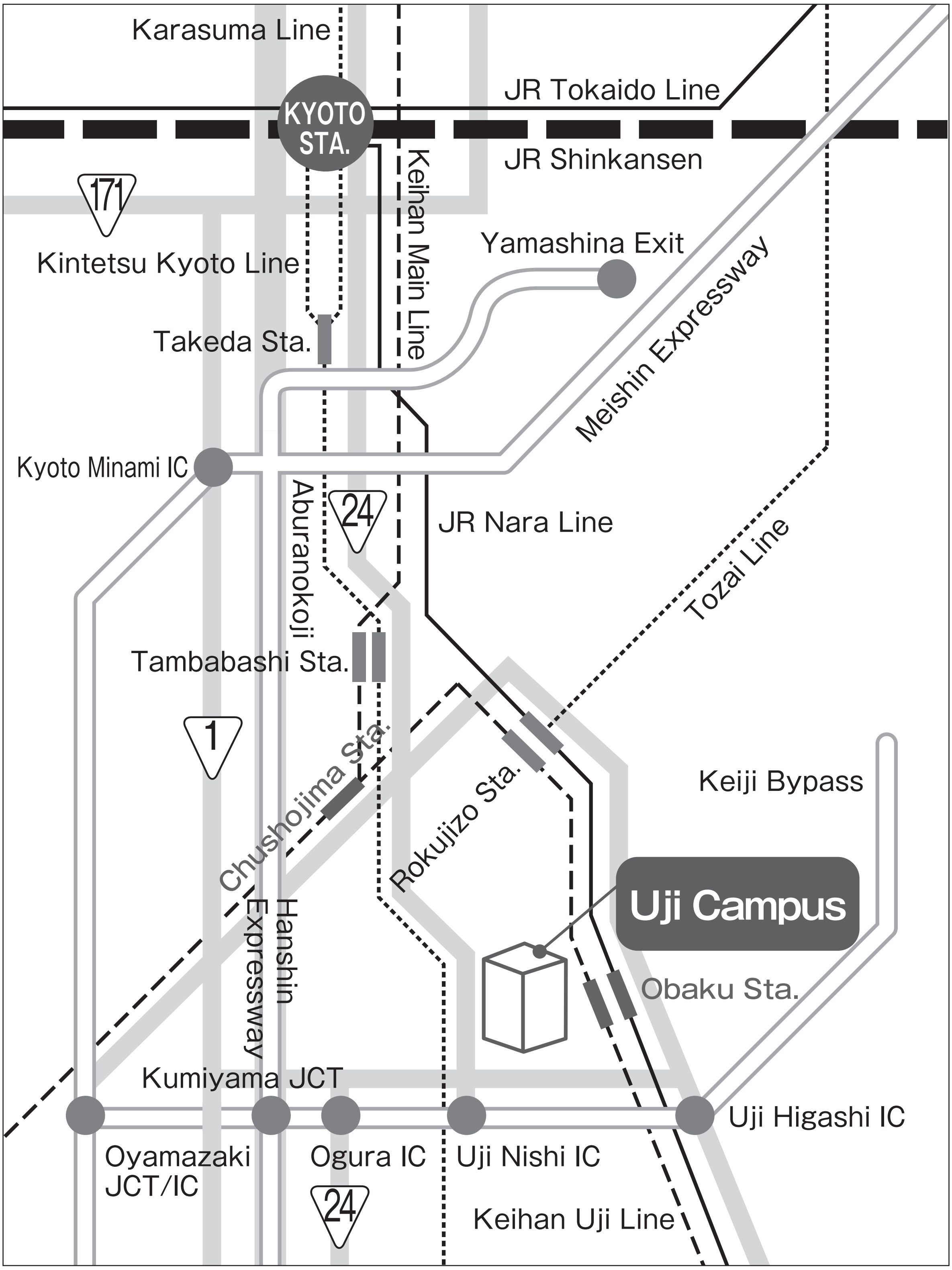
Magnetic configuration dependence of energy confinement properties and profile structure formation: The Heliotron J device has a feature of high freedom of magnetic confinement configuration compared to other stellarator/heliotron devices. We so far clarified the effect of the toroidal mirror component in the magnetic field spectrum, so called, the bumpiness, on neoclassical transport, MHD and confinement of energetic ions. Recently we have installed plasma diagnostics for profile measurement in Heliotron J, which makes it possible to analyze the physical mechanism of the configuration dependence. In this fiscal year, we have extended the configuration control parameters, and have conducted experiments of the bumpiness control and the rotational transform control.

In the magnetic configuration control experiment, we have extended the bumpiness parameter from conventional low, medium and high bumpiness to higher bumpiness, that is, ultra-high bumpiness. We have measured electron density and temperature profiles with a Nd:YAG Thomson scattering diagnostic with the launching angle of electron cyclotron heating and the magnetic field strength are adjusted for on-axis heating. The line-averaged electron density is kept constant, $n_e = 1\text{-}1.2 \times 10^{19}$ m^{-3}. We have observed that the stored energy measured with a diamagnetic loop is maximal at the standard (medium bumpiness) configuration.

The hollow density profile may be related to trapped electrons. According to the TRAVIS code calculation, the population of the trapped electrons is higher as the bumpiness is higher, related to the magnetic ripple structure. The transport of the trapped electrons may be reduced, resulting that the electron density profiles is flatter. We need to perform neoclassical analysis and turbulence simulation analysis to clarify the relationship between the profile shape and the magnetic configuration.

Formation of electron internal transport barrier (e-ITB) in NBI only plasmas: e-ITB was observed in helical plasmas typically in ECH plasmas. On-axis ECH heating forms a positive radial electric field determined by the neoclassical transport, forming aa large electron temperature gradient with reduced thermal transport coefficient. This phenomenon has been observed in many helical devices including Heliotron J. On the other hand, in NBI plasmas, ion ITB has been observed, but no e-ITB has been never observed. In this experimental campaign, we have observed an e-ITB in NBI-only plasmas in Heliotron J for the first time. The NBI is injected in co and/or counter direction. When a high intense gas puffing (HIGP) is applied to an NBI plasma without ECH, the electron density and the stored energy increases, and the increasing rate is changed a little 20 msec after the HIGP. In this timing, the electron temperature gradient changes at $r/a < 0.3$, and the central electron temperature rises up to 0.6 keV. The electron density profile is not flat but centrally peaked. A multi-channel AXUV measurement shows that the intensity at the core region increases with the edge intensity kept low. In conventional gas puffing, on the other hand, no increase in electron temperature is observed, and the electron temperature is as low as 200 eV. We will study the physical mechanism of the e-ITB formation in NBI-only plasmas by controlling the external parameters such as magnetic configuration and HIGP intensity.

7. HOW TO GET TO THE IAE



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