ISSN 1342-3177
IAE-AR-2017

Institute of Advanced Energy
Kyoto University

ANNUAL REPORT 2016

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

ANNUAL REPORT

2016

Institute of Advanced Energy
Kyoto University

Gokasho, Uji, Kyoto 611-0011
Japan

CONTENTS

FOREWORD

Institute of Advanced Energy (IAE) was established in 1996 for the investigation of energy science and technology, aiming at sophistication of every process during the energy generation, energy conversion, and energy utilization. The energy system for next generation have to be an environment-friendly (or ecologically sustainable) one. Crowned as the name of our institute is "Advanced Energy", which means an energy system that has high-level compatibility between the "Good Quality" ensuring the environmental-friendliness and the "Sufficient Amount" covering the global energy demand. Toward realization of such the Advanced Energy system, we have been preforming interdisciplinary studies to explore the future frontier of energy science and technology.

These works have been conducted by three research divisions of IAE, which have total 14 research sections including two for guest researchers, as well as the Laboratory for Complex Energy Processes. The Laboraroty specializes in highly project-oriented cross-disciplinary studies. In addition to the individual works in each research section, "cooperation with scientists from different academic fields" is also an important key word for our institute. We are conducting a lot of collaborative activity with researchers from inside and outside of IAE and also with domestic and international colleagues; Joint Usage/Research Center (JURC) Program, Collaboration works in the Laboratory for Complex Energy Processes, research projects with other universities and organizations, Research/Educational program with other departments in Kyoto University, etc.

As an innovative concept for Advanced Energy, we have proposed a concept of "Zero-emission Energy (ZE)" since FY2010. This idea of ZE comes from the fruitful results of individual and collaborative researches in IAE, including collaboration projects performed with a lot of member from relating departments in Kyoto University. Since FY2011, IAE has been qualified by the Ministry of Education, Culture, Sports, Science and Technology (MEXT) as Joint Usage/Research Center for Zero-emission Energy Research. This program supports over 90 collaboration subjects par a year, which are proposed by researchers from about 40 institutions. On the other hand, the collaboration program in the Laboratory for Complex Energy Processes supports the cross-division and/or cross-section activities mainly for the IAE researchers, which are producing the seeds for advanced collaboration subjects in JURC for ZE Research.

This annual report summarizes key activities in those IAE's research for FY2016 (April 2016 – March 2017). Although this report is edited based on the research section, some results from the collaborative investigations are also included.

Due to the space limitation, unfortunately, the details of each study is not discussed in the report. Please contact to each researcher for the details and for the possibility of future collaborations.

We would like to ask your continual support, guidance and cooperation for these activities. Thank you.

March 2017

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Director
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Guest Research Associate
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講師

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教授

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Associate Professor
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准教授

Kouichi Jimbo
Assistant Professor
神保光一
助　教

Shun Nakano
Assistant Professor
仲野　瞬
助　教

Tomohiko Hayashi
Researcher
林　智彦
研究員

Okinobu Hashitomi
Technical Staff
橋冨興宣
技術専門員

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Technical Staff
高塚真理
技術専門職員

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技術専門職員

Takamasa Ohmura
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研究支援推進員

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Research Support Staff
圓﨑さゆり
研究支援推進員

Sanae Iwamura
Research Support Staff
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教　授

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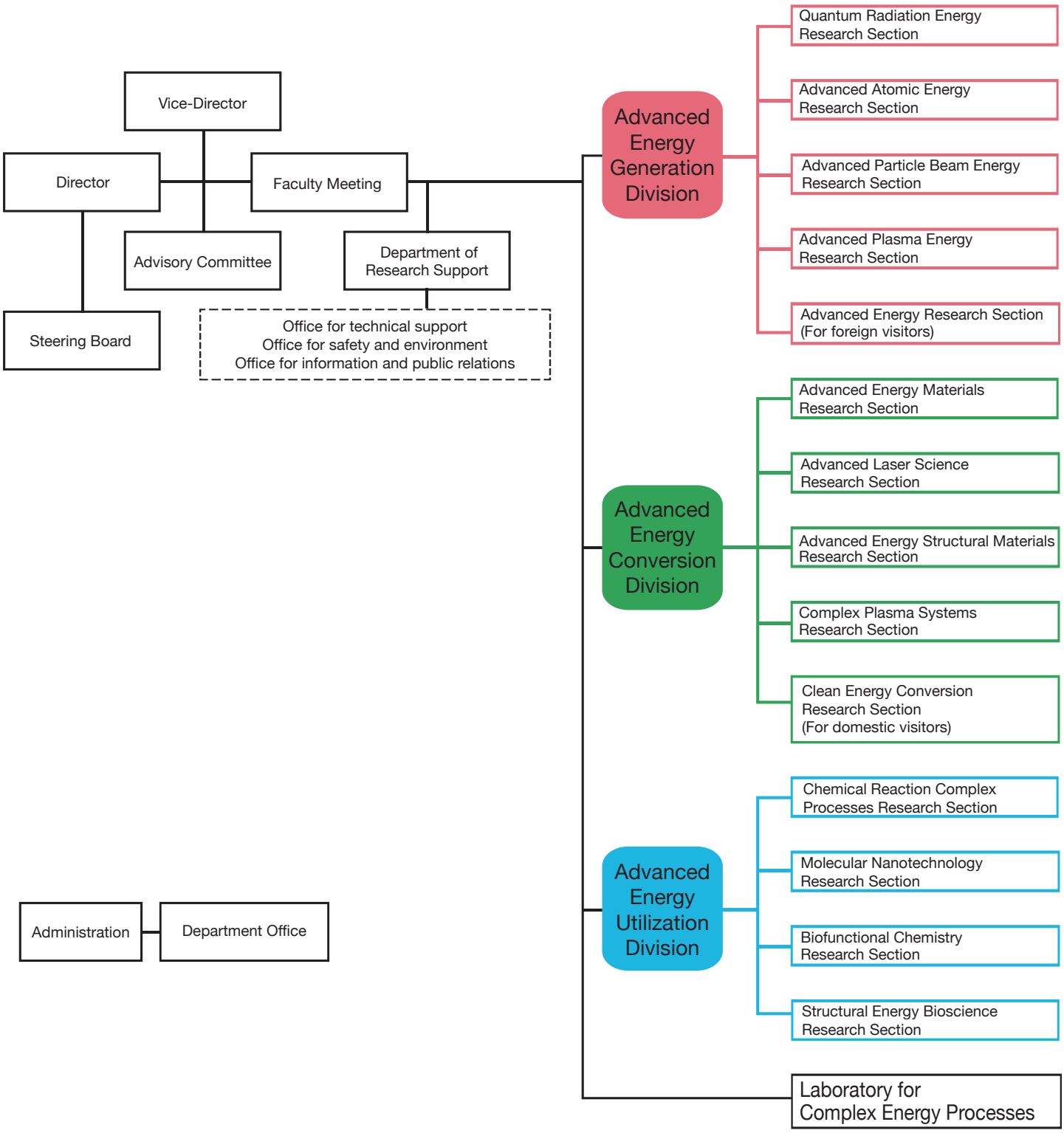
2. ORGANIZATION CHART



3. RESEARCH ACTIVITIES

3-1. RESEARCH ACTIVITIES IN 2016

Quantum Radiation Energy Research Section

H. Ohgaki, Professor
T. Kii, Associate Professor
H. Zen, Assistant Professor
H. Farzaneh, Program-Specific Junior Associate Professor Senior Lecturer
(K. Miura, Specially Appointed Professor)
(J. Wannapeera, Researcher)
(J. Yan, Researcher)

1. Introduction

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

2. Free-electron Laser

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

2.1 KU-FEL

The target wavelength of KU-FEL is MIR (Mid infra-red) regime, from 5 to 20 μm. The high power tunable IR laser will be used for basic researches on energy materials and systems. Figure 1 shows a schematic drawing of the KU-FEL system. The KU-FEL consists of a 4.5-cell thermionic RF gun, a 3-m travelling wave accelerator tube, a beam transport system, and a 1.8-m undulator and a 5-m optical resonator. The FEL device now can cover the wavelength range from 3.6 to 23 μm. The maximum macro-pulse energy which can provide is around 30 mJ in a 2-μs macro-pulse at the wavelength of 9 μm. The FEL is routinely operated and opened for internal and external users.

Another topic of KU-FEL development is introduction of photo-cathode RF gun, which enables us to generate higher peak power and wider tunable range MIR-FEL. Development of a UV-laser system for illuminating photo-cathode has been completed under collaboration with Dr. R. Kuroda, Researcher of AIST. In FY2014, we have achieved FEL lasing with photo-electron beam generated from LaB_6 cathode. Further study is undergoing to use this operation mode for user experiments.

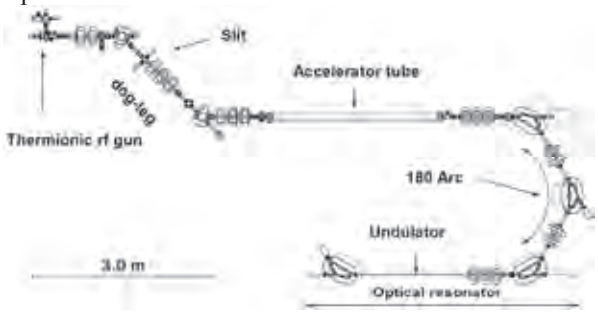


Fig. 1 Schematic drawing of the KU-FEL

2.2 MIR-FEL Application in the Energy Science

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

2.3 THz Coherent Undulator Radiation Source

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

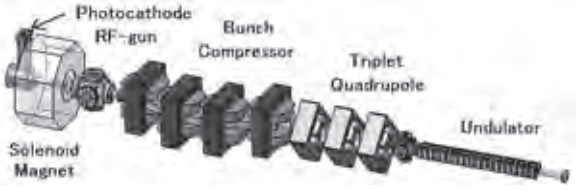


Fig. 2 3D image of THz coherent undulator radiation source.

Some commissioning experiments has been conducted to check the performance of the device. As the results, it was confirmed that the device can provide coherent undulator radiation in the frequency range from 160 to 550 GHz. The absolute intensity of the coherent undulator radiation will be measured in next fiscal year.

3. Bulk HTSC Staggered Array Undulator

An undulator with strong magnetic field will play an important role in future synchrotron light sources and free electron lasers. We constructed a new udulator which consists of stacked bulk high critical temperature superconductors array and a solenoid magnet. The bulk high-Tc superconductor staggered array undulator (Bulk HTSC SAU) can generate a stronger periodic field than that of conventional permanent magnet undulator.

4. Isotope Imaging for Nuclear Security

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

A demonstration experiment of the NRF-CT imaging by using LCS gamma-ray beam has been carried out at a newly developed LCS gamma-ray beamline, BL-1U, at UVSOR-III. The LCS gamma-ray beamline generates 5.4 MeV LCS gamma-rays with a flux of 1×10^7 photons/s without a collimation. The LCS gamma-ray beam irradiated a natural lead and we obtained a 5292-keV NRF peak in this beamline.

By using NRF absorption method a NRF-CT image has been taken for a sample target consists of aluminium, stainless steel, and lead rods of 8 mm in diameter which form a 5 × 5 rod array. X-axis of 1-cm interval and θ-axis of 36 degree interval have been scanned. The NRF signals from the witness target (natural lead) were measured by a Ge detector. At the same time, transmission gamma-rays have been measured by a $LaBr_3$(Ce) detector which gives a density distribution of the sample target. The CT reconstructions were performed to obtain ^{208}Pb distribution. Figure XX shows the ^{208}Pb distribution after the normalization by the atomic transmittance measured by the $LaBr_3$(Ce) detector. It is clear that ^{208}Pb distribution image was successfully reconstructed.

5. Assessing the benefits and impacts of clean energy development in Asian mega cities

This research focuses on demonstrating how clean energy policies and programs can help achieve multiple energy, environmental, public health and economic benefits in a cost-effective way in Asian mega cities. To this aim, a robust integrated modeling framework is developed which tends to be characterized by extensive underlying data and relatively complex formulation that

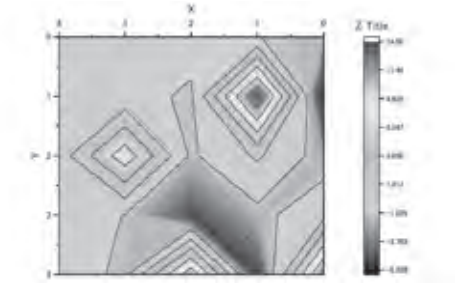


Fig. 3 ^{208}Pb distribution image reconstructed by the transmission of 5292-keV NRF peaks after the normalization.

represents the fundamental engineering and economic decision making of the society at a city level. The four mega-cities which will be evaluated in detail in this research are Tokyo, Seoul, Delhi and Shanghai. In the first phase of the research, activities will focus on evaluating the existing clean energy policy developments, countermeasures and challenges in selected cities. In the second phase, activities will concentrate on designing strategic plans that achieve greater or border benefits in selected cities.

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

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

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

Acknowledgment

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

Collaboration Works

NSTDA（タイ），JASTIP、WP2，大垣英明

Financial Support

1. Grant-in-Aid for Scientific Research

大垣英明，基盤研究（B），NRF を利用した同位体 3D イメージングに関する基礎研究

紀井俊輝，挑戦的萌芽研究，ベクトルポテンシャルと電子ボルテックスビームとの相互作用の探索

Farzaneh Hooman，基盤研究（C），Assessingthemultiplebenefitsofcleanenergypoliciesi-nAsianmega-cities

全炳俊，若手研究（A），超短バンチ電子ビームを用いた新奇 THz 自由電子レーザ発生手法の研究

2. Others

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Advanced Atomic Energy Research Section

S. Konishi, Professor
R. Kasada, Associate Professor
Y. Takeuchi, Assistant Professor

1. Introduction

Future of the humankind is strongly depending on the stable supply of energy, resource and recycling of waste within the environmental capacity. This section considers energy systems as a major part of this sustainability issue. The major objective of the study in this section is to pursue advanced energy systems for the sustainable development under global environmental constraints. The studies described below are featured by not only the innovative technology of energy genera-tion, conversion and utilization systems. The attractiveness of the total energy system considered by the socio-economic analysis of future society and markets in the global scale and the scope covering 21st century and beyond is reflected. Typically, we propose a Zero-emission energy scenario based on fusion energy for biomass-based recycling system.

The major studies performed in our laboratory this fiscal year were as follows:

(1) Design of small and realistic biomass-fusion hybrid energy system
(2) Development of advanced fusion blanket and divertor with liquid LiPb and SiC composite for high temperature heat
(3) Conversion of waste biomass by endothermic reaction to generate hydrogen and liquid fuel
(4) Design and analysis of electricity grid system for zero-emission generation technology
(5) Development of compact neutron beam using cylindrical discharge device and its innovative application.
(6) Analysis of radiologial impact of nuclides from fusion plants.
(7) Materials R&D for the above-mentioned issues

2. Evaluation of Life Cycle Analysis of tokamak fusion power reactors by improving system code

This study incorporate the Life Cycle Analysis (LCA) of fusion as an extension of a system code to calculate CO_2 emissions and environmental cost adding to the regular expenses for reactor construction, operation and decommissioning. Tokamak type DEMO reactor and following commercial reactors are analyzed and evaluated by the cost and environmental impact represented by the CO_2 emissions, and was compared with present and future power generating systems such as fossil, nuclear and renewables. Result indicated that (1) The objective of conceptual design of the tokamak fusion power reactor is moved by changing evaluation index. (2) The tokamak fusion reactor can reduce CO_2 emissions in the life cycle effectively by reduction of the amount involved in the replacement of internal components. (3) The tokamak fusion reactor achieves under 0.174$/kWh electricity cost, the tokamak fusion reactor is contestable with 1500 degrees-class LNG-fired combined cycle power plant, as shown in Table 1. Fusion energy was found to be attractive and competitive when environmental cost is significant.

[H. Kobori, R. Kasada, R. Hiwatari, S. Konishi, Fusion Engineering and Design, 109-111 (2016) 760-763.]

3. Limitation of fusion power plant installation on future power grids under the effect of renewable and nuclear power sources

Future electricity grids would be unstable because of the larger share of renewable and nuclear power sources those do not respond to demand. This instability might bring some additional difficulties to fusion plant installation. Therefore, the authors carried out a quantitative feasibility study from the aspect of grid stability through simulation. Results showed that the more renewable and nuclear sources are linked to a grid, the greater disturbance the grid would encounter upon a sudden output interruption of a fusion power plant, e.g. plasma disruption. The frequency deviations exceeds 0.2 Hz on some grids, suggesting potential limitations of fusion plant installation on future grids particularly in the developing countries. To clearly show the suggested limitations of fusion plant installations, a novel diagram was presented as shown in Fig.1.

Table 1 Calculated Electricity cost compared with various power sources [K. Tokimatsu, H. Hondo, Nucl. Fusion, 40 (3Y) (2000), pp. 653–659].

	Fusion1	Fission	LNG	Oil fired	Hdro-po wered	Geo-thermal	Photo-voltaics	Wind-po wered
Electricity cost [$/kWh]	0.1505	0.1000	0.1460	0.1750	0.1300	0.1050	1.4600	0.8
Carbon tax [$/kWh]	0.0017	0.0013	0.0293	0.0503	0.0007	0.0009	0.0026	0.0017
Total cost [$/kWh]	0.1522	0.1013	0.1753	0.2253	0.1307	0.1059	1.4626	0.8797

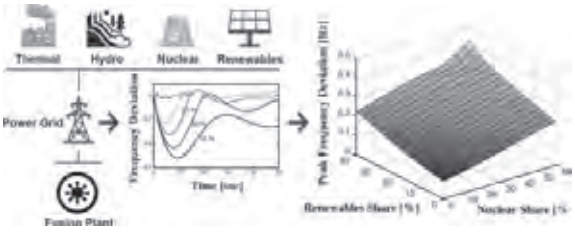

Fig. 1. Peak frequency deviation under the effect of renewable and nuclear power sources.

[S. Takeda, S. Sakurai, Y. Yamamoto, R. Kasada, S. Konishi, Fusion Engineering and Design 109-111 (2016) 1754-1758.]

4. Improvement of tensile properties of pure Cu and CuCrZr alloy by cryo-rolling process for divertor components of fusion reactor

This study investigated the effect of cryo-rolling process, i.e. cold-rolling at liquid-nitrogen temperature followed by heat treatment, on tensile properties of pure copper and precipitation-hardened CuCrZr alloy. The cryo-rolling process resulted in a simultaneous improvement of strength and ductility of pure copper. On the other hand, a cryo-rolled CuCrZr alloy showed higher tensile strength but comparable ductility with a conventional cold-rolled CuCrZr alloy. Microstructural analysis indicated that the drastically-beneficial effect of cryo-rolling on pure copper may be due to its heterogeneous size distribution of grains which consists of cryo-rolled fine grains, residual cryo-rolled grains and recrystallized coarse grains. The modest but certain benefit of cryo-rolling on CuCrZr alloy can be explained by different texture formation compared with conventional cold-rolling at room temperature. As shown in Fig. 2, neutron irradiation at 290 °C had no significant impact on tensile properties of cryo-rolled CuCrZr alloy.

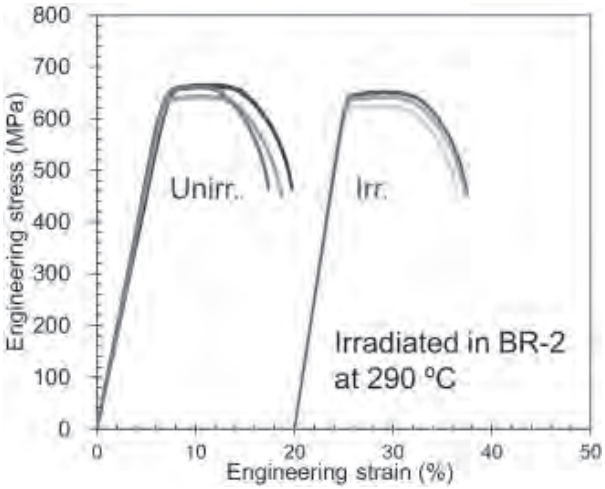

Fig.2 Engineering stress–strain curves of cryo-rolled CuCrZr alloy before and after neutron irradiation in BR2 at 290 °C.

[R. Ihira, H. Gwon, R. Kasada, S. Konishi, Fusion Engineering and Design 98-99 (2015) 1804-1807.]

5. Chemical state mapping of degraded B_4C control rod investigated with EPMA-SXES

Boron Carbide (B_4C) is widely used as control rods in light water reactors, such as the Fukushima Daiichi nuclear power plant, because it shows excellent neutron absorption and has a high melting point. However, B_4C can melt at lower temperatures owing to eutectic interactions with stainless steel and can even evaporate by reacting with high-temperature steam under severe accident conditions. To reduce the risk of recriticality, a precise understanding of the location and chemical state of B in the melt core is necessary. Here we show that a novel soft X-ray emission spectrometer in electron probe microanalysis (EPMA-SXES) can help to obtain a chemical state map of B in a modeled control rod after a high-temperature steam oxidation test as shown in Fig. 3. This work was reported in the domestic newspapers and in the scientific news in the world.

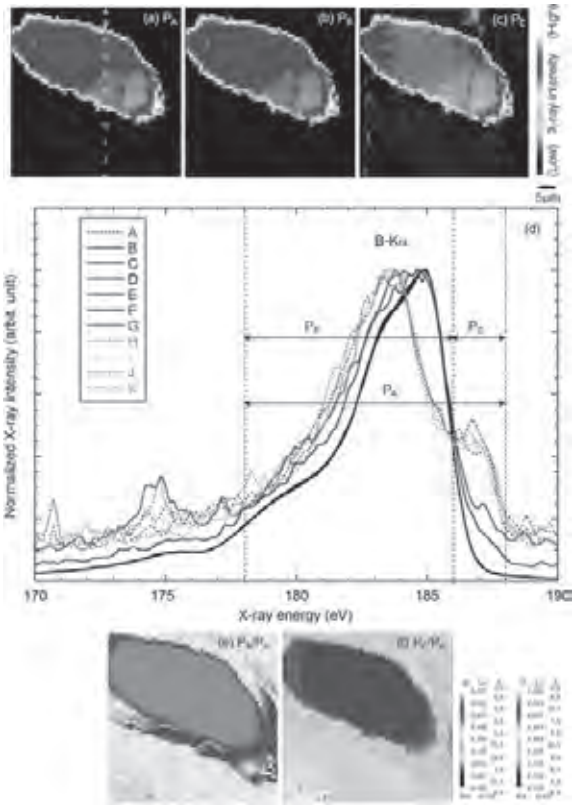

Fig.3 Elemental maps based on (a) P_A, (b) P_B, and (c) P_C of (d) B-Kα spectrum, obtained by EPMA-SXES and re-calculated by peak-area ratio as (e) P_B/P_A and (f) P_C/P_A.

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Financial Support

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Advanced Particle Beam Energy Research Section

K. Nagasaki, Professor
K. Masuda, Associate Professor
S. Ohshima, Assistant Professor

1. Introduction

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

2. Photoemission Property Measurement of LaB_6 and CeB_6 Photocathodes for FEL System

Quantum efficiency (QE) improvement of metal compound materials is expected to provide robust, long lifetime, and low cost photocathodes desired for free electron lasers. We studied thermionic excitation assisted photoemission aiming at QE improvement by extra excitation of electrons by heating the cathode. We focused on two metal compound materials, namely LaB_6 and CeB_6, both of which are widely used as thermionic cathodes for high brightness electron beam sources. Those materials have low work function, implying their better performance in photocathode operation than other low cost metal compound materials. To obtain basic knowledge about the thermionic excitation assisted photoemission for those materials, we carried out photoemission property measurements under a wide range of cathode temperature with three different incident laser wavelengths: 266, 355, and 532 nm, i.e. 2-4th harmonic of a Nd:YAG laser. Figure 1 shows results from the measurements. As the figure shows, photoemission property of LaB_6 for shorter wavelength is found to show 2-exponential temperature dependence to cathode temperature. The same tendency has been observed for CeB_6. It is also revealed that LaB_6 has higher QE than CeB_6, which is the same tendency as that of thermionic emission from those two materials. It is also revealed that, by heating the cathode, 532 nm laser, corresponding to a lower photon energy than the work function, can induce photoemission when the cathode is heated. We have confirmed that this photoemission is dominated by single photon process assisted by thermionic excitation as expected, rather than the other possibilities such as multi-photon excitation and thermionic emission enhancement by the laser-induced heating effect.

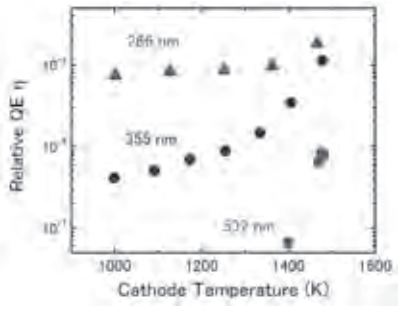

Fig. 1 Temperature dependence of relative quantum efficiency (measured electrons / incident photons) of LaB_6

3. Portable Detection System of Special Nuclear Materials by Use of D-D Fusion Neutron Source

Timely detection of special nuclear materials (SNMs) is of paramount importance for combatting global nuclear terrorism. As the passive radiation detectors deployed in the marketplace are known to be inadequate in practice especially for identifying SNMs like U-235, several active interrogation systems for deployment in seaports and airports have been proposed. Those systems, however, require highly intense sources and/or heavy shielding materials surrounding the detectors for blocking the background neutrons and/or gamma-rays, which make portable/transportable use impossible.

We are developing the world's first portable, active

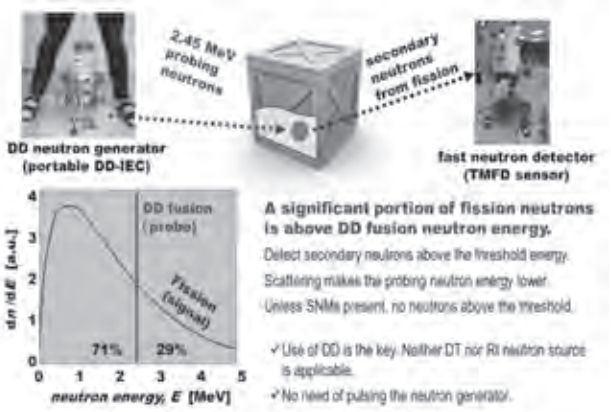

Fig. 2 The threshold energy neutron analysis (TENA) method for detecting SNMs.

SNMs interrogation system based on a newly developed method, that is the Threshold Energy Neutron Analysis (TENA) technique, comprising a lightweight D-D Inertial Electrostatic Confinement (IEC) fusion neutron source for interrogation of suspicious objects, coupled with Tensioned Metastable Fluid Detector (TMFD) technology.

The basic idea and features of the TENA method is illustrated in Fig. 2. The TENA requires D-D fusion as the probing neutron source. Neither RI, D-T nor other accelerator-driven neutron source is applicable. SNMs interrogated with thermal and/or epi-thermal neutrons originated from 2.45 MeV mono-energetic D-D neutrons emit high energy neutrons. The detection of neutrons with energies over 2.45 MeV (which amount to about 30% of all the induced fission neutrons generated) constitutes an unmistakable signature for conclusively identifying SNMs with a low rate of false positive signals, as energies of the probing neutrons are below 2.45 MeV. A portable (70 cm in length, <25 cm in diameter, <30 kg) IEC fusion neutron source (see a photo in Fig. 2) with a D-D neutron yield in excess of 5×10^7 sec^{-1} is under development for this purpose.

What is also crucially needed for the successful "portable" TENA system is the ability of TMFD sensor to reject the probing neutrons below 2.45 MeV and all background gamma-rays, while detecting above 2.45 MeV neutrons from fission reactions with high efficiency. The first experiments of the proposed TENA-TMFD scheme by use of a highly enriched uranium of 10 g as the target have proved promising capability to detect SNMs within the inspection time requirement for the practical use.

4. Improvement of Reflectometer and Measurement of Electron Density Fluctuation in Heliotron J

We have developed a reflectometer system to study turbulent transport in the Heliotron J device. The reflectometer system with two carrier frequencies measures electron density fluctuations at two radial positions, enabling us to the radial correlation length of plasma turbulence. A spike noise of about 80 kHz was observed so far in Reflectometer 2 with a fixed carrier frequency, which gives rise to a problem for turbulent/MHD fluctuation analysis. Through careful investigation of the system, we found that a tripler generated the spike noise. We replaced it by a doubler, and upgraded the system by considering this replacement. At the input frequency of 12.93 GHz, the LO power before a mixer is 11 dBm, and the power difference between upper and lower side bands is 16dB, which satisfies the condition for normal operation to measure the RF signal.

Figure 3 shows the Q signals of Reflectometer 1 and 2. The carrier frequency of Reflectometer 1 is 40.52 GHz, corresponding to the cutoff density of $2.04\times10^{19}m^{-3}$, while the carrier frequency of Reflectometer 2 is 25.82 GHz, corresponding to the cutoff density of $0.83\times10^{19}m^{-3}$. When the pellet is injected at t=218 msec, the electron density quickly increases. One can see that the Q signal of Reflectometer 1 rapidly increases, while the response of Reflectometer 2 is weak. A Nd:YAG Thomson scattering diagnostic shows that the electron density reaches the cutoff density for Reflectometer 1 *after* the pellet injection, and the electron density reaches the cutoff density for Reflectometer 2 *before* the pellet injection. This confirms that both reflectometers reflect the carrier waves at the cutoff density. We have calculated Power Spectrum Density (PSD) of the reflectometer signals, and coherence with a magnetic probe signal. Coherent modes have been observed at about 120 kHz, which are energetic particle driven MHD modes. Such modes should be eliminated the coherent modes when we evaluate turbulent radial structure including correlation length

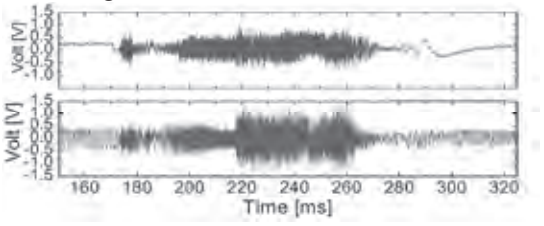

Fig.3 Electron density, Q signal (Reflectometer 1), Q signal (Reflectometer 2) at shot #64910

Collaboration Works

Univ. Wisconsin（米国），Oak Ridge National Laboratory（米国），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，水内亨，長﨑百伸，岡田浩之，小林進二，山本聡，南貴司

西南物理研究所（中華人民共和国），IPP, Greifswald（ドイツ），University of Wisconsin（米国），反射計を用いた電子密度分布・揺動解析，長﨑百伸

AUN（オーストラリア），データマイニングを用いた MHD 安定性解析，山本聡，長﨑百伸，

IPP, Greifswald（ドイツ），電子サイクロトロン電流駆動の理論解析，長﨑百伸

Stuttgart University（ドイツ），CIEMAT（スペイン），ヘリカル磁場配位における乱流揺動研究，大島慎介，長﨑百伸，佐野史道，水内亨，岡田浩之，南貴司，小林進二，山本聡

Stuttgart Univ.，CIEMAT（スペイン），先進閉じ込め配位，長﨑百伸，大島慎介，水内亨，岡田浩之，南貴司，小林進二，山本聡

CIEMAT（スペイン），Kurchatov Institute（ロシア），ORNL（米国），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, 山本聡, 小林進二，長﨑百伸，大島慎介，水内亨

Purdue Univ.（米国），張力準安定流体中性子検出器を用いた核燃料物質非破壊検知技術に関する研究，増田開

核融合科学研究所・双方向型共同研究，磁場分布制御を活用したプラズマ構造形成制御とプラズマ輸送改善，水内亨（代），長﨑百伸，岡田浩之，南貴司，門信一郎，小林進二，山本聡，大島慎介

核融合科学研究所・双方向型共同研究，ヘリオトロン J，CHS，LHED 装置における重水素プラズマの粒子輸送の研究，水内亨，山本聡，南貴司，大島慎介，小林進二，長﨑百伸，岡田浩之

核融合科学研究所・双方向型共同研究，低磁気シアヘリオトロン配位における磁気島に対するプラズマ応答の研究，水内亨，岡田浩之，長﨑百伸，山本聡，小林進二，南貴司

核融合科学研究所・双方向型共同研究，ヘリオトロン J における ICRF 加熱を用いたプラズマの高性能化研究，水内亨，岡田浩之，南貴司，小林進二，長﨑百伸，山本聡，木島茂，大島慎介，門信一郎

核融合科学研究所・双方向型共同研究，高速カメラを主体とした周辺乱流計測と乱流物理の解明 -Helical Heliotron 磁場装置 Heliotron J での乱流計測, 水内亨, 小林進二, 大島慎介, 岡田浩之, 長﨑百伸, 山本聡，南貴司，門信一郎

核融合科学研究所・双方向型共同研究，磁気シアが MHD 不安定性による閉じ込め性能劣化度に与える影響の研究，水内亨，岡田浩之，長﨑百伸，小林進二，山本聡，南貴司

核融合科学研究所・双方向型共同研究，多様な磁場配位を有するヘリカル系プラズマにおけるプラズマフローと磁気島の理解，水内亨，山本聡，小林進二，長﨑百伸，岡田浩之，南貴司，大島慎介

核融合科学研究所・双方向型共同研究，ヘリカル系プラズマにおけるアルヴェン固有モードに起因する高速イオン損失研究, 水内亨, 山本聡, 小林進二，大島慎介，岡田浩之，南貴司，長﨑百伸，門信一郎

核融合科学研究所・双方向型共同研究，有限ビーム幅を考慮した電子バーンシュタイン波放射計測，水内亨，長﨑百伸，大島慎介，南貴司，山本聡，小林進二，岡田浩之

核融合科学研究所・双方向型共同研究，Heliotron J 装置における電極バイアスにによるポロイダル粘性遷移研究，水内亨，岡田浩之，長﨑百伸，門信一郎，小林進二，南貴司，山本聡，大島慎介

核融合科学研究所・双方向型共同研究，複合揺動計測によるヘリオトロン J の乱流構造解析，水内亨，長﨑百伸，岡田浩之，南貴司，小林進二，大島慎介

核融合科学研究所・双方向型共同研究，アルベン固有モードによる高速イオン異常輸送の物理過程とその制御に関する研究, 水内亨, 岡田浩之, 南貴司，長﨑百伸，山本聡，大島慎介，小林進二

核融合科学研究所・双方向型共同研究，マルチチャンネルカロリーメーターによるダイバーター熱流束の計測, 水内亨, 大島慎介, 岡田浩之, 小林進二，門信一郎

核融合科学研究所・双方向型共同研究，ヘリカルプラズマの不純物輸送に対する同位体効果の影響，水内亨，門信一郎，小林進二，山本聡，大島慎介，南貴司，岡田浩之，長﨑百伸

核融合科学研究所・双方向型共同研究，ヘリオトロン J の NBI 加熱に対する再突入粒子の影響, 水内亨, 岡田浩之，南貴司，小林進二，長﨑百伸，山本聡

核融合科学研究所・双方向型共同研究，ヘリオトロンJにおけるVUV分光法を用いた不純物の計測と輸送の研究，水内亨，門信一郎，岡田浩之，山本聡，南貴司，小林進二，長﨑百伸，大島慎介

核融合科学研究所・双方向型共同研究，ヘリオトロンJにおけるプラズマ高密度化実験，水内亨，門信一郎，長﨑百伸，岡田浩之

Financial Support

長﨑百伸，量子科学技術研究開発機構，電子サイクロトロン周波数帯ミリ波の非吸収パワーの評価方法に関する検討

長﨑百伸，核融合科学研究所・一般共同研究，EC波の伝播・吸収に対する磁気シアの効果

長﨑百伸，核融合科学研究所・一般共同研究，マイクロ波アシストセラミック焼結の大量生産に向けた応用研究

増田開，新エネルギー・産業技術総合開発機構，戦略的基礎技術高度化支援事業（プロジェクト委託型）/世界に先駆けた次世代インフラの構築の実現に資する技術/ポータブル核分裂物質非破壊検知装置によるテロ対策インフラ強化

増田開，（株）アドバンテスト，電子銃周辺空間電荷効果計算

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Advanced Plasma Energy Research Section

T. Mizuuchi, Professor
T. Minami, Associate Professor
S. Kobayashi, Assistant 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 FY2016 is shown focusing on (1) role of magnetic configuration to form electron internal transport barrier (eITB) and (2) study of H-mode transition triggered by high intensity gas puffing.

2. Role of Magnetic Configuration to Form Electron Internal Transport Barrier in Heliotron J

The experiments have been performed on the medium bumpiness magnetic field configuration at $B_{axi.}$ = 1.25 T. Because the Heliotron J magnetic configuration has low magnetic shear, the vacuum rotational transform profile is almost flat and the value of central $\iota/2\pi$ is 0.558. The plasma with eITB is produced by centrally focused 70 GHz ECH ($P_{inj.} \sim$ 270 kW, the absorption ratio is above ~ 90%). The plasma current, which is mainly driven by bootstrap current due to $N_{||}$=0.0, ramps up to 1.5 kA.

Figure 1 shows the typical time evolution of electron temperature, density and plasma current. The electron temperature and density profiles from the Nd:YAG Thomson scattering measurement at 210ms, 240ms and 300ms are also shown. Because the experiment was carried out under a constant density condition, which fulfills the condition of a low density (line averaged $n_e \leq 1.2\times10^{19}$ m^{-3}) that is required to form the eITB[1], the eITB formation, which is characterized by a peaked electron temperature profile shape, is observed from t=200ms to t=330ms. When the plasma current increases up to 0.7kA at time of 223ms, a fast jump of the electron temperature at r/a~0.1 in the ECE signal is observed. Figure 2 shows the position of the eITB foot point, which is derived from the electron temperature profiles, as a function of the plasma current. Before the rapid rise, the eITB foot point is kept on the same location. When the plasma current reaches at 0.7kA, the location of the eITB foot point jumps to the outside of the plasma from r/a~ 0.13 to r/a~0.23. This increase is not the transition to the eITB formation, because the eITB has been already formed before the rapid rise of the ECE signal. The Nd:YAG Thomson scattering measurements show the enhanced confinement region in the eITB expands at the transitive increase.

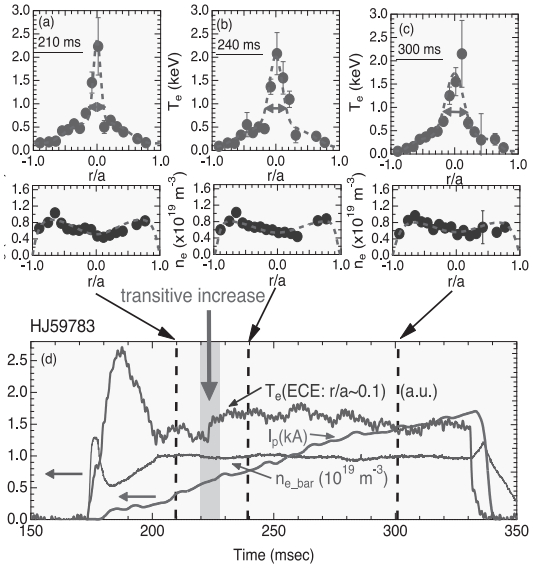

Fig.1 Rapid electron temperature rise has been observed during eITB formation with current ramp-up. (a) (b) (c) Electron temperature and density profiles. (d) Time evolution of electron temperature, density and plasma current.

After the rapid temperature rise, the location continues to move to the outside from r/a~0.2 to r/a~0.4 with the current increases. On the other hand, the changes of the electron density profiles are small

during the discharge. Although the central electron temperature slightly decreases at the end of the discharge, the kinetic stored energy increases after the electron temperature rapid rise due to the expansion of the enhanced confinement area.

The neoclassical calculation suggests that the movement of the eITB foot point has the relation with a n/m=4/7 rational surface formation. The eITB can be formed without the low-order rational surface in Heliotron J, however, this rational surface affects the behavior of the eITB formation and the enhanced confinement region expands. Because this rational surface is a candidate on which the magnetic island can be produces, the enhanced region of the eITB might be expanded by the magnetic island. These results show the possibility that there is the synergy effect of the eITB and the magnetic island for the expansion of the improved confinement region.

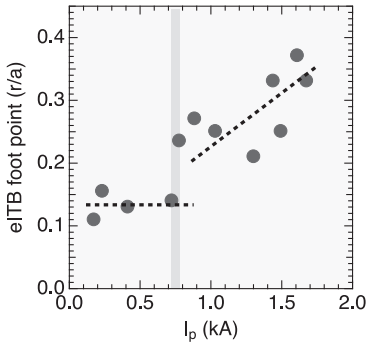

Fig.2 Foot point of eITB as a function of plasma current. Transition occurs at ~0.7 kA.

3. Study of H-mode transition triggered by high-intensity gas puffing in Heliotron J

In this section, the experimental study on H-mode transition triggered by high intensity gas puffing (HIGP) is reported. The HIGP method is short-pulsed (10-20ms) gas fueling with several times higher fueling rate using conventional Piezo-electric type valves. It has been reported that the H-mode transition has been observed in the Heliotron J NBI plasmas when an appropriate HIGP is applied. Before the transition, a bursting n =2 mode with frequency of f = 5-30 kHz appears in the density and magnetic fluctuations at the peripheral region (see Fig. 3). In the case that the amount of HIGP is insufficient to trigger the transition, on the other hand, a small amplitude of n = 1 mode is observed, which has no bursting.

The lower frequency (low-f) fluctuation corresponding to the burst frequency (f = 1-3 kHz) has larger structure (n = 0) in toroidal direction. The cross-correlation function analysis shows that the low-f fluctuation propagates outwardly to scrape-off-layer and the propagation is synchronized with the H_α/D_α intensity, which indicates the particle exhaust phenomena. The reduction in the particle exhaust and the rapid (~0.4 ms) evolution of the density gradient at the peripheral region are observed at the timing of the H-mode transition. Figures 4(a) and 4(b) show the intensity of low-f fluctuation and density gradient as a function of density increase by HIGP. The H-mode transition is observed when a significant intensity of low-f fluctuation appears. In this case, the steep density gradient is clearly formed. Then the low-f fluctuation appeared after the applying HIGP has a correlation to trigger the transition, reading to the formation of the steep density gradient at the peripheral region.

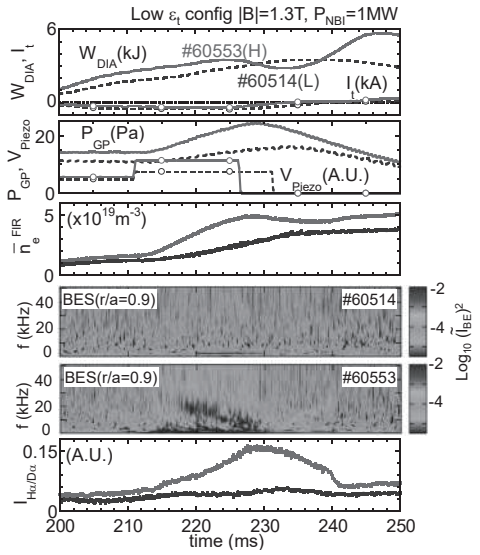

Fig. 3 Time evolution of plasma parameters obtained in H-mode transition (#60553) and no-transition (#60514) plasmas. For the H-mode plasmas, the transition occurs at t = 240ms.

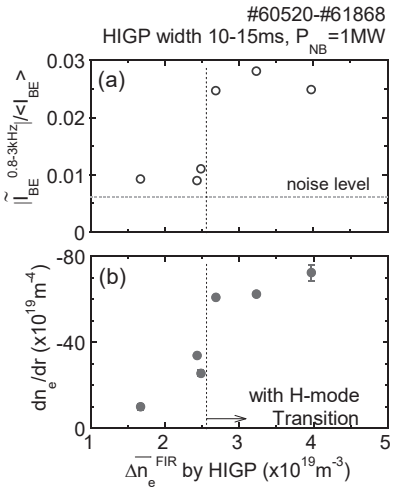

Fig. 4 (a) Root-mean-square of low-f fluctuation and (b) density gradient at peripheral region as a function of density increase by HIGP.

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Collaboration Works

西南物理研究所（中華人民共和国），CEIMAT（スペイン），SMBI 法の応用，水内亨

Univ. Wisconsin（米国），Oak Ridge National Laboratory（米国），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，水内亨，長﨑百伸，岡田浩之，小林進二，山本聡，南貴司

Stuttgart University（ドイツ），CIEMAT（スペイン），ヘリカル磁場配位における乱流揺動研究，大島慎介，長﨑百伸，水内亨，岡田浩之，南貴司，小林進二，山本聡

Stuttgart Univ.，CIEMAT（スペイン），先進閉じ込め配位，長﨑百伸，大島慎介，水内亨，岡田浩之，南貴司，小林進二，山本聡

CIEMAT（スペイン），Kurchatov Institute（ロシア），ORNL（米国），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，山本聡，小林進二，長﨑百伸，大島慎介，水内亨

PPPL（米国），低磁気シアヘリカルプラズマにおける高速イオンの異常輸送ならびに損失機構に関する研究，山本聡，小林進二

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核融合科学研究所・双方向型共同研究，磁場分布制御を活用したプラズマ構造形成制御とプラズマ輸送改善，水内亨（代），長﨑百伸，岡田浩之，南貴司，門信一郎，小林進二，山本聡，大島慎介

核融合科学研究所・双方向型共同研究，ヘリオトロン J，CHS，LHED 装置における重水素プラズマの粒子輸送の研究，水内亨，山本聡，南貴司，大島慎介，小林進二，長﨑百伸，岡田浩之

核融合科学研究所・双方向型共同研究，低磁気シアヘリオトロン配位における磁気島に対するプラズマ応答の研究，水内亨，岡田浩之，長﨑百伸，山本聡，小林進二，南貴司

核融合科学研究所・双方向型共同研究，ヘリオトロン J における ICRF 加熱を用いたプラズマの高性能化研究，水内亨，岡田浩之，南貴司，小林進二，長﨑百伸，山本聡，木島茂，大島慎介，門信一郎

核融合科学研究所・双方向型共同研究，高速カメラを主体とした周辺乱流計測と乱流物理の解明 -Helical-Axis Heliotron 磁場装置 Heliotron J での乱流計測，水内亨，小林進二，大島慎介，岡田浩之，長﨑百伸，山本聡，南貴司，門信一郎

核融合科学研究所・双方向型共同研究，高性能磁場閉じ込めプラズマを目指した粒子補給法の検討（ヘリオトロン J におけるプラズマ高密度化に向けた粒子補給法の模索），水内亨，小林進二，岡田浩之，長﨑百伸，南貴司，山本聡，大島慎介

核融合科学研究所・双方向型共同研究，磁気シアが MHD 不安定性による閉じ込め性能劣化度に与える影響の研究，水内亨，岡田浩之，長﨑百伸，小林進二，山本聡，南貴司

核融合科学研究所・双方向型共同研究，多様な磁場配位を有するヘリカル系プラズマにおけるプラズマフローと磁気島の理解，水内亨，山本聡，小林進二，長﨑百伸，岡田浩之，南貴司，大島慎介

核融合科学研究所・双方向型共同研究，ヘリカル系プラズマにおけるアルヴェン固有モードに起因する高速イオン損失研究，水内亨，山本聡，小林進二，大島慎介，岡田浩之，南貴司，長﨑百伸，門信一郎

核融合科学研究所・双方向型共同研究，有限ビーム幅を考慮した電子バーンシュタイン波放射計測，水内亨，長﨑百伸，大島慎介，南貴司，山本聡，小林進二，岡田浩之

核融合科学研究所・双方向型共同研究，Heliotron J 装置における電極バイアスによるポロイダル粘性遷移研究，水内亨，岡田浩之，長﨑百伸，門信一郎，小林進二，南貴司，山本聡，大島慎介

核融合科学研究所・双方向型共同研究，不純物輸送機構・同位体効果の理解に向けた新古典理論の拡張と応用，水内亨，岡田浩之，小林進二，山本聡，南貴司

核融合科学研究所・双方向型共同研究，複合揺動計測によるヘリオトロン J の乱流構造解析，水内亨，長﨑百伸，岡田浩之，南貴司，小林進二，大島慎介

核融合科学研究所・双方向型共同研究，アルヴェン固有モードによる高速イオン異常輸送の物理過程とその制御に関する研究，水内亨，岡田浩之，南貴司，長﨑百伸，山本聡，大島慎介，小林進二

核融合科学研究所・双方向型共同研究，マルチチャ

ンネルカロリーメーターによるダイバーター熱流束の計測, 水内亨, 大島慎介, 岡田浩之, 小林進二, 門信一郎

核融合科学研究所・双方向型共同研究，ヘリカルプラズマの不純物輸送に対する同位体効果の影響，水内亨，門信一郎，小林進二，山本聡，大島慎介，南貴司，岡田浩之，長﨑百伸

核融合科学研究所・双方向型共同研究，ヘリオトロンJのNBI加熱に対する再突入粒子の影響, 水内亨, 岡田浩之，南貴司，小林進二，長﨑百伸，山本聡

核融合科学研究所・双方向型共同研究，ヘリオトロンJにおけるVUV分光法を用いた不純物の計測と輸送の研究, 水内亨, 門信一郎, 岡田浩之, 山本聡, 南貴司，小林進二，長﨑百伸，大島慎介

核融合科学研究所・双方向型共同研究，ヘリオトロンJにおけるプラズマ高密度化実験，水内亨，門信一郎，長﨑百伸，岡田浩之

Financial Support

1. Grant-in-Aid for Scientific Research

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2. Others

水内亨，核融合科学研究所，双方向型共同研究

水内亨，（株）日立製作所，京都大学エネルギー理工学研究所における核融合研究に対する助成

水内亨，核融合科学研究所・一般共同研究，高性能核融合プラズマ閉じ込め理工学の深化に向けた先進ヘリカル研究の現状と展望

水内亨，核融合科学研究所・一般共同研究，京都大学におけるヘリオトロン型磁場配位による核融合プラズマ研究に関する歴史的資料収集･整理

小林進二，核融合科学研究所・一般共同研究，重水素放電における高速イオン荷電交換分光の検討

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Advanced Energy Research Section

Christine S. Chow, Foreign Visiting Researcher
(Professor of Chemistry, Wayne State
University, Detroit, MI 48202, USA)

1. Summary

The author spent three months (April 14, 2016 – July 22, 2016) as a visiting professor at the Uji campus of Kyoto University, hosted by the group of Prof. Takashi Morii.

Here the author reports on the investigation of peptide interactions with RNA and the study of platinated RNAs.

2. Introduction

A number of antibiotics in use today target bacterial ribosomes. Resistance to these naturally derived compounds is a common challenge, with the need to create unique inhibitors that are not derived from natural products. Furthermore, targeting biologically important regions within the bacterial ribosome is also difficult because a variety of resistance mechanisms involve modifications to these locations. The goal of this work is to identify new locations for inhibition of bacterial functions along with the discovery of compounds that can selectively target those regions. The bacterial ribosome is a well-known natural target for antibiotics and plays a critical role in protein synthesis. The antibiotics target key domains such as the aminoacyl-tRNA binding site and peptidyl transferase center. In efforts to study a unique region for antibiotic development, helix 69 (H69) of the 50S subunit of bacterial ribosomes was chosen. This 19-nucleotide stem-loop motif is located at the central region of the ribosome (Figure 1) [1].

Peptides are known to have favorable antimicrobial properties and can also target bacterial ribosomes. A heptameric peptide (NQVANHQ) was shown to be an H69 binder with moderate affinity (low μM) and selectivity for the bacterial over human H69 [2]. The goal of the work carried out during the author's stay in Uji was to analyze sequence variants in order to identify tighter-binding and more selective species, and also improve on the membrane permeability of these peptides by synthesizing a series of variants with cell-penetrating moieties attached at the ends. In addition, a series of platinum complexes were explored for their ability to target H69 RNA. The results of kinetic studies and binding-site characterization were presented at the 21st Annual Meeting of the RNA Society in Kyoto from June 28 – July 2, 2016.

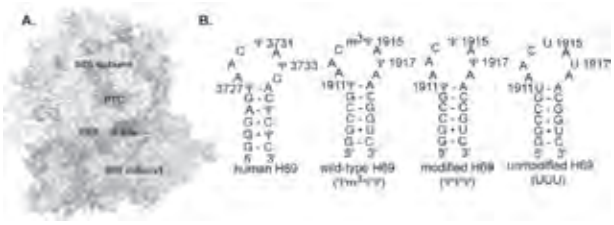

Figure 1. A) The 70S *E. coli* bacterial ribosome (PDB: 2AVY, 2AW4) is shown with H69 highlighted in cyan, aminoacyl-tRNA site (A site) in red, peptidyl transferase center (PTC) in purple, 30S subunit in light grey, and 50S subunit in yellow. B) The secondary structures of H69 are given (from left to right) to compare human H69, with wild-type H69 (with *E. coli* numbering), a modified H69 variant (ΨΨΨ), and unmodified H69 (UUU).

3. Experimental observations

As illustrated in Figures 2 and 3, positions 1 and 4–7 of the peptide were determined to be the most important for binding affinity with the modified variant of H69, ΨΨΨ. For example, at position 1, the preference is R > N >> A (in combination with positions 2–7, QVANHQ), in which replacement of N with R improves binding and the presence of A abolishes binding. In contrast, replacement of A with R in position 4 causes a greater than five-fold reduction of binding [3].

Figure 2. The relative binding affinities and selectivities of the peptide variants for ΨΨΨ (upper) or UUU (lower) are illustrated. Each position contains either A, R, or the parent amino acid along with the remaining parent amino acid sequence, which is indicated in blue. The size of the letter indicates the relative affinity or selectivity of that amino acid variant compared to the other amino acids at that position, with larger letters indicating tighter binding or more selective species.

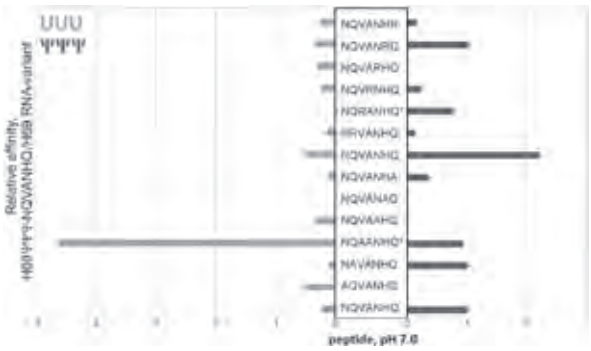

Figure 3. Graphical representation of modified peptide variant binding affinity relative to the parental peptide-modified H69 interaction (ΨΨΨ-NQVANHQ).

The results illustrated in Figure 3 support the idea that peptide ligands can be modified to achieve high selectivity and affinity to functionally important ribosomal RNA motifs and that these RNA-binding species have similar affinities to natural RNA-targeting compounds such as aminoglycoside antibiotics. With these results in hand, the author set out to generate compounds that could overcome the second challenge, which is cell penetration. The goal was to synthesize compounds that can cross bacterial cell membranes but not those of humans. The peptides NQAANHQ and RQVANHQ were chosen for further modification because they showed the highest affinity and selectivity for the unmodified and modified versions of H69. Preliminary results reveal that the short alkyl chain has a modest affect on the ability of the peptide to kill bacteria. Currently the impact of the longer alkyl chain on cell viability is being examined through the use of MIC studies.

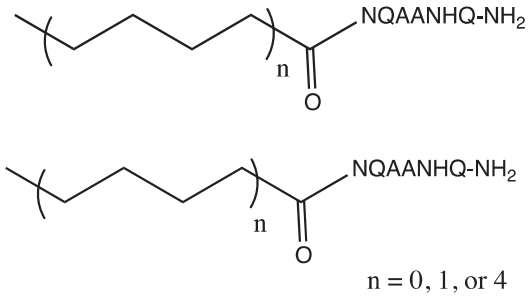

Figure 4. Peptide variants with cell-penetrating moieties at the N terminus are illustrated.

The second project involved the exploration of platinum compounds as new RNA-targeting agents. The well-known anticancer agent cisplatin and several of its analogues have been examined for their ability to bind to the H69 motif of ribosomal RNA (Figure 1) [4]. Cancer patients undergoing chemotherapy are known to be more susceptible to infections, including those caused by bacteria or viruses. While common side effects of chemotherapy are due to impairment of the immune system, there could be other molecular functions that are altered or inhibited by anticancer drugs. The impact of cisplatin on resistance to antibacterial drugs such as aminoglycosides was explored. More specifically, reaction rates of cationic platinum complexes with H69 constructs were determined in the presence of different antibiotics such as the aminoglycosides. The rates of platination with RNA decrease in the presence of aminoglycosides, suggesting a competition of the two compounds for RNA binding. This work demonstrates the utility of platinum binding kinetics as a tool to study RNA-drug interactions, and also provides insight into antibiotic resistance caused by cisplatin. Potential projects that could be developed from this work include examination of RNA or DNA structures following platination using techniques such as DNA origami. For example, DNA circles can be formed by ligating platinated oligonucleotides, which would allow specific structural changes to be visualized and measured by AFM.

4. Acknowledgements

The author thanks the Institute of Advanced Energy and Kyoto University for providing financial support and office space during her visit. She is grateful to Professor T. Morii and his entire research group for their generous support and many helpful discussions. She is particularly thankful to Drs. S. Nakano and E. Nakata, as well as Prof. I. Saito, for their collaborations, helpful discussions, and technical assistance, and to Ms. Kaori Hashimoto for all of her help with paperwork and pre-trip arrangements.

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Advanced Energy Research Section

Joon-Hwa Lee, Foreign Visiting Professor
(Professor in Department of Chemistry, Gyeongsang National University, 501 Jinju Boulevard, Jinju, Gyeongnam 52828, Republic of Korea)

1. Summary

The author spent three months (Aug. 9, 2016 - Nov. 8, 2016) as a guest professor at the Uji campus of Kyoto University, hosted by the Masato Katahira group.

Here the author reports about an NMR investigation on salt concentration dependency of B-Z transition of DNA induced by the Zα domain of the PKZ from *Carassius auratus* (caZα$_{PKZ}$).

2. Introduction

Z-DNA binding proteins (ZBPs) play important roles in RNA editing, innate immune response and viral infection [1]. ZBPs have been identified in an RNA editing enzyme (ADAR1), DNA-dependent activator of interferon-regulatory factor (DAI), the viral E3L protein and a fish protein kinase containing a ZBP (PKZ) [1]. structural studies in solution suggested an *active* mechanism of B-Z transition of a 6-bp DNA induced by ZBPs, in which (i) the ZBP (denoted as **P**) binds directly to B-DNA (denoted as **B**); (ii) the B-DNA in the complex is converted to Z-form; and (iii) the stable **ZP2** complex (the Z-form DNA denoted as **Z**) is produced by the addition of another **P** to **ZP** [2].

The crystal structures of the caZα$_{PKZ}$ in complex with dT(CG)$_3$ revealed that two caZα$_{PKZ}$ molecules bind to each strand of double-stranded Z-DNA using residues in their α3 helix and their β-hairpin (β2-loop-β3) [3]. The solution structure of the free form of caZα$_{PKZ}$ was mostly similar to its structure when bound to Z-form dT(CG)$_3$, with the exception of the orientation of the β-hairpin, which is involved in a charge-charge interaction with the phosphate backbone of the Z-DNA [4]. In a previous study, we performed the global analysis of chemical shift perturbation ($\Delta\delta_{obs}$) and relative Z-DNA population (f_Z) data at 10 mM and 100 mM NaCl using Eqs. (1) and (2), repsecetively:

$$\Delta\delta_{obs} = \frac{[BP]}{[P]_{tot}}\Delta\delta_B + \frac{[ZP] + 2[ZP_2]}{[P]_{tot}}\Delta\delta_Z \quad (1)$$

$$f_Z = \frac{[ZP] + [ZP_2]}{[N]_{tot}} \quad (2)$$

This study found that the protein had different binding affinities for B- and Z-DNA and that interaction with B-DNA was severely affected by the concentration of NaCl ([NaCl]).

In order to investigate the B-Z transition induced by caZα$_{PKZ}$ at high [NaCl], we analyzed the imino proton spectra of dT(CG)$_3$ during titration with caZα$_{PKZ}$ and monitored the ^{1}H-^{15}N chemical shift perturbations of caZα$_{PKZ}$ during titration with dT(CG)$_3$, both at 250 mM NaCl.

3. Experimental observations

(1) Relative Z-DNA population of dT(CG)$_3$ upon binding to caZα$_{PKZ}$ at 250 mM NaCl

We collected imino proton spectra of dT(CG)3 with different sets of $[N]_{tot}/[P]_{tot}$ ratios at 10, 100, and 250 mM NaCl and analyzed them to deduce relative Z-DNA populations (f_Z). Fig. 1A shows the f_Z values at 10, 100 and 250 mM NaCl as a function of $[N]_{tot}/[P]_{tot}$ ratio. Even with an excess amount of protein ($[N]_{tot}/[P]_{tot}$ ratio = 0.1), the f_Z reached only ~ 0.5 at 250 mM NaCl, whereas f_Z was nearly 1 at both 10 mM and 100 mM NaCl. Also, f_Z values at a $[N]_{tot}/[P]_{tot}$ ratio = 0.5 dropped significantly as [NaCl] increased, reaching a value of ~0.35 at 250 mM NaCl. This is consistent with previous data which showed that the B-Z transition rarely occurred at 250 mM NaCl, even with an excess molar ratio of caZα$_{PKZ}$.

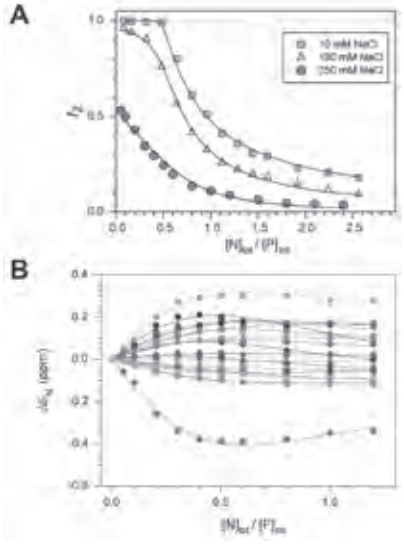

Fig. 1: (A) f_Z values of dT(CG)$_3$ induced by caZα$_{PKZ}$ at 10 (blue square) [4], 100 (yellow triangle) [4], or 250 mM NaCl (magenta circle, this study) as a function of $[N]_{tot}/[P]_{tot}$ ratio. (B) ^{15}N chemical shift changes ($\Delta\delta_N$) of HSQC cross-peaks of caZα$_{PKZ}$ upon dT(CG)$_3$ binding at 250 mM NaCl. Solid lines are the best fits to the Eqs. (1) and (2).

(2) Chemical shift perturbation of caZα$_{PKZ}$ upon binding to dT(CG)$_3$ at 250 mM NaCl

Fig. 1B shows the ^{15}N chemical shift changes in

the HSQC spectra of caZα$_{PKZ}$ at 250 mM NaCl as a function of $[N]_{tot}/[P]_{tot}$ ratio. The magnitude of each chemical shift change was reduced compared with that measured at 10 and 100 mM NaCl in the previous study [4]. For example, amide resonances of I22, T25, H40 and Q49 were less perturbed by dT(CG)$_3$ addition at 250 mM NaCl than at 10 and 100 mM NaCl (Fig. 2). This implies that the binding affinity is weaker at 250 mM NaCl than at the lower salt concentrations.

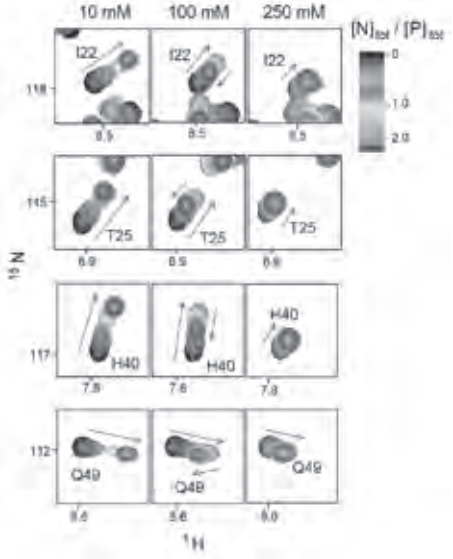

Fig. 2: Comparison of the 1H-15N HSQC peaks of the I22, T25, H40, and Q49 of caZα$_{PKZ}$ at 10 (left) [4], 100 (middle) [4], or 250 mM NaCl (right, this study). The cross-peak color changes gradually from blue (free) to red (bound) according to the $[N]_{tot}/[P]_{tot}$ ratio.

(3) Chemical shift differences in caZα$_{PKZ}$ upon binding to B-DNA and Z-DNA

By using the global fitting method, 1H and 15N chemical shift differences of the B-DNA-bound and Z-DNA-bound forms relative to the free form are also deduced. In the previous study [4], it was shown that the B-DNA and Z-DNA cause distinctive chemical shift perturbations at 100 mM NaCl whereas they do not at 10 mM NaCl. The differences between the chemical shift perturbations of the BDNA-bound form and the Z-DNA-bound form become more significant at 250 mM NaCl.

^{1}H chemical shift differences in Q49 of the free, B-DNA-bound, and Z-DNA-bound forms at the three NaCl concentrations were summarized in Fig. 3. The chemical shift perturbations clearly show that, at high salt, the conformation of the B-DNA-bound form is very like that of the free protein, but as the [NaCl] decreases, the Z-DNA-bound conformation predominates. This suggests that the chemical shifts of the B-DNA-bound form at each different salt concentration reflect the extent of the active conformation of caZα$_{PKZ}$ for B-Z transition.

In this study, we present the binding affinity for B- and Z-DNA of caZα$_{PKZ}$ and the resulting relative Z-DNA populations based on the global fitting of NMR data at 250 mM NaCl, indicating the significantly lower Z-DNA population at all $[N]_{tot}/[P]_{tot}$ ratios at 250 mM NaCl, compared to the other salt concentrations (Fig. 1A). CaZα$_{PKZ}$ has a unique salt concentration-dependent B-Z transition activity, unlike other ZBPs such as hZα$_{ADAR1}$ and yabZα$_{E3L}$ [3]. We suggested that the reduced B-Z transition activity at high salt concentrations resulted from the weaker intermolecular interactions associated with the reduced binding surfaces. Structural features of the B-DNA-bound form at 250 mM NaCl are different from those at 10 and 100 mM NaCl, which is revealed as distinctive chemical shift changes (Fig. 3). When we assumed the B-DNA-bound form at 10 mM NaCl as the fully active BP conformation, the active population decreased as the salt concentration increased.

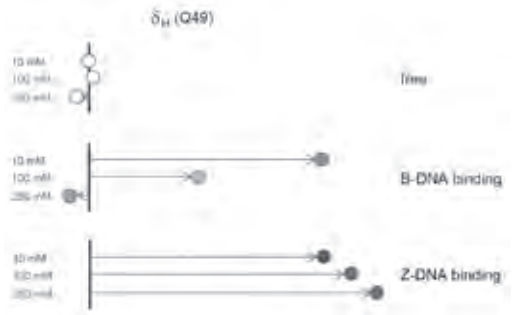

Fig. 3: ^{1}H chemical shift differences of Q49 for free, B-DNA bound, and Z-DNA bound forms at 10, 100 and 250 mM NaCl. The ^{1}H chemical shift value of Q49 for the free form at 10 mM NaCl is the reference point.

In summary, we have studied the B-Z transition induced by caZα$_{PKZ}$ at 250 mM NaCl by NMR spectroscopy. The B-Z transition activity of caZα$_{PKZ}$ was severely impaired and the binding affinity for B-DNA was critically reduced by increased salt. Chemical shift differences for the B-DNA-bound form of caZα$_{PKZ}$ reflected the proportion of active B-DNA-bound conformation present in solution, which is modulated by the salt concentration. Our results emphasize that the B-DNA-bound form of caZα$_{PKZ}$ can be used as molecular ruler to quantify the degree of B-Z transition.

This study has been published in *Biochemical and Biophysical Research Communications* in January, 2017 [5].

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Advanced Energy Research Section

Geir Martin Haarberg, Visiting Professor
(Professor at Norwegian University of Science and Technology, NO-7491 Trondheim, Norway)

1. Summary

The author spent three months at Kyoto University, Uji Campus in Prof. Nohira group. A review of the most promising technologies for electrochemical production of silicon for photovoltaic applications is presented. Recent efforts are summarised and discussed here, and a new method is proposed.

2. Introduction

Solar energy is one of the best options for future generation of renewable and sustainable electricity. The challenge is that solar cells are very expensive to produce. Silicon is abundant and non-toxic. Industrial production of solar grade silicon is energy intensive and the product has a high price. Many research projects have been carried out to develop alternative processes for SoG-Si, and they are either metallurgical or electrochemical. A review on electrochemical approaches in molten salts was recently published [1]. The main challenge is to reduce the levels of phosphorus and boron to less than 1 ppm.

3. Electrochemical approaches

Silicon cannot be deposited from aqueous electrolytes due to the negative deposition potential which will give hydrogen as the main cathode product. Electrolytes of molten salts, molten oxides and ionic liquids have been proposed as electrolytes. The most common approach is electrolysis with decomposition of a dissolved raw material where silicon is deposited on a cathode substrate and a gas, mainly Cl_2, CO_2 or O_2, is evolved at the anode. Alternatively electro-decomposition of solid SiO_2 in molten $CaCl_2$ based electrolytes can be used, as proposed by Nohira et al. [2]. Other principles are based on electrorefining using impure Si as the anode or depositing a liquid silicon containing alloy.

4. Electrolyte

Molten oxide electrolytes or molten slags have the advantage of depositing liquid silicon. However the high temperature and corrosive environment represent major challenges. More research have been carried out in different molten salt electrolytes; mainly chlorides, fluorides or a mixture of these. Low water solubility in many fluorides may cause problems removing solidified salt. Mixtures of KF and chlorides have successfully been studied [3]. Fluorides are generally known to give better quality deposits than chlorides, due to the formation of stable complexes which may prevent diffusion controlled deposition. Another possibility is to use ionic liquid electrolyte [4]. A promising electrolyte is 1-butyl-1-methyl-pyrrolidiniumbis(trifluoromethylsulfonyl)-imide ([BMP]Tf_2N). Cyclic voltammetry is shown in Fig. 1. The main challenge at low temperatures is that silicon is a poor conductor which will limit the thickness of the deposit.

5. Raw material

Silica powder, SiO_2, is the most convenient raw material in terms of price and availability, but metallurgical grade silicon (MG-Si) is a good alternative. Also a silicon containing salt may be used; the best candidates being K_2SiF_6 and $SiCl_4$. The advantage of using MG-Si is that electro-refining may be applied method. This may give the desired purity after a few repeated refining step and could be competitive if each refining step has a low energy consumption. Reports have shown that silicon should be present as a complex in molten salts to avoid evaporation of $SiCl_4$ or SiF_4, and adding SiO_2 may give rise to the formation of stable dissolved oxide complexes. $SiCl_4$ is probably the best choice for ionic liquids.

6. Electrodes

High purity Si is very reactive, and this has especially been observed when depositing Si from ionic liquids [5]. The deposits frequently reacted spontaneously with water. High purity Si electronic grade was found to dissolve spontaneously in molten $CaCl_2$ with dissolved CaO and SiO_2 [6]. The cathode substrate should be inexpensive and inert with respect to silicon. Silver is a good candidate due to its inertness, but it is somewhat expensive. Results from voltammetry on silver are shown in Fig. 2. Candidate elements for producing liquid alloys are copper, zinc and aluminium. Deposition of silicon on aluminium may be a way of simplifying the production of solar cells, since Al is expected to replace Ag as the contacting metal for solar cells [8]. Various forms of carbon are available and inexpensive, and graphite or glassy carbon could be an excellent cathode

substrate. One problem is intercalation of alkali metals, especially potassium. At the anode, chlorine evolution may be acceptable when using chloride based electrolytes. In molten salts containing dissolved silicon oxide graphite anodes may be used, but CO_2 may cause formation of carbonate ions which may be reduced to carbon at the cathode. The best inert anode candidate for oxygen evolution may be tin oxide, which should be inert at temperatures up to ~800 °C. A liquid silicon-copper has successfully been used as a dissolving silicon anode for electrorefining of metallurgical grade silicon [6]. Some interesting results have fairly recently been published by Maldonado and co-workers [9-11]. They have focused on depositing semiconductor materials of nano size scale by using a novel approach employing a liquid cathode such as gallium or mercury. Successful deposition of silicon nanowires from propylene carbonate electrolyte with $SiCl_4$ at temperatures as low as 60 °C by using liquid gallium droplets as cathode was reported [11]. In this case silicon precipitates inside the liquid Ga cathode from a supersaturated solution and there is very little alloy formation. The active cathode is liquid Ga, so the poor electric conductivity of Si at low temperature will not cause any limitation of the process.

7. Conclusion - Concept for a new process for electrochemical production of SoG-Si

The proposed concept is based on the use of a liquid cathode which does not alloy with silicon. A good cathode candidate is gallium, which is liquid from 30 °C to 2204 °C. Solid silicon will precipitate inside the liquid cathode. Using ionic liquid electrolytes $SiCl_4$ should be the raw material and chlorine gas will be evolved at the anode. Molten salt electrolytes should be based on $CaCl_2$-NaCl-CaO or KCl-KF. The best option for obtaining silicon of high purity is to use metallurgical grade silicon as the raw material in an electrorefining process using a liquid Si-Cu anode.. Alternatively the raw material can be high purity SiO_2 in a process using an inert oxygen evolving anode. The process should be further optimised by exploring other liquid cathodes which may alloy with impurities of boron and phosphorus.

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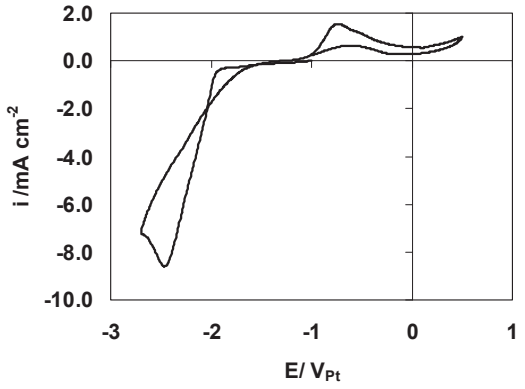


Figure 1. Cyclic voltammetry on Al in [BMP]Tf_2N saturated with $SiCl_4$ (~1 M) [5]. Potential scan rate: 10 mV s^{-1}

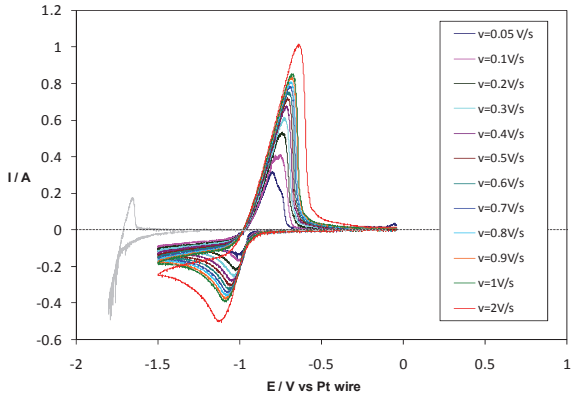


Figure 2. Cyclic voltammetry on Ag in molten KF-LiF-K_2SiF_6 at 800 °C [7].

Advanced Energy Research Section

Saravanan Chinnusamy, Visiting Research Scholar
(Assistant Professor & Head
Centre for Advanced Organic Materials
Department of Chemistry
Sona College of Technology, Salem-636 005
Tamil Nadu, India)

1. Summary

The author spent three months (July 1, 2016-September, 2016) as a visiting research scholar at the Uji campus of Kyoto University, hosted by the Professor Hiroshi Sakaguchi.

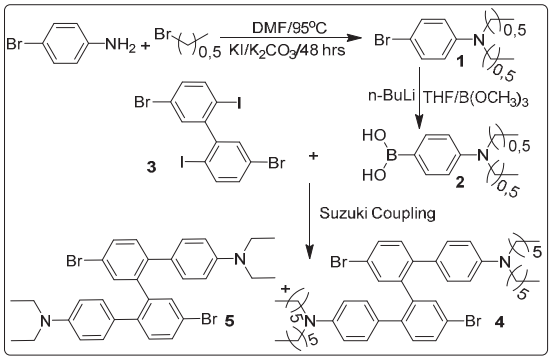
Here the author reports about a design and synthesis of new precursors for graphene nanoribons (GNRs) synthesized through the chemical vapour deposition (CVD) to Hirosi Sakaguchi.

2. Introduction

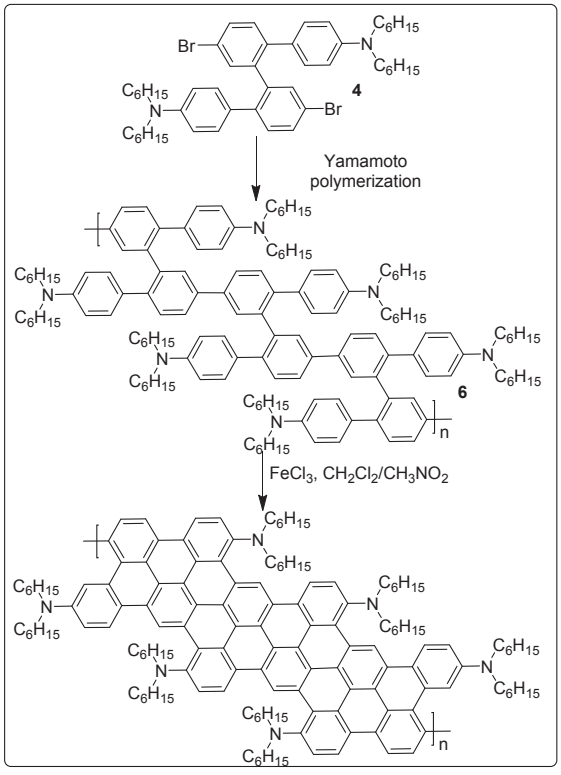
Because of high charge carrier mobility and conductivity properties related to its honeycomb lattice, graphene has emerged as a promising candidate material for nanoelectronics. However, graphene is a zero-bandgap semimetal, which limits its application as channel material for field-effect transistors (FETs).[1] One route to circumvent this problem is to shape graphene into strips known as nanoribbons (GNRs), which can be made by several efforts either through top-down or bottom-up approaches. Since the band gap of GNRs mainly depends inversely on the width of the ribbon, the scientist in a position to prepare atomically precise structure with different edges such as armchair, zigzag etc. In the case of top-down approaches, the GNRs can be etched from 2D graphene sheets using both self-assembled and lithographically defined masks. These methods, however, usually introduce rough edges and lack of structural precision into the GNRs, which undermines their electrical performances.[2] Unzipping the carbon nanotubes yields narrow GNRs with good quality, but the low throughput of this approach severely limits its scalability. Alternatively, atomically precise GNRs can be fabricated via bottom-up method through thermally induced polymerization of halogen containing molecular precursors on metal surfaces, mainly on Au and Ag, which is known as chemical vapour deposition (CVD). However, this method can yield a limited amount of GNR material on the surface of metal, which impedes its wider applications in electronic devices.[3] Alternatively, the GNRs have also been prepared by solution process, which pave the way for large scale production.[4] In this regard, we have designed and synthesized various types of precursors for the preparation of solution processed GNRs.

3. Experimental observations

The synthetic for the preparation of preparation of precursors and their GNRs are shown in Scheme 1 and 2.



Scheme 1. Synthetic route for the preparation of precursors 4 and 5.



Scheme 2. Synthetic route for the preparation of GNRs.

4-Bromoaniline was alkylated in the presence of potassium carbonate to compound 1 with the yield of 65% as white coloured powder and the corresponding boronic acid derivative 2 was achieved using n-butyllithum. The compound 3 was prepared according to the reported procedure.[5]

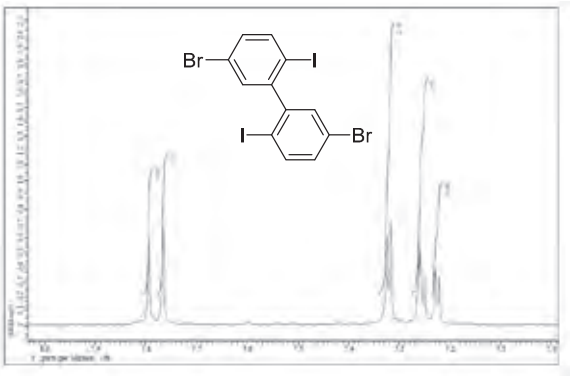


Figure 1. ^{1}H-NMR spectrum of compound 3.

The Suzuki coupling reaction between 1 and 3 yields precursor 4 and 5 as a white coloured solid with the yield of 25 and 27%, respectively. Particularly, the purification of precursor 4 and 5 is highly complicated due to the presence of many side product confirmed through the observation of many spots with close R_f in its thin layer chromatography. After column purification, we injected into MPLC for further purifications.

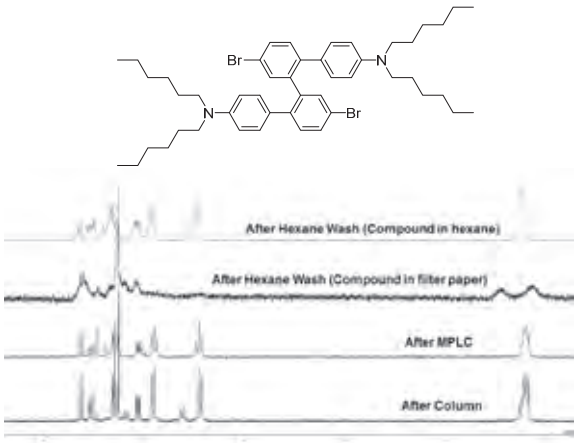


Figure 2. ^{1}H-NMR spectrum of compound 3 with various purification process.

After the Yamamoto polymerization of 4 to yield polyphenylene precursor **6** with good yield. The cyclisation of 6 as well as characterization is ongoing in professor Sakaguchi laboratory.

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Advanced Energy Materials Research Section

K. Matsuda, Professor
T. Hinoki, Associate Professor
Y. Miyauchi, Associate Professor
K. Jimbo, Assistant Professor

1. Introduction

We are working on basic and applied science 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, graphene related materials, and layered transition metal dichalcogenides for efficient utilization of light energy and development of future optoelectronic devices with ultra-low energy consumption. The Multi-Scale Testing and Evaluation Research Facility is also used for development of new composite materials. Followings are main research achievements in the year of 2016.

1. Anisotropic Optical Properties of Layered Germanium Sulfide

Two-dimensional (2D) layered materials, transition metal dichalcogenides and black phosphorus, have attracted much interest from the viewpoints of fundamental physics and device applications. The establishment of new functionalities in anisotropic layered 2D materials is a challenging but rewarding frontier, owing to their remarkable optical properties and prospects for new devices. Here, we studied the anisotropic and thickness dependent optical properties of layered 2D monochalcogenide of germanium sulfide (GeS). Figure 1 shows the Schematic crystal structure of GeS. Three Raman scattering peaks corresponding to the B_{3g}, A_{1g}, and A_{2g} modes with strong polarization dependence are demonstrated in the GeS flakes, which validates polarized Raman spectroscopy as an effective method for identifying the crystal orientation of anisotropic layered GeS.

Photoluminescence (PL) is observed with a peak at around 1.66 eV that originates from the direct optical transition in GeS at room temperature. The significantly decrease of the PL intensity with decrease of GeS thickness is observed, which suggests the presence of surface defect states. Moreover, determination of the polarization dependent characteristics of the PL and absorption reveals an anisotropic optical transition near the band edge of GeS, which is also supported by the density functional theory calculations. This anisotropic layered GeS presents the opportunities for the discovery of new physical phenomena and will find applications that exploit its anisotropic properties.

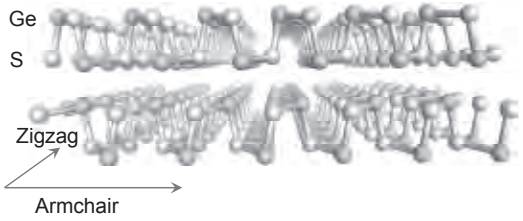

Fig. 1 Schematic crystal structure of 2D monochalcogenide of germanium sulfide (GeS). GeS has an anisotropic crystal structure along zigzag and armchair direction.

2. Highly Efficient and Stable Perovskite Solar Cells by Interfacial Engineering Using Solution-Processed Polymer Layer

Solar cells based on methylammonium lead halide pervoskites ($CH_3NH_3PbX_3$, X=I, Br, Cl) have been attracted much attention in recent several years. Since 2010, the power conversion efficiency of perovskite solar cells has improved drastically through improvements and engineering of solvents, interfaces, and materials. However, some emergent issues in $CH_3NH_3PbX_3$ remain to be solved for the future industrial applications. Large crystallites have been observed to result in the formation of large voids (pinholes) and boundaries in the perovskite layer, which may produce shunt-leakage paths that reduce

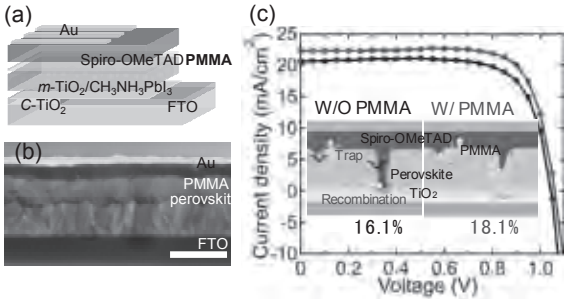

Fig. 2 (a) Schematic of device structure. (b) Cross-sectional SEM image of the device. (c) Photovoltaic performance of perovskite solar cell with and without PMMA layer. Inset shows carrier recombination dynamics.

the photovoltaic performance.

Here we studied a facile method for improving the performance in perovskite solar cells by insertion of a solution-processed polymer layer between the perovskite and the hole-transporting layer. Figure 2 (a) and (b) show the schematic of device structure, and cross-sectional SEM image of the device. The photovoltaic conversion efficiency of perovskite solar cell increases increased to 18.1% and stability is only about 5% decreased during 20 days exposed in moisture ambient conditions by a poly-methyl methacrylate (PMMA) polymer layer incorporation, as shown in Fig. 3(c). The improved photovoltaic performance of devices by a PMMA layer is attributed to reducing the carrier recombination loss from pinholes, boundaries and surface states of perovskite layer. The significant gain generated by this simple procedure supports the use of this strategy in further applications of thin film optoelectronic devices.

3. Evaluation of photoluminescence quantum yield of monolayer WSe2 using reference dye of 3-borylbithiophene derivative

Since discovery of unique properties of graphene, research interests on atomically thin-layered two-dimensional (2D) semiconductors have been stimulated extensively. The monolayer transition metal dichalcogenides (TMDs) with a chemical formula of MX_2 (M = transition metal atom and X = chalcogen atom; M = Mo, W; X = S, Se, and Te) as atomically thin-layered 2D semiconductors have attracted much interests both from viewpoints of fundamental physics and applications in recent years. The photoluminescence (PL) quantum yield is defined as the ratio of photons absorbed and emitted from the materials, which is an essential value for the optical analysis of semiconductors.

We studied an evaluation method of photoluminescence quantum yield of monolayer transition metal chalcogenides on a transparent substrate using a reference dye. A 3-borylbithiophene derivative ($C_{58}H_{49}BN_2S_4$) reference dye shows a high PL quantum yield of 36% even in the solid form and the high quantum yield is kept in a Poly(methyl methacrylate) (PMMA) matrix. Moreover, the photon energy of PL is similar to those of monolayer TMDs. These PL characteristics of the reference dye are useful for an evaluation of PL quantum yield in monolayer TMDs. The PL quantum yield of 0.18 ± 0.03% was evaluated for mechanically exfoliated monolayer WSe_2 on glass substrate at room temperature.

4. Novel Silicon Carbide Composites with Particle Dispersion in Matrix

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

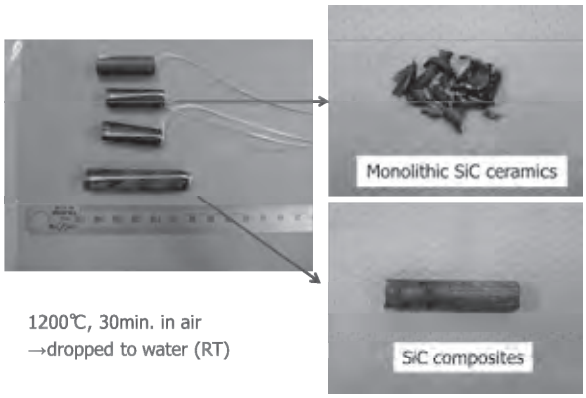

Fig. 3 Monolithic SiC ceramic tubes and BN particle dispersion SiC composite tube before and after thermal shock tests from 1200 ^{o}C to ambient temperature.

Silicon carbide composites were fabricated by CVI method and LPS method. Silicon carbide with C matrix was formed by mixture of SiC source gas and C source gas in CVI composites. Silicon carbide with BN matrix was formed by mixture of SiC powder and BN powder in LPS composites. Mechanical properties were characterized by tensile test and flexural test before and after exposure in air up to 1750C. Microstructures and fracture surfaces were characterized by FE-SEM.

Both SiC composites with C and with BN in matrix have uniform microstructure through thickness. They showed ductile fracture behavior with fiber pullouts. The technique was applied to fabricate 10 mm diameter tube for fuel cladding of light water reactor. Thermal shock test was carried out using the composite tube. The tube was heated to 1200 ℃ in air, kept 30 min and dropped to ambient temperature water. The composite tube kept original shape without apparent damage, although the monolithic ceramic SiC tube was completely fractured. Figures 3 show monolithic ceramic tube and the composite tube before and after the thermal shock tests.

Collaboration Works

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

Politecnico di Torino（イタリア）、Oak Ridge National Laboratory（米国），セラミックス材料の接合強度評価技術開発，檜木達也

Politecnico di Torino（イタリア），Mechanical and sealant joining of SiC/SiC composites for high temperature applications，檜木達也

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

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

OECD NEA, THE EXPERT GROUP ON ACCIDENT TOLERANT FUELS FOR LIGHT WATER REACTORS (EGATFL), 檜木達也

東北大学金属材料研究所，原子力用セラミックス及びセラミックス複合材料の中性子照射効果，檜木達也

核融合科学研究所・LHD 計画共同研究，LHD ダイバータのタングステン化に向けたコーティング技術の開発と膜特性評価，檜木達也

量子科学技術研究開発機構，SiC/SiC 複合材料の照射下強度予測のための SiC の動的照射特性評価，檜木達也，近藤創介

Financial Support

1. Grant-in-Aid for Scientific Research

松田一成，新学術領域研究，原子層人工ヘテロ構造における新規光物性と光学応用

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ニクスの創生と応用

松田一成，挑戦的萌芽研究，遷移金属ダイカルコゲナイドの新規光電変換機能とその応用

松田一成，特別研究員奨励費，原子層ヘテロ構造の光科学と太陽電池応用

宮内雄平，新学術領域研究，偏光分解分光イメージングによる原子層局所形態・光物性相関の研究

宮内雄平，挑戦的萌芽研究，遷移金属ダイカルコゲナイドにおける光誘起バレー分極の制御に関する研究

宮内雄平，若手研究（A），極限ナノ物質の複合化による新奇創発量子物性の誘起とその応用

2. Others

松田一成，（公財）旭硝子財団，極限二次元単層ナノ物質におけるグリーンフォトニクスの開拓

檜木達也，核融合科学研究所・PHENIX 事業，原型炉プラズマ対向機器開発のための要素技術の工学的評価

檜木達也，核融合科学研究所・LHD 計画共同研究，LHD ダイバータのタングステン化に向けたコーティング技術の開発と膜特性評価

檜木達也，日伊エグゼクティブプログラム，”Protective joining and coating of new porous matrix SiC/SiC composites for high temperature applications,” Politecnico di Torino（イタリア）

檜木達也，近藤創介，量子科学技術研究開発機構，SiC/SiC 複合材料の照射下強度予測のための SiC の動的照射特性評価

宮内雄平，村田学術振興財団，原子層半導体におけるバレー分極状態の空間マッピングとその制御

宮内雄平，（公財）光科学技術研究振興財団，カーボンナノチューブの近赤外アップコンバージョン発光を用いた生体深部の高解像イメージング手法の開拓

宮内雄平，（公財）中谷医工計測技術振興財団，カーボンナノチューブの近赤外アップコンバージョン蛍光を用いた生体イメージング

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Advanced Laser Science Research Section

T. Nakajima, Associate Professor

1. Introduction

The main objective of our research is to develop the laser-related theory and experimental techniques to contribute to the efficient use of laser-based devices in energy science. The targets we employ for our studies ranges from nanoparticles (NPs), metallic films, and polymer films with the goal to develop new techniques to monitor the dynamics upon irradiation of lasers and also fabricate new materials.

2. Observation of number-density-dependent growth of plasmonic nanobubbles

In recent years intense studies on the optical properties of NPs have led to various interesting applications in biophysics and many other fields. For most of the applications an effective use of laser-induced surface plasmon (SP), a collective motion of free electrons on the NP's surface, is the key, since most of the applications are based on the photothermal heating of NPs via SP. In many applications the surrounding medium is water (or liquid), and as a natural consequence of the plasmonic heating of NPs, plasmonic nanobubbles (NBs) are formed. In this work we experimentally study the temporal growth of plasmonic NBs, and find that its growth exhibits a striking dependence on the number density of NPs.

The experimental setup consists of the second harmonic (532nm) of the Q-switched Nd:YAG laser, which serves as a pump and also probe pulse, 50 μL quartz cuvette filled with the Ag NP solutions as a sample, and two photodiodes to measure the temporal profiles of the 532nm pulse before and after the cuvette. Since the irradiation of single laser pulse can result in the size reduction of NPs we use a fresh NP solution for every single laser pulse so that the well-defined NP solution interacts with the laser pulse. Figure 1 shows the procedure to obtain the time-resolved NB radius from the optical detection. Briefly, the temporal profiles of the 532nm pulse before and after the cuvettes (Fig. 1(b)) are converted to the time-dependent extinction cross sections (red curve in Fig. 1(c)), which are further recast into the time-dependent NB radius (black curve in Fig. 1(c)) with the aid of the relation between the extinction cross section and NB radius calculated by the Mie theory (Fig. 1(a)). We repeat the measurements, and obtain the NB radius at the end of the pulse (7 ns) for

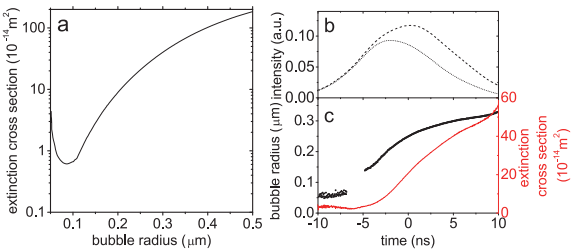

Fig. 1 (a) Extinction cross section of the NB at 532 nm as a function of bubble radius calculated by the Mie theory. (b) Typical temporal profiles of 532 nm pulses before (dashed) and after (dotted) the cuvette. (c) Time evolution of extinction cross section (red) calculated from the curves in graph (b) and time evolution of bubble radius (black) obtained using the red curve and graph (a).

the different laser fluences and number densities of Ag NPs, and the results are summarized in Fig. 2. Obviously, at any number density of Ag NPs, the bubble radius is larger when the incident laser fluence is higher. This is simply because more heating of surrounding water as well as Ag NPs takes place when the incident laser fluence is higher. Surprisingly, we find that the growth of NBs has a striking dependence on the number density of Ag NPs when the laser fluence is high. In contrast, the growths of NB radius are very similar, irrespective of the number density, when the laser fluence is low. At the number densities of NPs we study in this work, the inter-particle distance is in the range of 14-30 μm , and the question is what kind of interaction can influence the bubble dynamics.

We attribute this anomalous behavior of NBs to the effect of the shock wave, and carry out the nu-

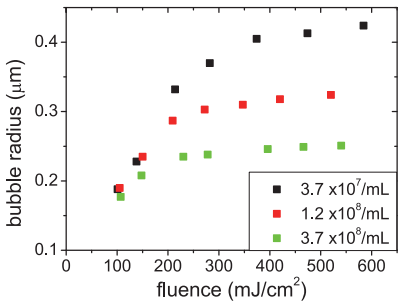

Fig. 2 Bubble radius at the end of the pulse for the different laser fluences and number densities of Ag NPs.

merical calculations. The results reasonably agree with the experimental ones.

Our findings imply that the number density can be a new doorknob to control laser-nanobubble as well as laser-nanoparticle interactions.

3. Laser-induced nanostructures on thin Au films

NPs have been of great interest due to its wide application in various fields. In spite of their tremendous usefulness, uniform placing of NPs on a substrate is not easy, because aggregation can take place. In some cases, fabricating a thin film first on a substrate, and then induce nanostructures (NS) on it by thermal or laser annealing may be more cost-effective and convenient.

Conventional thermal annealing can surely induce NS on Au films, but it takes some time. Laser annealing is another way, but it also takes some time, in particular if ultraviolet or visible lasers are employed. This can be well-understood if one recalls that the use of such lasers requires the focus of the beam onto the film down to the sub-mm diameter, which means that the beam spot has to be scanned on the film for the large-area processing. If one employs a mid-infrared laser, thin metallic films can be annealed differently, because the mid-infrared laser is well absorbed by glass substrates, as a result of which the metallic film on it is indirectly heated.

In this study we investigate the effects of CO_2 laser annealing of magnetron-sputtered Au films with a thickness of 5-10 nm on glass substrates with a thickness of ~0.15mm. Thicker glasses require much more laser power to induce NS. Figure 3 shows the AFM images and absorption spectra of 5nm Au films sputtered on cover glass substrates irradiated at different laser powers, 0, 2.5, 4, and 6W, for 5 minutes. We notice that the laser power of 2.5 W is too small to induce NS. The AFM image shows very sparse NS (Fig. 3(b)), and consistently, the absorption spectrum hardly exhibits SP resonance (SPR) of Au (Fig. 3(f)). However, the use of 4W laser power induces the significant change on the surface morphology, as shown in Fig. 3(c), and a clear SPR is observed in the absorption spectrum (Fig. 3(g)). Further increase of laser power to 6W induces more NS (Fig. 3(d)) and larger SPR (Fig. 3(h)). Now, we fix the laser power to 6W, and change the irradiation time. The results are summarized in Fig. 4. At only 6 seconds after laser irradiation the SPR begins to appear, and it grows to the maximum at ~20 seconds. Further increase of irradiation time up to 1 minute only slightly changes the position SPR to the red side with a bit broader resonance width. This indicates that the size of NS is growing between the irradiation time of 20 seconds and 1 minute. At the irradiation time of 5 minutes the SPR becomes broader and has a long tail at the long-wavelength side. This implies that the coalescence of NPs is taking place.

Thus, we have found that CO_2 laser annealing is very efficient to induce NS on Au films, and for the 5 nm Au films on a thin glass substrate only 20 second irradiation at 6W is sufficient to observe notable SPR. This simple technique can be conveniently used to prepare substrates for surface enhanced Raman scattering.

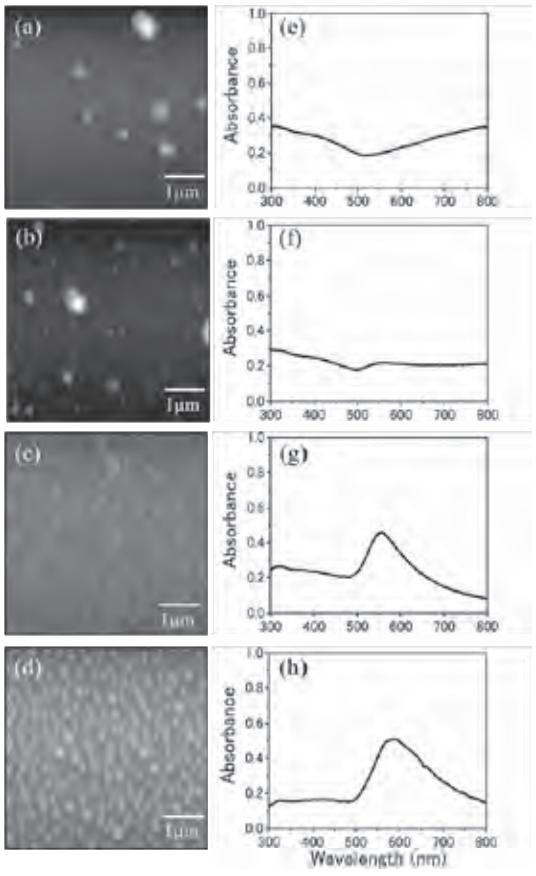

Fig. 3 AFM images (left column) and optical absorption spectra (right column) of 5 nm Au films on cover glasses after CO_2 laser annealing at different laser powers. The employed laser powers are (a, e) 0, (b, f) 2.5, (c, g) 4, and (d, h) 6 W, respectively. Irradiation time is 5 minutes for all cases.

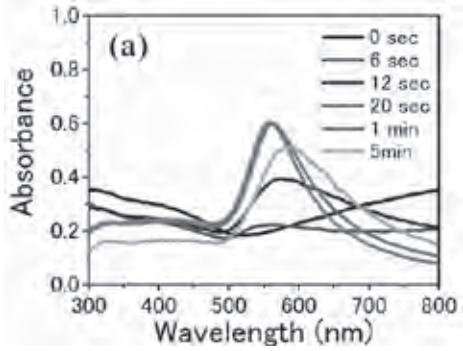

Fig. 4 Absorption spectra of 5nm Au films after CO2 laser annealing with different irradiation times. Annealing times are (b) 6, (c) 12, and (d) 20 sec, and (e) 1 and (f) 5 minutes, respectively, and the laser power is 6 W for all cases.

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Advanced Energy Structural Materials Research Section

A. Kimura, Professor
K. Morishita, Associate Professor
K. Yabuuchi, Assistant Professor
Z. Zhexian, Researcher
J. Gao, Researcher

1. Introduction

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

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

(2) Tungsten (W) diverter R&D: The feasibility of W diverter has been assessed along with fracture toughness evaluation after ion-irradiation. Since W is brittle, both the effects of heat loading and ion-irradiation may cause recrystallization and radiation hardening which often results in embrittlement. In order to understand irradiation hardening of W, crystal orientation dependence of irradiation hardening and microstructural evolution were investigated with W single crystals.

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

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

2. Ion-irradiation hardening in W single crystals

Pure tungsten (W) single crystals of {001} and {011} surface orientation have been irradiated with 6.4 MeV Fe3+ ions up to 0.1, 1 and 2 dpa at 573 K to investigate the hardening and microstructural evolution in W as a function of crystal orientation orand damage level. The thesis consists of the eight chapters.

The ion-irradiation affected zone size of pure W single crystals of {001} and {011} surface orientations were evaluated as a function of damage level (0.1, 1 and 2 dpa) and crystal orientation. At the irradiation dose of 2 dpa as well as 1 dpa, a double black band structure was observed as shown in Fig.1. The main defects are ordered networks of dislocation loop rafts. The width and depth of the high defect density bands were orientation and damage level dependent. The NI hardness profiles of all the samples conditions showed that ion-irradiation hardening depended more on crystal orientation than on damage level. The ion-irradiation hardening depth profile in all the damage level of W{001} was deeper than W{011}. A double black band structure can be interpreted on the bases of SRIM code calculation results indicating two different depth profiles of lattice damages and implanted Fe^{3+} ions. The shallower black bands may consist of lattice damages and/or vacancy clusters, while the deeper one may consists of Fe interstitial

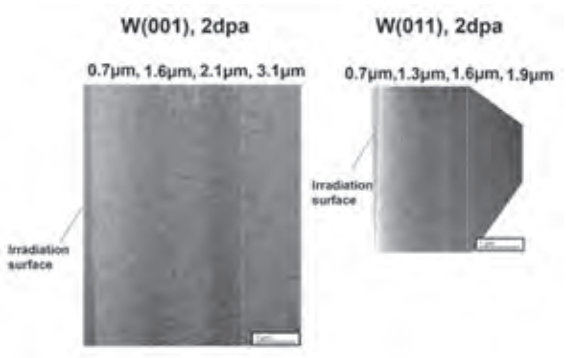

Fig. 1: Microstructure of 2 dpa irradiated W{001} and W{011}. The position of deeper ion-irradiation affected zone is much deeper in W{001}.

loops.

As for the orientation dependence of the NI hardness profile, a possible interpretation of the crystal orientation dependence can be addressed to the 1D motion of very fine interstitial loops which are invisible by TEM up to 1 dpa irradiation and becomes large enough to be visible at 2 dpa and responsible for irradiation hardening irrespective of the dpa level, where the longer distance of the 1D motion of interstitial loops in W{001} than in W{011} is considered to be due to the difference in the geometrical orientation of the direction of the 1D motion along the direction parallel to the Burger's vector, b, of the loops.

3. Theoretical evaluation of formation kinetics of defect clusters in nuclear materials

Radiation-induced embrittlement is one of the most significant degradation modes for structural materials used in nuclear plants, which may affect the integrity and lifetime of the plant. This is attributed to microstructural changes in materials during irradiation, in which athermal displacement defects such as vacancies and self-interstitial atoms are created. These defects act as carriers for the transfer of solute atoms and impurities in materials, and concurrently, those atoms and displacement defects themselves become components of defect clusters. The clusters thus formed play significant roles as obstacles to dislocation movement in materials during deformation, leading to irradiation-induced hardening, ductility loss, and embrittlement.

In recent decades, much experimental effort has been made to investigate the formation of Cu-rich precipitates, solute atom clusters and so-called matrix defects in reactor pressure vessel steels during irradiation, which may be candidate species for causing irradiation hardening and embrittlement. Specifically, an investigation of the formation of Cu-V clusters in α-Fe has been essential to understanding RPV embrittlement mechanisms. From those studies, many new findings have been obtained; however, what should now be considered is the fact that the embrittling species investigated so far were, in many cases, produced under accelerated irradiation conditions with high-energy neutrons, ions and electrons, wherein the damage rate was higher than that experienced in nuclear power plants. Are the embrittling species identified so far really produced in the actual irradiation environment? To answer this question, a careful interpretation of experimental data by theoretical and modeling techniques is required.

In the present study, a theoretical investigation is conducted to understand the formation process of Cu-V clusters in Fe from the viewpoint of thermodynamics. First, a procedure is established to describe the formation energy of Cu-V clusters in bcc Fe, where several unknown parameters in the formula are determined to fit cluster energy values obtained by MD calculations with empirical interatomic potentials. Using the formula thus obtained, the nucleation free energy is then evaluated as a function of the damage rate and temperature. KMC simulations are also performed to investigate the dependence of the damage rate on nucleation processes. We finally found that there are two different nucleation paths on the energy surface; one is the nucleation process of empty voids, and the other corresponds to the nucleation of pure-Cu clusters by a roundabout process. Lower energy nucleation path may depend on the damage rate. This fact is very important when considering microstructural evolution in materials during irradiation under a wide variety of damage rates.

4. Interaction between a faceted void and a dislocation in bcc Fe

Irradiation hardening is one of the mechanical property changes induced by the irradiation defects. Generally, the interactions between dislocations and the defects play an important role in the hardening and the plastic deformation is controlled by the dislocation motion overcoming the defects: for instance, it is well known that irradiation hardening stems from the elastic interaction between dislocations and radiation defects, such as voids and interstitial dislocation loops of which the strength factors are considered to be different each other .

In our study, the strength factor of faceted voids in body-centered cubic (BCC) Fe was evaluated experimentally by two different approaches: one based on the Orowan equation to link the measured irradiation hardening with the average size and number density of irradiation-induced voids, and the other involving direct observation of the interaction between a dislocation and a void by transmission electron microscope (TEM). As a result of preliminary study, it was shown that the strength factor of voids estimated for ion-irradiation hardening by the Orowan equation was 0.6, whereas the strength factor estimated by the direct TEM approach, where the strength factor was obtained from the bowing angle of the dislocation line overcoming the void, was 0.8. The difference in the strength factors measured by the two approaches is considered to be due to the positional relationship between dislocations and voids: the central region of a void is stronger than the tip. Moreover, the gliding plane and the direction of dislocation may also affect the strength factor of voids.

In order to assess the assumption, the mechanisms of interaction between dislocations and different type of faceted voids were investigated by molecular dynamics (MD) calculations. The MD calculations showed that the cutting strength and its mechanisms were different in each type of void.

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FEI STU（スロバキア），IAEA-CRP Pound robin test，木村晃彦

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

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

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

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

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Complex Plasma Systems Research Section

S. Kado, Associate Professor
S. Yamamoto, Assistant Professor

1. Introduction

Magnetic fusion has some key features which make it an attractive option in a future energy mix: (1) inherent safety features; (2) waste which will not be a burden for future generations; (3) no greenhouse gases; and (4) the capacity for large scale energy production. The required raw materials for the fuel are abundantly and widely available in the Earth. The combination of these features provides magnetic fusion the potential to make a substantial contribution to satisfying world energy demand later this century and beyond. The development of magnetic fusion as a commercial reactor of electricity requires the solution to the physics problems of plasma transport and magneto-hydrodynamics. The goal of the fusion plasma research is the discovery of a magnetic configuration that can efficiently confine a high density plasma at a high temperature for a sufficiently long confinement time to produce net thermonuclear power. The point is to deepen the understanding of fusion plasma dynamics and to create key innovative technologies to make magnetic fusion a practical energy source. This research section seeks to investigate the confinement optimization of high-temperature plasmas in the helical-axis heliotron line. For the experimental and theoretical investigation of this theme, the plasma device of Heliotron J has been operated to study the magnetic configuration effects of ”hot plasma” confinement in Heliotron J. In particular, heating and fuelling, confinement and diffusion mechanisms and their diagnostics are of great importance. Recent results of this section in FY2015 are as follows:

2. Evaluation of Intensity Calibration Method for VUV Spectrometer Using Bremsstrahlung Spectrum

Imperfectly ionized impurity atoms of medium to high atomic number enhance a cooling of plasma, since these atoms absorb electron energy by further excitation or ionization, followed by a radiative decay. Many of the line spectra from these atoms/ions are in the vacuum ultraviolet (VUV) region. In order to monitor these impurity spectra in Heliotron J, we use a VUV spectrometer system at 16 - 40 nm.

Intensity calibration is regarded as an important issue to evaluate the spectral line intensity.

In this work, we applied bremsstrahlung spectrum in high-density plasmas, that has been proposed as an indirect yet useful intensity calibration method. We made use of a high density plasma produced by high intensity gas puffing (HIGP) experiments.

The bremsstrahlung spectral intensity, at wavelength λ, is a function of electron density(n_e), electron temperature(T_e), and the effective charge(Z_{eff}) which is indicative of the contribution of the impurity ions. On the other hand, a Nd:YAG laser Thomson scattering measurement only offers the spatial distribution of n_e and T_e.

Therefore, we have proposed the following calibration equation,

$$I^{abs}(1;\lambda) = \frac{I^{abs}(Z_{eff};\lambda)}{\langle Z_{eff}\rangle} = I^{meas}(Z_{eff};\lambda)\frac{CF(\lambda)}{\langle Z_{eff}\rangle}$$

where I^{abs} and I^{meas} represent the line-averaged absolute and measured spectral intensities, respectively, and CF is the calibration factor. $<Z_{eff}>$ is the emission-averaged value and cannot straightforwardly be evaluated.

Based on the Thomson scattering data, we first calculated the intensity of the bremsstrahlung for $<Z_{eff}> = 1$, namely $I^{abs}(1;\lambda)$, which we assumed to be equivalent to the intensity normalized to $<Z_{eff}>$. According to this formulation, CF is only available as the form of the calibration factor per $<Z_{eff}>$, namely $CF/<Z_{eff}>$. When we obtain $<Z_{eff}>$ by some other methods, then we can achieve the absolute calibration.

Figure 1 shows the result for the calibration at the

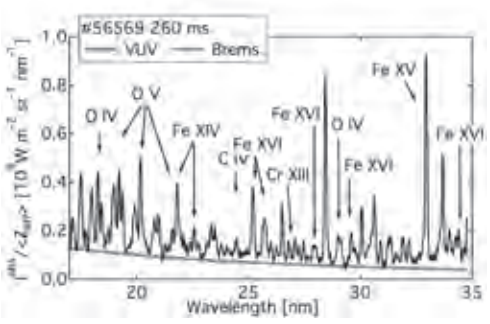

Fig. 1 Calibrated VUV spectrum for high density experiment (#56569) in Heliotron J, for unknown $<Z_{eff}>$.

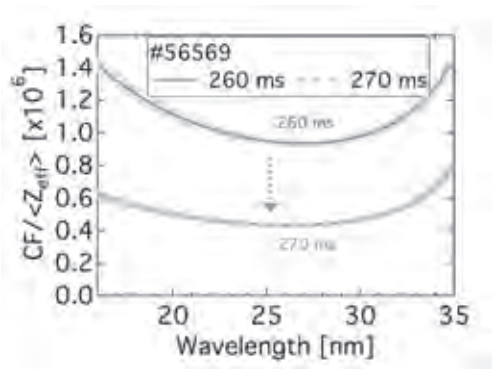

Fig. 2 Obtained *CF* per $<Z_{eff}>$ for 260 and 270 ms. Bands at each line represent error-bars.

experimental sequence time, 260 ms. Baseline indicated by the blue line was used for the bremsstrahlung spectrum.

One can see in Fig. 2 that the CF/ $<Z_{eff}>$ is considerably decrease between 260 and 270 ms. Since *CF* does not depend on the plasma parameters, this change is attributable to the change in $<Z_{eff}>$. In fact, we observed during this period that the n_e and T_e profiles were not changed that much, while many line spectra from the heavy ions such as iron and chromium were enhanced.

In future, we are planning to determine $<Z_{eff}>$ by an absolutely calibrated visible spectrometer to complete the absolute calibration of the VUV spectrometer.

3. Development of Scintillator-type lost fast ion probe

Good confinement of fusion-born energetic alpha particles is required before their thermalization since alpha particles are a primary heating source and sustain self-ignited Deuterium-Tritium (D-T) fusion reactions in a fusion reactor. Fast ions including the alpha particle can resonantly couple with Magnetohydrodynamics (MHD) waves such as shear Alfvén wave and excite them by the energy transfer from the fast particles to the waves. On the other hand, this resonant wave-particle interaction affects fast particle orbit and leads to a redistribution and a loss of fast particles. This phenomenon would prevent to sustain self-ignited D-T fusion plasmas. We have to clarify the mechanism of resonant wave-particle interaction, and minimize the effect of fast particles and fast ion losses in fusion plasmas.

We newly developed a scintillator-type lost fast ion probe (SLIP) which can directly measure an energy and pitch angle of lost fast ions escaping from plasma confinement region in order to clarify the mechanism of anomalous losses of fast ions due to MHD instabilities in Heliotron J. We target on both co-going passing and trapped fast ions produced by the tangential neutral beam injector (NBI) because fast ion driven MHD instabilities such as energetic particle modes (EPMs) and global Alfvén eigenmodes (GAEs) are usually observed in the co-NBI-heated plasmas in Heliotron J.

Lost fast ion flux was observed in SLIP in NBI heating plasmas at several magnetic configurations. Figure 3 shows a typical observation of scintillation light corresponding to lost fast ions obtained from ICCD. The observed light indicates that lost fast ions have an energy of about 20 keV close to the NBI injection energy and about 10 keV after both slowing-down and pitch angle scattering processes, and pitch angle of about 120 deg. According to full orbit calculations of measured ions by SLIP, a part of the observed lost fast ions seems to have an orbit of transit particles. The nine circles and numbers in each circle in the fig. 3 indicate the measurement region and channel number of the PMT respectively. Figure 4 shows the time evolution of the auto power spectrum of PMT #5 signal, and the low-pass filter (LPF) of 10 kHz is applied to PMT #5 is also shown.

A bursting loss fast ion flux was observed in the frequency range of 100 kHz shown in Fig. 4. They have high coherence with the magnetic fluctuation corresponding to EPMs and their appearance synchronized with also EPMs. SLIP signals indicate that lost fast ions are caused by bursting EPMs. We will clarify the resonant wave-particle interactions using not only SLIP measurement, but also nonlinear hybrid code for the MHD and particle.

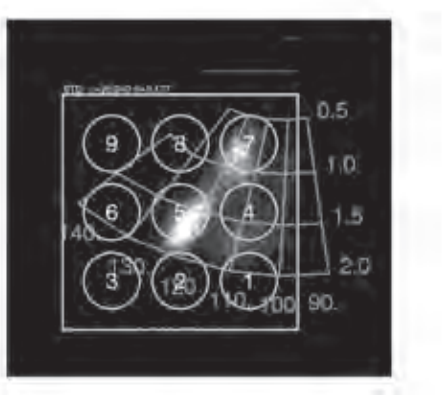

Fig. 3 Observation of lost ion by ICCD image

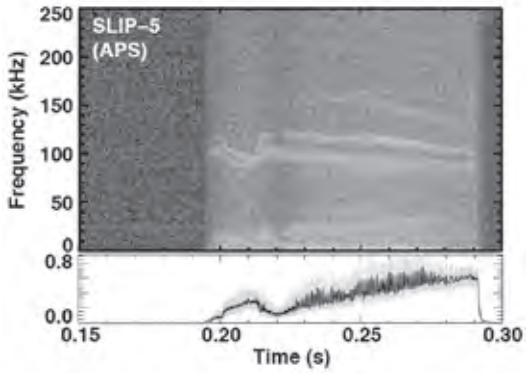

Fig. 4 Observation of bursting lost ion flux synchronized with bursting EPMs

Collaboration Works

Univ. Wisconsin（米国），Oak Ridge National Laboratory（米国），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，水内亨，長﨑百伸，岡田浩之，小林進二，山本聡，南貴司

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Stuttgart University（ドイツ），CIEMAT（スペイン），ヘリカル磁場配位における乱流揺動研究，大島慎介，長﨑百伸，水内亨，岡田浩之，南貴司，小林進二，山本聡

Stuttgart Univ.，CIEMAT（スペイン），先進閉じ込め配位，長﨑百伸，大島慎介，水内亨，岡田浩之，南貴司，小林進二，山本聡

CIEMAT（スペイン），Kurchatov Institute（ロシア），ORNL（米国），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，山本聡，小林進二，長﨑百伸，大島慎介，水内亨

PPPL（米国），低磁気シアヘリカルプラズマにおける高速イオンの異常輸送ならびに損失機構に関する研究，山本聡，小林進二

核融合科学研究所・双方向型共同研究，磁場分布制御を活用したプラズマ構造形成制御とプラズマ輸送改善，水内亨（代），長﨑百伸，岡田浩之，南貴司，門信一郎，小林進二，山本聡，大島慎介

核融合科学研究所・双方向型共同研究，ヘリオトロン J，CHS，LHED 装置における重水素プラズマの粒子輸送の研究，水内亨，山本聡，南貴司，大島慎介，小林進二，長﨑百伸，岡田浩之

核融合科学研究所・双方向型共同研究，低磁気シアヘリオトロン配位における磁気島に対するプラズマ応答の研究，水内亨，岡田浩之，長﨑百伸，山本聡，小林進二，南貴司

核融合科学研究所・双方向型共同研究，ヘリオトロン J における ICRF 加熱を用いたプラズマの高性能化研究，水内亨，岡田浩之，南貴司，小林進二，長﨑百伸，山本聡，木島茂，大島慎介，門信一郎

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核融合科学研究所・双方向型共同研究，磁気シアが MHD 不安定性による閉じ込め性能劣化度に与える影響の研究，水内亨，岡田浩之，長﨑百伸，小林進二，山本聡，南貴司

核融合科学研究所・双方向型共同研究，多様な磁場配位を有するヘリカル系プラズマにおけるプラズマフローと磁気島の理解，水内亨，山本聡，小林進二，長﨑百伸，岡田浩之，南貴司，大島慎介

核融合科学研究所・双方向型共同研究，ヘリカル系プラズマにおけるアルヴェン固有モードに起因する高速イオン損失研究，水内亨，山本聡，小林進二，大島慎介，岡田浩之，南貴司，長﨑百伸，門信一郎

核融合科学研究所・双方向型共同研究，有限ビーム幅を考慮した電子バーンシュタイン波放射計測，水内亨，長﨑百伸，大島慎介，南貴司，山本聡，小林進二，岡田浩之

核融合科学研究所・双方向型共同研究，Heliotron J 装置における電極バイアスによるポロイダル粘性遷移研究，水内亨，岡田浩之，長﨑百伸，門信一郎，小林進二，南貴司，山本聡，大島慎介

核融合科学研究所・双方向型共同研究，不純物輸送機構・同位体効果の理解に向けた新古典理論の拡張と応用，水内亨，岡田浩之，小林進二，山本聡，南貴司

核融合科学研究所・双方向型共同研究，アルベン固有モードによる高速イオン異常輸送の物理過程とその制御に関する研究，水内亨，岡田浩之，南貴司，長﨑百伸，山本聡，大島慎介，小林進二

核融合科学研究所・双方向型共同研究，マルチチャンネルカロリーメーターによるダイバーター熱流束の計測，水内亨，大島慎介，岡田浩之，小林進二，門信一郎

核融合科学研究所・双方向型共同研究，ヘリカルプラズマの不純物輸送に対する同位体効果の影響，水内亨，門信一郎，小林進二，山本聡，大島慎介，南貴司，岡田浩之，長﨑百伸

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Financial Support

Grant-in-Aid for Scientific Research
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Clean Energy Conversion Research Section

Takayuki Uchihashi, Visiting Professor
(Kanazawa University)

1. Introduction

Since the establishment of high-speed atomic force microscopy (HS-AFM), its performance has been demonstrated by imaging studies on various proteins in dynamic action [1]. The HS-AFM technique has become a routinely used tool in biological science. Actually we strongly collaborate with Prof. Katahira's and Prof. Morii's groups in Institute of Advanced Energy for various biological samples.

Nevertheless, the current HS-AFM that adopts the sample stage-scanning mode has limitations in some regards. To achieve the fast scanning speed, a small sample stage with a light weight has to be used and then this small size of the sample stage restricts the range of specimens to be placed. To remove this restriction, HS-AFM should adopt the tip-scanning configuration, in which the cantilever itself is scanned in the three dimensions. Furthermore, tip-scanning HS-AFM has another advantage because it can be easily combined with optical microscopy, including fluorescence microscopy techniques such as a total internal reflection fluorescence microscopy (TIRFM). AFM visualizes the surface structure of objects but lacks the capability of identifying the target molecules when the molecules exist in a crowded system containing multiple species, whereas fluorescence microscopy can identify the labeled molecules. As such, the combination of the two microscopy techniques would complement their weaknesses.

To make HS-AFM more versatile for the use in more biological applications, we have developed combined system of HS-AFM and single-molecule fluorescent microscopy and demonstrated the potential of the new system [2].

2. Tip-scanning HS-AFM Combined with TIRFM

In tip-scanning AFM, the laser beam to detect the cantilever deflection has to be scanned so that the laser beam is always focused on the cantilever during the scanning. The laser tracking system has been developed using a two-dimensional mirror tilter. The two directional angles of the normal line to the mirror plane are changed in synchrony with XY-scanning of the cantilever, as depicted in Fig. 1(a). The mirror tilter is composed of two base plates and four piezo actuators (Figs. 1(b)). The dichroic mirror is supported by the two X-piezoactuators glued on the base plate 2 through a beveled block. This whole unit is further supported by the two Y-piezoactuators glued on the base plate 1. The respective pairs of piezoactuators are displaced in the opposite directions, by which the respective tilt angles of the dichroic mirror are scanned. The maximum change of the tile angle was estimated to be approximately $\pm 4.8 \times 10^{-4}$ radian for X-directions, giving the maximum displacements of the focused spot, approximately 19 μm.

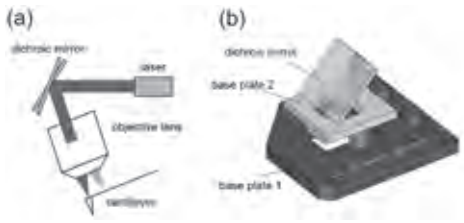

Fig. 1 Dichroic mirror tilter for laser-beam tracking. (a) Schematic showing the working principle of laser-beam tracking by mirror-tilting method. (b)Perspective view of the two-dimensional mirror tilter.

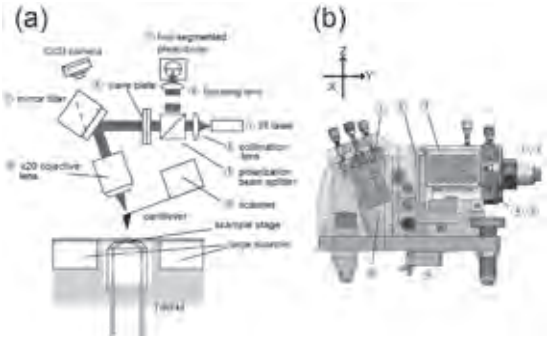

Fig. 2 Schematics and photograph showing the tip-scan HS-AFM unit. (a) Configuration of OBD detector with dichroic mirror tilter. (b) Whole structure of the tip-scan HS-AFM unit. The numbers attached to respective parts correspond to the numbers shown in (a). (c) A photograph of the tip-scan HS-AFM unit mounted on the optical stage in which the wide-area XY-scanner is installed.

Figure 2(a) shows a schematic diagram of the optical-beam-deflection system for tip-scanning HS-AFM. An infrared (IR) laser of wavelength 980 nm is used for the optical-beam-deflection (OBD) system. The optical components are optimized for the IR wavelength, including the collimation lens, λ/4 plate, polarization beam splitter, and the focusing lens placed at the front of the two-segmented photodiode. Figures 2(b) shows the side view of the tip-scanning HS-AFM unit. The frame that supports the unit consists of the top and base parts. All components in the OBD detector including the mirror tilter are

assembled in the top frame and hung from its roof to ensure mechanical stability. The positions of the IR laser, the two-segmented photodiode, and the scanner with the cantilever can be adjusted with precise screws in the XZ-, YZ- and XY-planes, respectively. The whole assembly is supported by a tripod consisting of two adjustable screws and a screw connected to the revolving shaft of the stepper motor. As optical microscopy to be combined with the tip-scanning HS-AFM, objective-lens type TIRFM was employed for single-molecule fluorescence imaging. The tip-scanning HS-AFM unit is simply mounted on a stage of the inverted optical microscope.

3. Simultaneous HS-AFM/TIRFM Imaging

Figure 3(a) shows a TIRFM image of rhodamine-labeled actin filaments that are partially biotinylated and immobilized on a cover slip sparsely covered with avidin molecules, while Figs. 3(c) and (d) show HS-AFM images of the same sample captured for narrow areas located within the region shown with the rectangle in Fig. 3(a). Figure 3(b) shows a wide-area AFM image acquired with a slow scanner incorporated into the optical stage. By comparing the TRIFM and wide-area AFM images, we can easily find the positional correlation between the TIRFM image and the HS-AFM images captured for the narrow areas, as indicated with the small rectangles in the overlaid image between the TIRFM image and the wide-area AFM image, as shown in Fig. 3(e).

We also succeeded in simultaneous observation of HS-AFM and TIRFM for processive movement of chitinase A which is an enzyme that degrades chitin microfibrils by hydrolysis [3]. For fluorescence imaging, chitinase A was labeled with Cy3. Crystalline chitin microfibrils suspended in water were immobilized onto a glass cover slip by spin coating. Figure 4 shows successive images of chitinase A moving along a chitin microfibril, which were simultaneously captured by HS-AFM and TIRFM at an imaging rate of 3 fps. The HS-AFM images (upper panel in Fig. 4) show binding of a single chitinase A molecule to the chitin microfibril (0.99 s) and its afterwards movement on the microfibril towards the upper-right (1.98 s and 2.64 s). A fluorescent spot also appeared at 0.99 s in the TIRFM image (lower panel in Fig. 4). The fluorescent spot slightly moved with time toward the right side, although the movement is much less discernible, because the field of view in TIRFM is much wider than that in HS-AFM.

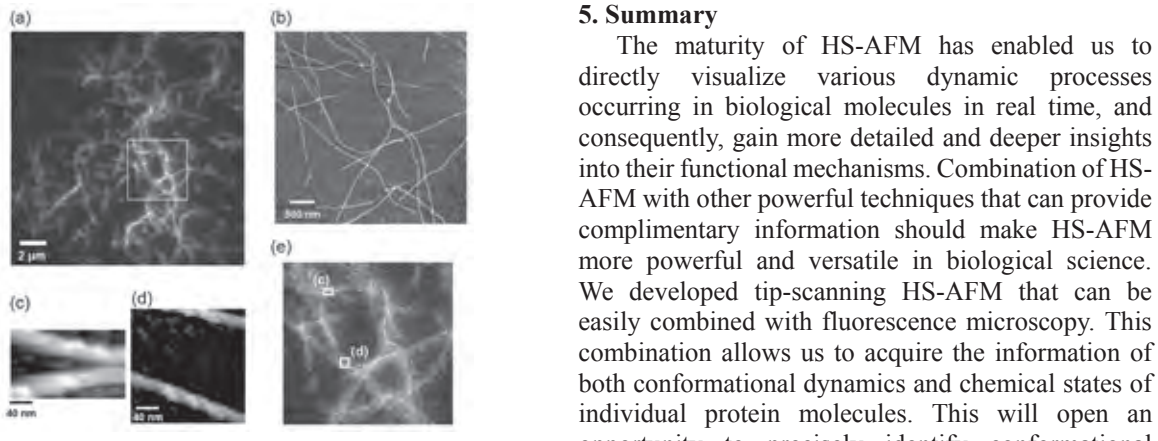

Fig. 3 Positional correlation between TIRFM, AFM, and HS-AFM images of rhodamine-labeled actin filaments. (a) TIRFM image. The white rectangle indicates the region for which (b) a wide-area AFM image. (c) HS-AFM image captured at an imaging rate of 8.3 fps with 100 × 45 pixels. The position of tip was set by reference to the TIRFM image. (d) HS-AFM image captured at an imaging rate of 2 fps with 100× 100 pixels. The position of cantilever tip was set by reference to the TIRFM image. (e) The overlaid TERM and AFM image.

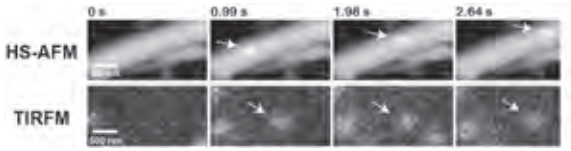

Fig. 4 Simultaneous HS-AFM/TIRFM imaging of proteins in action. (a) Cy3-labeled chitinase A on a chitin microfibril. The HS-AFM images (upper panel) captured at 3 fps with 150 × 35 pixels show a single chitinase A molecule moving towards the top-right (arrows). The TIRFM images (lower panel) with 40 × 15 pixels also show the same moving chitinase A molecule (arrows).

5. Summary

The maturity of HS-AFM has enabled us to directly visualize various dynamic processes occurring in biological molecules in real time, and consequently, gain more detailed and deeper insights into their functional mechanisms. Combination of HS-AFM with other powerful techniques that can provide complimentary information should make HS-AFM more powerful and versatile in biological science. We developed tip-scanning HS-AFM that can be easily combined with fluorescence microscopy. This combination allows us to acquire the information of both conformational dynamics and chemical states of individual protein molecules. This will open an opportunity to precisely identify conformational changes of a protein molecule triggered by, for example, nucleotide binding, hydrolysis, and product release.

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Clean Energy Conversion Research Section

Yasuhiro Suzuki, Visiting Associate Professor
(National Institute for Fusion Science)

1. Introduction

Generating and keeping clear flux surfaces are an aim of magnetic confinement researches, because magnetic islands and stochasticity of magnetic field leads the degradation of the confinement connecting and overlapping filed lines. In tokamaks, the degradation of the confinement due to generating islands like the locked mode and neoclassical tearing mode (NTM) were observed and studied [1,2]. The same degradations are also observed in helical system [3]. Thus, understanding and controlling of island dynamics are urgent and critical issues to aim the fusion reactor.

A method to identify magnetic islands is measuring electron temperature and density. However, if islands are rotating or healing, the profile measurement cannot identify island structure. Another method is the magnetic diagnostics. Since the magnetic diagnostics detects the change of magnetic flux directly, above problems are resolved but the diagnostics must be installed appropriately to detect perturbed field of islands.

In this study, we study island dynamics using the magnetic diagnostics in Heliotron J plasmas. Heliotron J is an L=1 and M=4 helical axis Heliotron configuration. A characteristic is the rotational transform profile with low magnetic shear of almost constant $\iota \sim 0.55$. This means there is a possibility of generating of large magnetic islands with coupling the resonant magnetic perturbation (RMP). If low-n RMP fields are superposed, big magnetic islands corresponding to low-n / m rational might be appeared. This is an advantage of Heliotron J device to study the plasma response on the magnetic islands. In particular, the nonlinear 3D equilibrium response is a critical issue in the stellarator. Thus, in order to generate low order magnetic islands and study the impact of the nonlinear 3D equilibrium response, external perturbation coils are designed and installed in Heliotron J device. In next section, the external coil to produce low-n perturbation field and magnetic diagnostic system are explained. Then, results of the island experiment are discussed. Lastly, we summarize this study and show the outlook.

2. Heliotron J device

The Heliotron J device is a medium sized helical-axis Heliotron device (R_0 = 1.2[m], a_p = 0.17 [m], B_0 < 1.5 [T]) with an L = 1 and M=4 helical coil. Figure 1 shows a schematic view of the experimental system. In this experiment, the initial plasma is produced by using the second harmonic X-mode ECH (70 GHz, < 0.45 MW, focused Gaussian beam) launched from a horizontal port.

To measure the plasma response field, four magnetic probes (MP01 ~ 04) are installed along the toroidal direction. These probes detect the perturbation along the toroidal direction. In addition, the normal field and the phase of the magnetic island are measured by two poloidal arrays of the flux loop.

3. Installation of external perturbation coils

The magnetic island is generated by the perturbed field from the 'MHD instability', which is the resistive instability, and the 'nonlinear 3D equilibrium response'. Usually, the identification of the perturbation on the MHD instability is easy because only detection of the perturbed field from the unperturbed field, which is the equilibrium field, is necessary. However, the identification of the perturbed field on the nonlinear 3D equilibrium response is difficult. The nonlinear 3D equilibrium response is driven by the equilibrium current (the Pfircsh-Schlüter (P-S) current, net toroidal current driven) along three-dimensionally rippled field lines. In addition, if the magnetic island is opened, the P-S current flow is distorted and further equilibrium response might be driven. To detect the perturbed field and identify the mode, the improvement of the magnetic diagnostic is necessary. As a first step, we measure the distortion of the P-S current flow on a low-n (n = 1) magnetic island. In theoretical analyses, spontaneous generation of the magnetic island by the equilibrium response is only for n >= 4 because of M = 4. In order to appear the distortion of the P-S current on the low-n island, the external perturbation

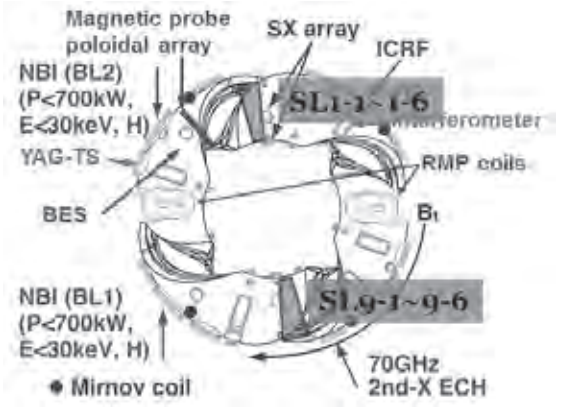

Fig.1: Experimental Setup

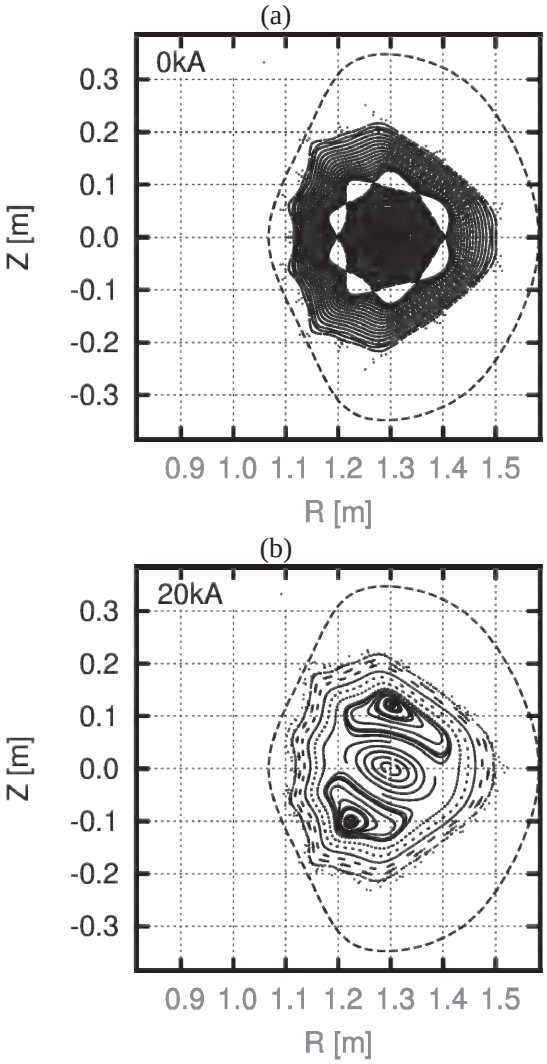

Fig.2: Poincaré plots of magnetic field lines with and without the RMP are shown at a poloidal cross section of $\phi = 0$.

with n = 1 is necessary. Thus, we designed and installed two pair of resonant magnetic perturbation (RMP) coils in Heliotron J device. RMP coils to generate n = 1 and 2 perturbations are installed at hatched positions in fig. 1. Poincaré plots of magnetic field lines are plotted at $\phi = 0$. Dashed lines in the figures indicate the wall of the vacuum vessel. In figs. 2 (a), an island chain by n / m = 4 / 8 natural resonance appears. On the other hand, in figs. 2 (b), large magnetic islands with n / m = 1/2 appear by the external perturbed field and the phase of islands is different in both cases. The phase of islands can be controlled by changing the current of the RMP coil.

4. Equilibrium response on low-n islands

Since the plasma pressure becomes flat on the island, the P-S current is distorted by flattering pressure profile. The distortion of the P-S current leads the nonlinear 3D equilibrium response. The magnetic diagnostic identifies the response localized along the toroidal direction.

To identify the nonlinear 3D equilibrium response, the pressure-induced perturbed field on the first wall is simulated. In fig. 3, the normal component of pressure-induced perturbed field, B_n, is shown. Poloidal and toroidal angle are normalized by 2π and $\theta = 0$ is the outermost position on $Z = 0$ plane. The marginal difference appears along $\phi = 0.9$ line. The order of the perturbed field of the nonlinear 3D equilibrium response is 10^{-3} (mT). The measurement is very difficult task. Therefore, the flux loop is necessary to measure the signal.

Finally, the result of the experiments with the RMP field is discussed. For typical shots, the density is kept constantly $n_e \sim 10^{19}$ m^{-3} and small net-toroidal current (< 1 kA) flowed in the plasma. Unfortunately, in these experiments, profiles of the electron temperature and density could not be measured. However, on signals of flux loops, differences with and without the RMP field are observed. This is consistent to the prediction from the numerical simulation. This suggests a possibility that the P-S current flow is distorted by the magnetic island.

5. Summary

We study the RMP coils in Heliotron J device and the nonlinear 3D equilibrium response. These coils can produce low-n magnetic island in the plasma. The distortion of the P-S current flow by large magnetic islands may make the pressure-induced perturbed field. The difference on signals of flux loops is observed with and without RMP field. This is consistent to the prediction from the numerical simulation but the quantitative study is a future subject.

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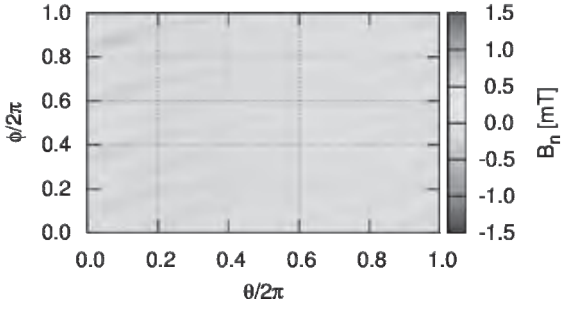

Fig.3: The normal field component on the first wall of the vacuum vessel.

Chemical Reaction Complex Processes Research Section

T. Nohira, Professor
T. Kodaki, Associate Professor

1. Introduction

In this research section, we study on electrochemistry, materials science, genetic engineering and protein engineering. We also apply them to the development of efficient solar-grade silicon production process and the efficient utilization of bioenergy.

In this fiscal year, we have researched the development of a novel production process of solar-grade silicon and the highly efficient production of bioethanol.

2. Development of a Novel Production Process of Solar-grade Silicon Using Molten Salt Electrolysis

Photovoltaic (PV) power generation has been developed as one of the key technologies that can mitigate the energy and environmental issues. High-purity Si used for crystalline Si solar cells are called as a solar-grade Si (SOG-Si), which exceeds the purity of 5N-7N.

To develop a next generation production process of SOG-Si, we have been studying the direct electrolytic reduction of solid SiO_2 to Si in molten $CaCl_2$ at 1123 K [1-3]. Recently, we proposed a new electrolytic production process for SOG-Si by utilizing liquid Si–Zn alloy cathode [4]. Figure 1 shows a schematic illustration of the proposed process. The overall process is composed of three major processes: an electrolysis process, a precipitation process, and a refining process. In the electrolysis process, solid SiO_2 is reduced to form Si–Zn liquid alloy on the cathode.

$$SiO_2\ (s) + Si\text{–}Zn\ (l,\ low\ Si\ conc.) + 4e^- \rightarrow Si\text{–}Zn\ (l,\ high\ Si\ conc.) + 2O^{2-} \quad (1)$$

In the precipitation process, metallic Si is recovered by lowering the temperature.

$$Si\text{-}Zn\ (l,\ high\ Si\ conc.) \rightarrow Si\ (s) + Si\text{-}Zn\ (l,\ low\ Si\ conc.) \quad (2)$$

After the precipitation process, the Si–Zn alloy with low Si concentration is reused as the cathode in the electrolysis process. The produced Si is further transferred to the refining process. An ingot of SOG-Si is manufactured by a directional solidification of the Si treated after leaching and vacuum refining.

This process is expected to have several advantages in terms of productivity and purification ability. In contrast to the Siemens process, the proposed process can be operated semi-continuously, which contributes to the high productivity. High purification efficiency is expected in the two-times segregation step; the deposition of solid Si from Si–Zn liquid alloy in the precipitation, and the precipitation of solid Si from liquid Si in the refining processes. Furthermore, the remaining Zn can be easily removed to several ppms even by the evacuation techniques used more than 30 years ago [5]. In this study, the electrochemical reduction of SiO_2 on Zn cathode was investigated at 1123 K.

Figure 2 shows the cyclic voltammograms for a liquid

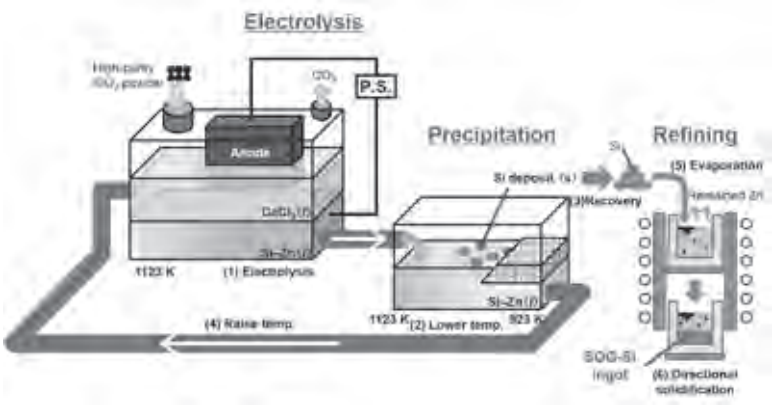

Fig. 1. A schematic drawing of solar-grade Si production utilizing an electrochemical reduction of SiO_2 powder on a liquid Si–Zn alloy cathode in molten $CaCl_2$.

Zn electrode with/without SiO_2 granules. The solid curve for Zn metal only indicates the negative current around 50 mA cm^{-2} from the rest potential (1.48 V) and the sharp current increase at 0.9 V. Since Ca and Zn forms a liquid phase over the all composition range at 1123 K, this current is likely due to the formation of liquid Ca–Zn alloy. The broken curve in Fig. 2 shows the voltammogram for the Zn electrode after the addition of SiO_2. While the rest potential is almost identical before the addition of SiO_2, the larger cathodic currents of 100 mA cm^{-2} are observed during the scan to the negative direction. Thus, the formation of Si–Zn alloy is expected at 0.9–1.45 V.

Based on the above result, potentiostatic electrolysis was conducted for a liquid Zn electrode after adding SiO_2 granules with a diameter of 0.1 mm at 0.90 V for 5.5 h in molten $CaCl_2$ at 1123 K. The sample was observed after cross-sectioning in the vertical direction. By SEM/EDX analysis, Si particles with a diameter of 2–30 μm have been confirmed in Zn matrix.

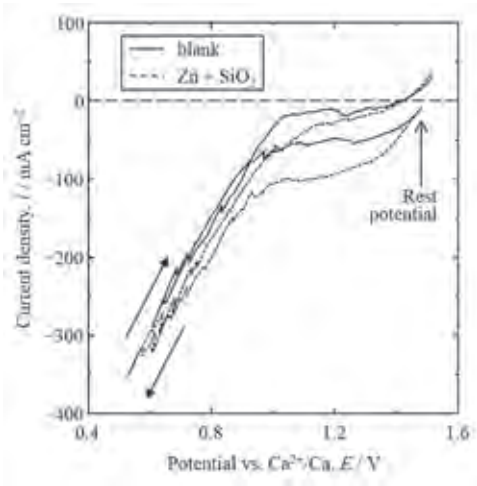

Fig. 2. Cyclic voltammograms for liquid Zn electrodes in molten $CaCl_2$ at 1123 K. Scan rate: 0.2 V s^{-1}.

3. Efficient Bioethanol Production from Cellulose using Ionic Liquid

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

In this fiscal year, effects of an ionic liquid, 1-Butyl-3-methylimidazolium Chloride ([bmim]Cl), on cellulose structure, cellulase activity, yeast growth and ethanol fermentation were examined extensively.

Cellulose was soaked into [bmim]Cl at 100°C with various ratios of cellulose and [bmim]Cl. Then cellulose was recovered as regenerated cellulose by the addition of excess water. X-ray diffraction (XRD) analysis (Fig. 3) showed that characteristic peaks of crystal cellulose were changed depending on the ratio of cellulose and [bmim]Cl. Glucose production from cellulose by cellulase was also examined under various ratios of cellulose and [bmim]Cl (Fig. 4). Under the conditions of crystal structure of cellulose disrupted (10 and 20% cellulose concentrations), about 50% of cellulose was hydrolyzed to glucose by cellulase. Furthermore, effects of [bmim]Cl on yeast growth and ethanol fermentation were examined. Considering these results, we are seeking the best conditions for efficient ethanol production from cellulose using ionic liquid.

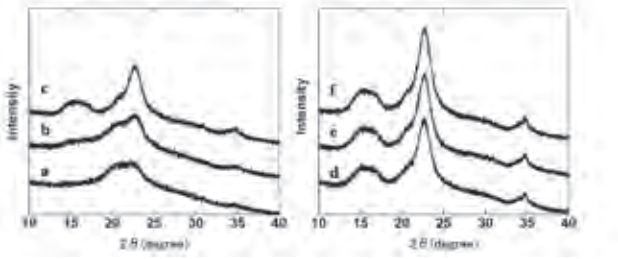

Fig. 3. XRD spectra of regenerated cellulose. Cellulose concentrations at soaking were 10%(a), 20%(b), 40%(c), 50%(d), 66%(e) and 80%(f).

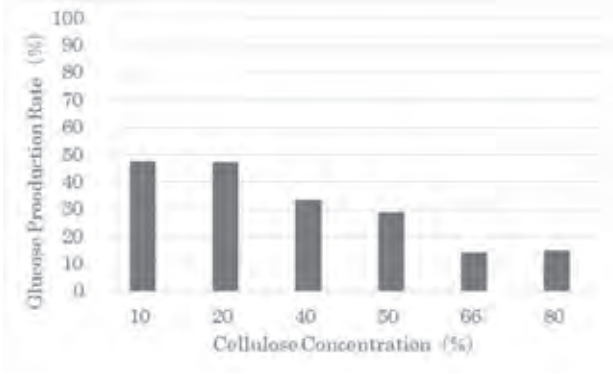

Fig. 4. Glucose production from cellulose by cellulase in various ratios of cellulose and [bmim]Cl.

These researches were partly supported by grants to T. N. from JST-CREST and MEXT (16H02410).

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Molecular Nanotechnology Research Section

H. Sakaguchi, Professor
T. Kojima, Assistant Professor
T. Nakae, 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 2016 are described below.

2. Synthesis of acene-type graphene nanoribbons from the Z-bar linkage precursor by 2Z-CVD

Graphene nanoribbons (GNRs), quasi-one-dimensional graphene strips, have shown great potential for electronics, optoelectronics, and photonics. These properties strongly depend on width and edge structure of them. Therefore, precisely controlled width and edge structure are required for desired properties. Bottom-up synthesis of GNRs is a one of suitable method to satisfy these requirements because of definition of their edge structures and widths by the shape of precursors. Atomically precise synthesis of armchair-edged GNRs have already been achieved under ultra-high vacuum (UHV) condition. However, given GNRs in this method were low yield and density was still low. Therefore, it was difficult to develop organic electronic devices with them. To develop devices, high-yield fabrication of assembled GNR films, isolation, and device fabrication are required.

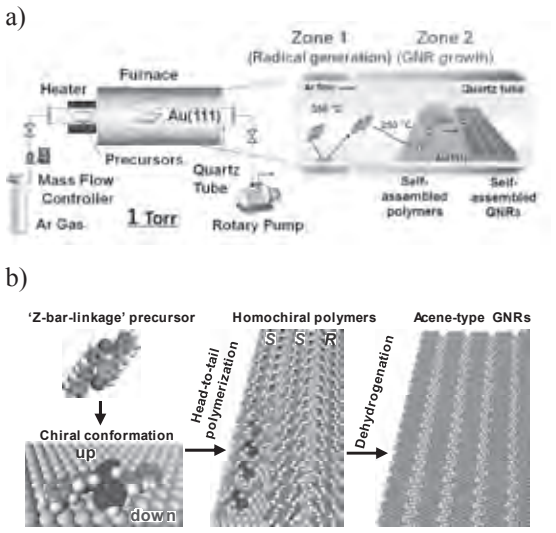

Fig. 1 Schematic illustrations of a) 2Z-CVD instrument and b) synthesis of acene-type GNRs from the Z-bar linkage precursor.

We have developed 2Z-CVD to produce densely-packed, parallelly-aligned self-assembled GNRs on Au(111) under low vacuum condition from halogenated polycyclic aromatic hydrocarbon (PAH) precursors. This technique successfully produced a series of armchair-edged GNRs in high yield. Attractive features of this method originate from an independent temperature-control of radical-generation process (zone 1) and the growth process (zone 2) (Figure 1a), 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. Although Au(111) surfaces have been reported to assist the dehydrogenation of polymers to afford GNRs, the detail mechanism of such catalysis, especially the role of metal surface, is unclear whether it is due to the electronic effect on the polymers or the conformational effect on the polymers. In addition, acene-type GNRs, which have the same chain axis as zigzag-edged GNRs, have been predicted to show high carrier mobility by theory. Thus, the precursor design to produce well organized acene-type GNRs on surface is desired.

Recently, we demonstrate 'conformation-controlled surface catalysis'; the 2Z-CVD of the 'Z-bar-linkage' precursor, which represents two terphenyl units are linked like a 'Z', results in the efficient formation of acene-type GNRs with a width of 1.45 nm through optimized cascade reactions (Fig.

1b). These surface reactions consist of the production of self-assembled homochiral polymers in a chain with a planar conformation, followed by efficient stepwise dehydrogenation. Interestingly, produced polymers have chirality regardless of no chiral catalyst and chiral precursors. More surprisingly, polymers were chosen only one conformation from huge number of them which exist 10^{100} types of conformations at least on the Au(111). The Z-bar-linkage precursor was considered to adopt chiral conformations with height asymmetry on Au(111), and thereby form self-assembled homochiral polymers in a chain with a planar conformation, followed by efficient stepwise dehydrogenation into GNRs via a conformation-controlled mechanism. In addition, high-density self-assembled homochiral polymers that stabilized the planar conformation could promote dehydrogenation. Finally, the FET devices fabricated using acene-type GNRs showed excellent semiconducting properties.

This study provided a new concept in conformation-controlled surface catalysis, in which the conformational adaptation of precursors and polymers on Au(111) could lead to an optimized reaction pathway to produce acene-type GNRs. This is conceptually analogous to enzymatic catalysis and will be useful for the fabrication of new nanocarbon materials.

3. Synthesis of strained nonbenzenoid-GNR by 2Z-CVD

Nonbenzenoid aromatic hydrocarbons, which contains five-membered rings, have attracted much attention due to their optical and redox properties. A five-membered ring in graphenic structure introduce curvature, which found in carbon nanotubes and fullerene. Therefore, production of carbon nanowires by using a nonbenzenoid precursor could introduce perturbation into their geometric and electronic properties.

Here, 2Z-CVD enables to use the nonbenzenoid precursor; dibromodibenzopentalene, which has two fused five-membered rings (provided from Prof. M. Saito, Saitama University). Fabricated polymers on Au(111) at 250 °C showed dot-like-shaped wires, which observed by scanning tunneling microscopy (STM). Raman spectra of the polymers was consistent with the calculation of dibenzopentalene polymer. Thus, the production of dibenzopentalene polymers was confirmed from these results. Furthermore, STM observation of annealed polymers at 500 °C showed carbon nanowires which supposed to be produced by intramolecular dehydrogenation. Thus obtained carbon nanowires might maintain five-membered rings, and expect to show unique properties due to their strained structure.

This result indicates that 2Z-CVD allows to adopt various precursors for fabricating carbon nanostructures with unique geometries. Thus, 2Z-CVD is the one of the most promising strategy of fabricating new class of carbon-based materials.

4. Strain-induced skeletal rearrangement of a PAH on a copper surface

Controlling the structural deformation of organic molecules can drive unique reactions that cannot be induced only by thermal, optical, or electrochemical procedures. Strain-induced rearrangements of aromatic carbon rings have been observed in graphene structures. As a typical example, a mechanical stress in graphene triggers a Stone–Wales rearrangement, a typical reaction of carbon allotropes that yields a defect composed of two heptagonal and two pentagonal rings fused together. Such defects play an important role in the formation of curved graphene, carbon nanotube, and fullerenes, which have shown potential for optoelectronics and photonics. Therefore, it is crucial to control the rearrangements of sp^2-carbon skeletal structures in order to synthesize functional nanocarbon materials for energy applications. However, in conventional organic synthesis, including mechanochemical procedures, it is difficult to control skeletal rearrangement in PAHs.

Recently, we demonstrate an unprecedented scheme for the skeletal rearrangement of PAHs on a metal surface, which driven by the intramolecular structural strain. The precise molecular structure were observed using high-resolution noncontact atomic force microscopy by collaboration with Assoc. Prof. Y. Sugimoto (the University of Tokyo).

To derive a highly strained PAH, we conducted a sequential procedure: (i) organic synthesis of a precursor PAH, diazuleno[1,2-*c*:2',1'-*g*]phenanthrene (**DAPh**), with two azuleno moieties in proximity to each other, and (ii) thermal cyclodehydroganation of **DAPh** adsorbed onto a Cu(001) surface. The product diazuleno[1,2,3-*cd*:1',2',3'-*fg*]pyrene (**DAPyr**) adopts a planar configuration on the surface, in spite of the fact that the azuleno moieties are sterically hindered by further mutual proximity. Therefore, the azuleno moieties flattened on the surface are highly strained. In order to eliminate the local strain instability, the **DAPyr** is thermally induced to react predominantly into an intrinsically flat PAH with a fulvaleno moiety, which has never been yielded by conventional organic synthesis. Such strain-induced reactions of organic molecules on surfaces would be a new approach to synthesizing unprecedented, functional chemical products.

Our proposed thermally-driven, strain-induced synthesis on surfaces will pave the way for the production of a new class of nanocarbon materials that conventional synthetic techniques cannot attain.

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Biofunctional Chemistry Research Section

T. Morii, Professor
E. Nakata, Junior Associate Professor
S. Nakano, Assistant Professor

1. Introduction

A transition to renewable energy technologies requires new chemistry to learn from nature. Nature has found fantastic solutions to convert solar energy to produce chemicals and to utilize them in the exceptionally efficient manners for almost 3 billion years. It is our challenge to understand the efficient bioenergetic processes of nature and to construct bio-inspired energy utilization systems. The research interests in our group focus on the design of biomacromolecules and their assemblies for molecular recognition, catalysis and signal transduction in water, the solvent of life. We take synthetic, organic chemical, biochemical and biophysical approaches to understand the biological molecular recognition and chemical reactions. Proteins and protein/nucleic acids assemblies are explored to realize biomimetic function of biological systems, such as visualization of cellular signals by fluorescent biosensors, directed self-assembly of peptides and proteins to build up nanobiomaterials, tailoring artificial receptors and enzymes based on the complex of RNA and a peptide or a protein, and reconstitution of the functional assemblies of receptors and enzymes on the nanoarchitectures. Followings are main research achievements in fiscal year 2016.

2. Construction of a library of structurally diverse ribonucleopeptides with catalytic groups

Highly specific recognition ability of the biomacromolecule to the target molecules is a key factor for the conversion of energy and materials with high efficiency in the living cells. Biomacromolecular receptors provide useful frameworks for constructing biosensors or enzymes with high specificity for a particular ligand. Efforts have been taken to rationally construct these artificial functional biomacromolecules through modification of proteins and nucleic acids receptors with appropriate fluorophores or with a catalytic group to achieve proximity effect between the substrate and the catalytic group. However, naturally occurring receptors do not always provide the recognition characteristics for the molecule of interest, and rational design of a receptor with desired specificity is still a challenging task. A library of RNA molecules that differ in their three dimensional structures by means of randomized nucleotide sequences has been applied for the selection of receptors for the target ligands. Although the library-based selection offers one of the promising methods to obtain aptamers with the specific recognition characteristics for the molecule of interest, further modification of the selected aptamers to exert a newly desired function is often difficult due to the lack of their structural information. In addition, the original substrate binding characteristics of the aptamer could be impaired by the introduction of a new functional group. Synthetic functional groups were incorporated to biomacromolecules in the library by modification of proteins or nucleic acids via chemical modification or genetic mutation. These chemical or genetic methods require laborious tasks to generate a library with limited size. Therefore, an alternative method is required to construct a large size library to increase the possibility of selecting a ‘‘hit” biomacromolecule with the function of interest. Ribonucleopeptide (RNP) is one of the appropriate scaffolds to construct a library with structurally diverse RNA-peptide complexes. We have reported a method to obtain ATP-binding RNP receptors by in vitro selection of a library of RNP with randomized RNA sequences. Because the RNA subunit works as a receptor for the substrate, the selected ATP-binding RNP receptor was further converted into a new RNP library by complexation of the RNA subunit and a library of Rev peptides, in which a peptide loop with randomized amino acid residues was incorporated at the N-terminus of Rev peptide. An ATP-binding RNP receptor selected from this peptide-based RNP library exerted higher ATP-binding specificity than the original RNP (Fig. 1a). A fluorescent RNP library was also constructed by combining the RNA subunit library and a library containing fluorophore-modified Rev peptides (Fig. 1a). The original substrate-binding ability of the RNP receptor was maintained in the selected RNP sensor even upon modification of the Rev peptide by a fluorophore. By taking advantage of the noncovalent complex formation of RNP, combination of the RNA library and the peptide library would dramatically increase the size of the RNP library. Therefore, RNP is a good candidate of scaffolds to construct a library of structurally diverse biomolecular assemblies containing a substrate-binding pocket and a synthetic functional group.

We reported the construction of a library of structurally diverse RNP receptors equipped with a synthetic functional group. A series of RNA subunits obtained by the in vitro selection of ATP-binding RNP receptors afforded a library of structurally diverse RNAs consisting of the ATP-binding region and the RRE (Rev Responsive Element) nucleotide sequence. A library of peptides was constructed by modification of the Rev peptide with catalytic groups through various peptide linkers (Fig. 1b). Combination of these two types of libraries by the complex formation between the RRE RNA and the Rev peptide generated a library of functionalized and structurally diverse RNPs, in which the catalytic group would align with various orientations against the ATP binding pocket of RNA subunits. In total, 609 RNPs were obtained by the combination of 29 RNAs and 21 peptides.

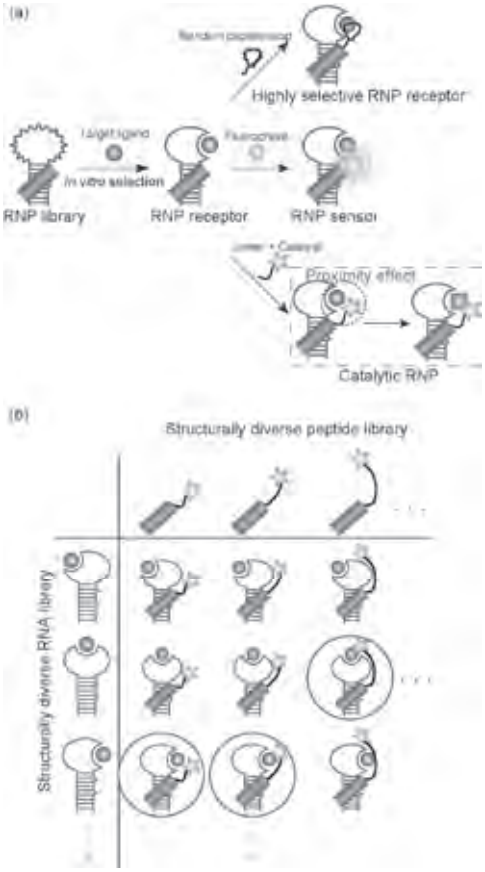

Figure 1. (a) Schematic illustration of the stepwise molding of RNP receptors. An RNP library containing catalytic groups in the peptide subunit could provide catalytic RNPs. (b) Combination of a structurally diverse RNA library and a structurally diverse peptide library affords the construction of a library of RNPs, in which the catalytic group aligns with various orientations to the substrate-binding pocket.

The functionalized and structurally diverse RNPs were expected to exhibit the ATP-binding ability. Umbelliferyl ester of adenosine (Umb-Ado) was utilized to select the RNPs that could accelerate the ester hydrolysis reaction by the proximity effect between the ATP binding domain and the catalytic group on the peptide (Fig. 1a). Facile screening of the structurally-diverse RNP library was successfully performed by the fluorescent detection of the hydrolyzed product of the ester derivative of adenosine to obtain catalytic RNPs. One of selected RNPs, consisting from An15 RNA and dmap-pa1-Rev, showed the highest acceleration of the hydrolysis. An15 RNA or dmap-pa1-Rev by itself showed no acceleration of the ester hydrolysis reaction, indicating that the RNP complex formation by An15 and dmap-pa1-Rev was necessary to accelerate the reaction. In addition, hydrolysis of 7-acetoxycoumarin, an umbelliferyl ester without the adenosine moiety, did not show any acceleration in the presence of An15/dmap-pa1- Rev RNP. These results indicated that the proximity effect between Umb-Ado in the binding pocket of An15 and the catalytic group, dmap of dmap-pa1-Rev upon the RNP complex formation likely accounts for the observed acceleration of the ester hydrolysis.

It is noteworthy that catalytic RNPs albeit with moderate activity were selected from the small size library, less than 1000, in this study. Because the numbers of ATP-binding RNA and/or the Rev peptide with catalytic group are readily increased, the size of RNP library would be expanded conveniently by the combination of these two subunits. Alternatively, introduction of random mutation to RNA of the selected RNP would afford a focused library for further selection of catalytic RNP. The functionalized and structurally diverse RNPs library would be quite useful for exploring catalytic RNPs not only for the ester hydrolysis but also for various other chemical reactions.

The presented work was supported in part by the Grants-in-Aid for Scientific Research (KAKENHI) from the Ministry of Education, Culture, Sports, Science and Technology (MEXT), Japan to S.N. (No. 26810090) and T.M. (25248038). And the other works in progress were also supported by KAKENHI from MEXT to E.N. (15H05492), T.M. (15H01402). T.T. acknowledges the Japan Society for the Promotion of Science (JSPS) for the fellowship (No. 15J09936).

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Structural Energy Bioscience Research Section

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

1. Introduction

We explore the way how biomolecules such as proteins (involving enzymes) and functional nucleic acids (DNA and RNA) work at atomic resolution based on structural biology with NMR. We determine both static and dynamical structures with the aid of our own development of the new methodology and elucidate the underlying mechanism of functions of these biomolecules. Structural biological approach is also applied to analyze enzymes involved in degradation of wood biomass at atomic resolution. The analysis is useful to develop the way to extract energy and valuable materials that can be used as starting materials of various products from the wood biomass. Thus, we pursue to contribute to the paradigm shift from oil refinery to biorefinery. Followings are main research achievements in the year of 2016.

2. Structural and functional analysis of wood degrading enzymes for better utilization of woody biomass

Woody biomass, which is composed of cellulose, hemicellulose, and lignin, is regarded as a "carbon neutral" source of energy and materials. Hemicellulose and lignin contain a variety of structural units and can be converted into medical and cosmetic substances. However, rigidity and complexity of the structure hinder their efficient isolation from woody tissue, thereby development of physically and chemically mild treatment that should also be environmentally friendly is awaited. In this line, we have been investigating the protein enzymes that are expressed in selective white-rot fungi. In this fiscal year, we investigated the functional and structural aspects of two enzymes, ligninolytic manganese peroxidase (MnP) and polysaccharide monooxygenase (LPMO).

MnP comprises three subfamilies, which are short-, long-, and extra-long MnPs. Their functional differences are still elusive. Previously, we had established a several methods to produce MnP from *E. coli*. Here we applied these methods to MnPs, each selected from the three subfamilies, respectively; we found that the low temperature expression, in which hemin was continuously provided during cultivation, gives the highest yield of soluble and active MnPs. We then investigated the activities of MnPs against DMP and ABTS in the presence and absence of Mn^{2+}. As we expected, all MnPs showed activity against DMP only in the presence of Mn^{2+}. However, surprisingly, two MnPs showed activity against ABTS both in the presence and absence of Mn^{2+}. Thus, MnPs of different subfamilies may have distinct functional characteristics. Structural study is now underway.

LPMO has recently been shown to be a copper-dependent metalloenzyme that on reduction generates a copper-oxyl radical, which cleaves mainly crystalline cellulose. Structure-function relationship, however, is still poorly understood. We had previously obtained LPMO using *P. pastoris* and established the crystallization conditions. This year, we have successfully obtained a better quality crystal and collected X-ray diffraction data at SPRING-8 (in collaboration with Prof. Mikami). Data were collected from 50.0 to 2.3 Å resolution range of reflections with an overall completeness of 92.1%. Structural analysis and refinement is currently in progress.

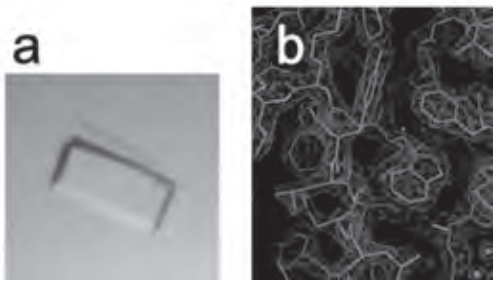

Figure 1. (a) Crystal of LPMO grown by sitting drop vapor diffusion. (b) A selected region of the density map of LPMO. Structural analysis and refinement is currently in progress.

3. Large conformational change of TLS upon binding of promoter-associated non-coding RNA

Translocated in liposarcoma (TLS) protein, also known as fused in sarcoma (FUS), is a nucleic acid-binding protein that is involved in diverse cellular events. TLS has a low-complexity (LC) domain at the N-terminal region followed by the RNA-binding domains at the C-terminal region. The C-terminal region binds to promoter-associated non-coding RNA (pncRNA) that is transcribed from the 5′ upstream region of *cyclin D1* (*CCND1*). This interaction allows the N-terminal region of TLS to inhibit histone

acetyltransferase activity of CBP/p300 on *CCND1*, but a structural mechanism of its allosteric regulation has been little understood. We have started a structural analysis of the regulation by using fluorescence resonance energy transfer (FRET) technique. We prepared the fusion protein in which blue fluorescent protein (BFP, donor) and green fluorescent protein (GFP, acceptor) were linked to the N- and C-termini of TLS, respectively. In the absence of pncRNA, strong fluorescence of GFP was observed as a result of an efficient FRET. In contrast, the FRET efficiency decreased upon addition of pncRNA. This result suggests the increase in distance between N- and C-termini of TLS upon binding of pncRNA. Our findings support a hypothesis that the interaction of TLS with pncRNA results in the conformational change of TLS from a closed form to an extended form and that thus the N-terminus of TLS can inhibit the histone acetyltransferase activity of CBP/p300.

4. The first successful observation of in-cell NMR signals of nucleic acids in human cells

It is recently widely recognized that the structure and function of biomolecules in living cells, which is very crowded, may deviate from those *in vitro*, which is much less crowded. As a suitable method to address this issue, in-cell NMR study, in which NMR signals originated from intact cells are directly observed and analyzed, is attracting much attention. So far, however, the in-cell NMR studies have been reported mostly for proteins. There are only a few reports on nucleic acids. Particularly, there is no report on nucleic acids signals of human cells. This time, we succeeded in observing the in-cell NMR signals of nucleic acids originated from intact human cells for the first time. In-cell NMR spectrum of the quadruplex formed by telomeric DNA is basically the same as *in vitro* one, but the difference between the two spectra was also noticed. The addition of a typical crowding agent, polyethylene glycol (PEG), to the in vitro sample could not perfectly reproduce the in-cell NMR spectrum, which implies that the structure in cells is not completely identical to that *in vitro* even with the crowding agent. This suggests the importance to study the structure and interaction of nucleic acids in human cells by in-cell NMR method. Further investigation is now in progress.

5. Determination of the stem-loop structure located in 3' UTR of Stat3 mRNA by NMR

Arid5a protein directs native $CD4^+$ T cells to differentiate into inflammatory $CD4^+$ T cells. Arid5a binds to the mRNA of Stat3 protein and thereby protects the mRNA from degradation by RNase, Regnase-1. Then, Arid5a maintains the amount of Stat3 and regulates the fate of $CD4^+$ T cells. We identified and determined the stem-loop structure in 3' UTR of Stat3 mRNA. This stem-loop turns out to be responsible for binding of Arid5a to Stat3 mRNA. The mutation that destroys the stem-loop structure abolished the binding. Thus, the determined stem-loop structure was concluded to play a key role in fate decision of the $CD4^+$ T cells. This study suggests the possibility that autoimmune disorder might be cured by inhibiting the elucidated function of Arid5a.

6. The findings of an RNA molecule that disrupts the Alzheimer's disease-related interaction of Aβ oligomer with prion protein

Amyloid beta peptide (Aβ) is considered to be a central factor for Alzheimer's disease. Aβ can form a soluble oligomer and insoluble fibril, and the oligomeric form is thought to be more toxic than the fibril. Recently, it was reported that prion protein (PrP) on cell membrane is bound by the Aβ oligomer and acts as a receptor of the Aβ oligomer, resulting in Alzheimer's disease. This year, we found that an RNA molecule (R12) that tightly binds to PrP can disrupt the interaction of the Aβ oligomer with PrP. It is known that thioflavin-S (ThS) binds to the amyloid fibril and emits strong fluorescence. In the absence of PrP, after lag-phase of ~50 h, the fluorescence increased rapidly, indicating that Aβ polymerizes to form the Aβ fibril (Figure 2a). In the presence of PrP, the fluorescence of ThS decreases with increase in concentration of PrP (Figure 2a). These results indicate that PrP interacts with Aβ and inhibits the Aβ fibrillization. When R12 was added, however, the fluorescence intensity of ThS rapidly increases even in the presence of PrP (Figure 2b). This indicates that R12 snatches PrP from the Aβ oligomer-PrP complex and that then the released Aβ oligomer restarts the fibrillization. We proposed that R12 has a therapeutic potential against Alzheimer's disease by inhibiting the formation of the Aβ oligomer-PrP complex.

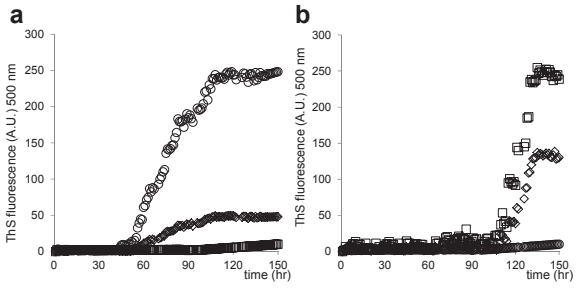

Figure 2. The effects of PrP and R12 on Aβ fibrillization. (a) Aβ was incubated either alone (circle) or with PrP at the concentration of either 0.5 μM (diamond) or 1 μM (square). (b) Aβ was incubated with 1 μM PrP. After 100 hours, R12 was added at a final concentration of either 0 μM (circle), 1 μM (diamond), or 2 μM (square).

Collaboration Works

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Gyeongsang University（韓国），タンパク質との相互作用による核酸の構造遷移に関する解析，片平正人

Université Laval（カナダ），核内 RNA 結合タンパク質の NMR による構造及び機能の解析，永田崇

Financial Support

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Advanced Energy Utilization Division

A. Rajendran, Junior Associate Professor

1. Introduction

Among the various types of DNA-binding proteins, topoisomerases (Topos) are quite attractive due to their importance in cancer therapy.[1] Though there are several investigations focused on the function of Topo enzymes and the development of drug molecules targeting these enzymes, the mechanism of action is still not well understood.[2] For instance, Topos involve several step-by-step processes in releasing the topological stress of DNAs. It is not well known at which step of the enzyme reaction is inhibited by a particular drug molecule. Typical methods, such as ethidium bromide assay, to measure the Topos inhibitory activity are not reliable. Thus, to understand the function of Topo enzymes and the mechanism of the drug inhibition, it is necessary to develop a novel and versatile method which differs significantly from the traditional indirect methods.

2. Preparation of DNA catenane and rotaxane inside a DNA origami frame

Since the Topo enzymes target the topologically constrained DNAs, the interlocked DNA structures could be the potential targets to investigate the Topo functions and their inhibitors. Topologically interesting structures such as Borromean rings, catenanes, and knots have already been prepared by using DNA.[3] Also, the complexity of the catenane[4] and rotaxane[5] structures were increased by constructing them by the DNA origami method[6]. However, integration of the duplex DNA catenanes and rotaxanes to the relatively larger and complex DNA nanostructures such as DNA origami has not yet been realized. These molecular assemblies have potential applications such as the functional components for molecular switches and motors, novel platforms for the investigation of the function of proteins, analysis of protein inhibitors, and so on.

In this project, I have developed a novel method by the combination of DNA origami and high-speed atomic force microscopy (HS-AFM)[7-13] for the screening of Topo-inhibitors. As for the target structure for the Topo reactions, I have constructed the topologically interlocked DNA catenane- and rotaxane-like structures inside a frame-shaped DNA origami (Figure 1). The formation of the DNA origami frame and the insertion of the catenane- and rotaxane-like structures were successfully characterized by agarose gel electrophoresis and HS-AFM (Figure 1). The optimization of the conditions for the formation and insertion of the catenane inside the DNA origami frame were carried out. To increase the stability of these functional structures, the nicks in these structures were sealed by using T4 DNA ligase. The ligation was also confirmed by the thermal treatment of these structures, where the ligated samples were stable at high temperature incubation while the non-ligated samples failed to keep the topologically interlocked structures. Further, I have investigated the stability of the DNA origami frame and the catenane/rotaxane ring structures in the presence of various kinds of Topo inhibitors. Both the origami and the DNA ring are stable against the Topo inhibitors for several hours at room temperature. This indicated that the DNA origami based analysis of Topo inhibitors could be successfully carried out. These functional structures inside the DNA origami frame contain the binding site for Topos. The Topo reaction and the function of Topo-inhibitors are under investigation.

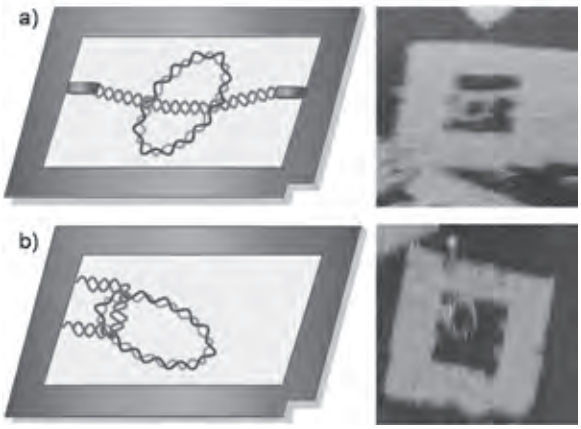

Figure 1. Left: Schematic illustration of the DNA origami frame with DNA rotaxane (a) and catenane (b) inside the frame. Right: AFM images in each case are given. Image size: 150 × 150 nm.

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Financial Support

Grant-in-Aid for Scientific Research
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Laboratory for Complex Energy Processes Research Section

M. Kinoshita, Professor
H. Okada, Associate Professor

1. Introduction

A. Theoretical Biophysics

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

B. Plasma Physics

The major subjects are to study fast-ion confinement in plasma confinement devices and to investigate interactions between fast-ions and materials, such as a first wall and a vacuum vessel. The fast-ion confinement is a critical issue for the fusion reactor since the alpha particles produced in the D-T reaction should be utilized to heat plasma efficiently. The interactions between fast-ions and materials cause the impurity problem for the plasma energy confinement and the damage for the vessel or the first wall materials occurs. Fast-ion profile and velocity distribution are investigated using ion cyclotron range of frequency (ICRF) minority heating in Heliotron J with special emphasis on the effect of the toroidal ripple of magnetic field strength (‘bumpiness’). Optimization of the ICRF heating is important for the three-dimensional magnetic configuration. We also investigate the effect of the position of the ion cyclotron resonance layer on the fast ion formation and confinement.

(A-1) Identification of thermostabilizing mutations for membrane proteins: Rapid method based on statistical thermodynamics [1]

Membrane proteins are responsible for the communication between cells and their environments. They are indispensable to the expression of life phenomena and also implicated in a number of diseases. Nevertheless, the studies on membrane proteins are far behind those on water-soluble proteins, primarily due to their low structural stability. Introduction of mutations can enhance their thermostability and stability in detergents, but the stabilizing mutations are currently identified by experiments. The recently reported computational methods suffer such drawbacks as the exploration of only limited mutational space and the empiricism whose results are difficult to physically interpret. Here we develop a rapid method which allows us to treat all of the possible mutations. It employs a free-energy function (FEF) which takes account of the translational entropy of hydrocarbon groups within the lipid bilayer as well as the protein intramolecular hydrogen bonding. The method is illustrated for the adenosine A_{2a} receptor whose wild-type structure is known and utilized. We propose a reliable strategy of finding key residues to be mutated and selecting their mutations which will lead to considerably higher stability. Representative single mutants predicted to be stabilizing or destabilizing were experimentally examined: The success rate was remarkably high. The melting temperature T_m for two of them was substantially higher than that of the wild type. A double mutant with even higher T_m was also obtained. Our FEF captures the essential physics of the stability changes upon mutations.

(A-2) Effects of salt or cosolvent addition on solubility of a hydrophobic solute in water: Relevance to those on thermal stability of a protein [2]

The solubility of a nonpolar solute in water is changed upon addition of a salt or cosolvent. Hereafter, “solvent” is formed by water molecules for pure water, by water molecules, cations, and anions for water-salt solution, and by water and cosolvent molecules for water-cosolvent solution. Decrease and increase in the solubility, respectively, are ascribed to enhancement and reduction of the hydrophobic effect. A plenty of experimental data are available for the change in solubility of argon or methane arising from the addition. We show that the integral equation theory combined with a rigid-body model, in which the solute and solvent particles are modeled as hard spheres with different diameters, can reproduce the data for the following items: salting out by an alkali halide and salting in by tetramethylammonium bromide, increase in

solubility by a monohydric alcohol, and decrease in solubility by sucrose or urea. The orders of cation or anion species in terms of the power of decreasing the solubility can also be reproduced for alkali halides. With the rigid-body model, the analyses are focused on the roles of entropy originating from the translational displacement of solvent particles. It is argued by decomposing the solvation entropy of a nonpolar solute into physically insightful constituents that the solvent crowding in the bulk is a pivotal factor of the hydrophobic effect: When the solvent crowding in the bulk becomes more serious, the effect is strengthened, and when it becomes less serious, the effect is weakened. It is experimentally known that the thermal stability of a protein is also influenced by the salt or cosolvent addition. The additions which decrease and increase the solubility of a nonpolar solute, respectively, usually enhance and lower the thermal stability. This suggests that the enhanced or reduced hydrophobic effect is also a principal factor governing the stability change. However, urea decreases the solubility but lowers the stability. Bromide and iodide ions decrease the solubility but lower the stability of a protein with a large, positive total charge. In these cases, the urea- or ion-protein van der Waals interaction energy as well as the hydrophobic effect needs to be taken into account in arguing the stability change. We also present a new view on the so-called Hofmeister series: We show how it is expressed when the change in hydrophobic effect dominates and how it is modified when other factors are also influential.

(B-1) Study of Fast Ion Generation by Combination Heating of ICRF and NBI in Heliotron J [3]

The fast ion generation and confinement are studied by using ICRF minority heating (hydrogen minority and deuterium majority) for the simulation study of alpha particles, whose heating is essential for fusion reactors. In a three-dimensional magnetic field device, Heliotron J (R_0 = 1.2 m, a = 0.1-0.2 m, $B_0 \leq$ 1.5 T), fast ion generation and confinement by ICRF minority heating are studied in combination with neutral beam injection (NBI) heating. Injected particle is hydrogen, and the minority ratio is about 0.1 for this experiment. Fast ions are measured using a charge-exchange neutral particle analyzer (CX-NPA) with ten energy channels for hydrogen and ten channels for deuterium.

The pitch angle dependence of minority proton energy spectra during ICRF pulse are investigated in the ECH target plasmas with NBI heating (injection energy, E_0: 25 keV, injected power: about 0.4 MW) for the case of low-ε_t and high bumpiness configurations. NBI direction is co-direction. The power of ECH and ICRF is 0.25 MW and 0.3 MW, respectively and the electron line-averaged density is 1×10^{19} m^{-3}. In the energy spectrum at pitch angle 128°, the peaks of E_0, $E_0/2$ and $E_0/3$ of the NBI energy appear in the no ICRF pulse phase. These peaks decrease from the higher energy as the pitch angle moves away from the injection angle of NB. When the ICRF pulse is injected, the high-energy tail beyond E_0 is extended. The energy spectrum at 128°, which is near the NB injection angle, the high-energy ion with energy beyond 50 keV is observed. The energy of fast ions is almost doubled from the original energy of NB. The difference of the energy between 128° and 123° of pitch angle is very small, however, at 120° the high-energy tail decreases obviously and the observed flux is below 40 keV. In the counter NBI case without ICRF pulse, the E_0 component is very small in comparison to co-NBI case. The chord of the CX-NPA measurement is not the same as the NB injection line, then the observed energy spectrum attributes to the confinement of fast ions. It is noted that the energy spectrum near the injection angle during ICRF pulse is almost same for co and counter cases. However, the high-energy component decreases rapidly as the pitch angle for the counter-injection case.

Using Monte-Carlo method with the experimental magnetic field and plasma parameters, the numerical calculation including orbit tracing, Coulomb collisions and ICRF acceleration is done in order to estimate the averaged behavior in whole torus for various configurations since the measurement area of the CX-NPA is limited. The test ions (protons) in the calculation, which represent the NBI particles, start at the middle point of the NB path in a plasma with the NB injection energy.

Injected ions with the mono energy collide with bulk particles in a plasma and are accelerated or decelerated by the ICRF wave, then, ions spread in velocity space. The acceleration by ICRF wave is modeled as the “kick” in velocity space. The particles in the calculation are summed up during 0.5 ms after 1.5 ms from the beginning because of the statistical reason. The ratio of lost ions in the counter-injection case is larger by 20% than that in the co-injection case. The spread in velocity space for the counter-injection case is larger than that in the co-injection case. However, the bulk part near the injection energy gets larger energy in the co-injection case and the energy spread for the bulk part is larger in the co-injection case. Then, only small number of high-energy ions in the very high energy region are observed in the counter-injection case. These result is qualitatively consistent with the experimental result.

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Collaboration Works

Univ. Wisconsin（米国），Oak Ridge National Laboratory（米国），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，水内亨，長﨑百伸，岡田浩之，小林進二，山本聡，南貴司

Stuttgart University（ドイツ），CIEMAT（スペイン），ヘリカル磁場配位における乱流揺動研究，大島慎介，長﨑百伸，水内亨，岡田浩之，南貴司，小林進二，山本聡

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核融合科学研究所・双方向型共同研究，磁場分布制御を活用したプラズマ構造形成制御とプラズマ輸送改善，水内亨（代），長﨑百伸，岡田浩之，南貴司，門信一郎，小林進二，山本聡，大島慎介

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ADMIRE project
(Application of DuET and MUSTER for Industrial Research and Engineering)

S. Kondo, Program-Specific Associate Professor

1. Introduction

The ADMIRE project (Application of DuET and MUSTER for Industrial Research and Engineering, current project leader; Prof. Kimura) is originally launched at IAE, Kyoto University in early 2006 as a MEXT supported program "Open Advanced Facilities Initiative for Innovation (Strategic Use by Industry)". Our primary objective is providing and sharing our resources, such as laboratory equipment, scientific knowledge, and the corresponding techniques, to private companies for encouraging their innovation. The representative facilities, DuET & MUSTER, were historically dedicated for the research on energy science and technology, with the special emphasis on R&Ds for fusion reactor materials. Due to this reason many of nuclear material relevant subjects are continuously running from the beginning of the ADMIRE. The current project, however, is flexible to accept any new ideas from the industries and ventures for supporting their R&D efforts, in so far as they are innovative. Indeed, most subjects currently running are not related to the nuclear applications, but related to advanced energy- and/or nano-science. Note that many inputs from these exciting new research fields drastically stimulate our original work.

2. Activities with DuET (Dual-Beam Irradiation Facility for Energy Science and Technology)

As an important part of fusion material research, evaluation of radiation damage in materials has been emphasized more than three decades. Under the current situation with no 14 MeV neutron irradiation facilities available for materials research, the Multiple Beams–Materials Interaction Research Facility has to have a very important role in many years to come. In order to obtain fundamental understandings of the radiation damage in fusion materials, as the dynamic material behavior under severe environments in advanced energy systems, such as fusion reactors, fission reactors, a Multiple Beams–Material Interaction Research Facility (DuET facility: Fig. 1) has been constructed at the IAE in 1998. The facility consists of a 1.7 MV tandem accelerator system with a pair of ion sources (a cesium sputter type heavy ion source and a duo-plasmatron type light ion source), a 1.0 MV single-end accelerator system with a light ion source and three target stations.

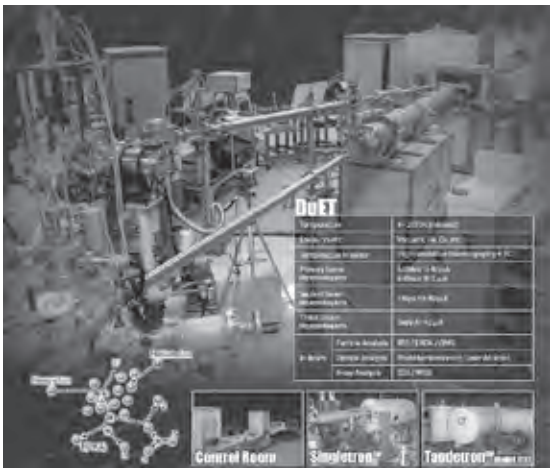


Fig. 1 Summary of the DuET facility set-up.

Testing by ion-irradiation is extremely useful to R&D of the nuclear materials because the flux “or damage rate” is extremely high (and it is easily controllable!) and conditions are accurate comparing to the testing in research reactors. Thus, many advanced materials, such as silicon carbide, tungsten alloys, and nuclear grade graphite, pro-vided by multiple commercial companies were tested within the ADMIRE framework. For example, the dimensional change of the graphite materials during irradiation have been unclear because of the difficulty of the testing due to the high porosity. However, our developed methods (WO2014034829 A1) successfully revealed a unique irradiation effects observed in those materials, such as the anisotropic dimensional change.

The creation of the functional materials, such as gradient materials, by implanting the specific ions on the materials is the other side of DuET work. Unfortunately, the detail of most topics cannot be introduced here because of the fixed-term classified contract between the ADMIRE and companies. However, those works help us to create new idea for the DuET application.

Fig. 2 Summary of the MUSTER equipment (selected).

3. Activities with MUSTER (Multi-scale testing and evaluation research) facility

Various analytical devices and mechanical testing machines are participated in the MUSTER facility; each covers different time-scale and/or time-scale range, respectively. Especially for the ADMIRE related work, an analysis of thin foils, coating materials, nanosized particles, and the control of nanoscale textures seem to be the key words of the recent users' demands. Two powerful analytical systems, KU-FEL (Kyoto University mid-infrared free electron laser facility managed by Prof. Ohgaki, Quantum Radiation Energy Section, Advanced Energy Generation Division, IAE) and NMR (three high-sensitive NMR systems managed by Prof. Katahira, Advanced Energy Utilization Division, Advanced Energy Utilization Division, IAE), have participated in the MUSTER in early 2013. Some upgrading and expanding of the MUSTER equipments, such as the instllation of new soft-XRD detector, high-resolution-TEM CCD camera, and GD-OES were achevived as well in 2013 to satisfy a recent user need. The latest available resources can be found in ADMIRE official site (http://admire.iae.kyoto-u.ac.jp).

Offering the right device for the right research objective is one of our key missions in addition to the technical advices for the device operation. One can say these analytical devices are the essential for most ADMIRE subjects, currently 24 subjects are running, where the percentage of operating time for the ADMIRE related work is more than 40% (1 year averaged, estimated on MAR 2016) of the total hours of use. Some have strong connection to the DuET experiments because the ion irradiation typically modify the atomic-scale structure. Some of ADMIRE subjects, such as the microstructural analysis of the grain boundary diffusion in neodymium magnet, led to the collaboration research with IAE, and those were presented at conferences and published in scientific journals by our faculty stuff.

The followings are the key analytical electron microscopies of the MUSTER.

• Field Emission Transmission Electron Microscope (JEOL JEM-2200FS): This is designed for both high resolution TEM/STEM and analytical microscopy with a 200 kV field emission gun. Point and line resolutions are 0.23 nm and 0.1 nm, respectively. The attachments or analytical methods which can be utilized are EDX, EELS, HAADF, Z-contrast imaging, etc.

• Field Emission Scanning Electron Microscope (Zeiss ULTRA55): This is a field emission scanning electron microscope (FE-SEM) incorporating a cold cathode field emission gun. Voltage range is from 0.5 kV to 30 kV. The resolution is 1 nm at 15 kV. The attachments are EDX and EBSD.

4. People

Human resources are the most important assets of the ADMIRE project. The followings are the members providing direct supports for all subjects currently running (MAR 2017, faculty professors are excluded in the following list).

- Okinobu Hashitomi (IAE Technical Staff), Administrator of DuET accelerators.

- Takamasa Ohmura (IAE Technical Staff), Administrator of MUSTER facility and more.

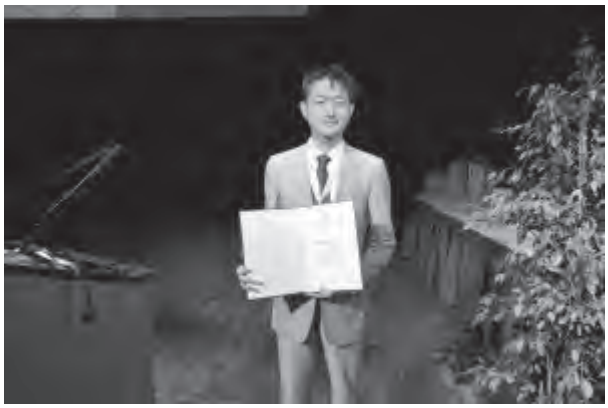
- Yasunori Hayashi (Program-Specific Researcher), Specialist of electron microscopy.

3-2. AWARD

PhD Poster Prize at 29th Symposium on Fusion Technology (SOFT).

Advanced Atomic Energy Research Section
Shutaro Takeda (D1)

At the 29th Symposium on Fusion Technology (SOFT) held in Prague, Czech Republic, Shutaro Takeda presented a paper on "Environmental Life Cycle Assessment of Nuclear Fusion Biomass Gasification Plant: A Promising Option for the Sustainable Future of Humanity?" and won the PhD Poster Prize. The conference covered topics on Socio-Economics, which, however, was not a major focus. Therefore, it was an achievement to obtain understanding from about 1,000 participants of the conference and chosen as one of the only three winners. This study was based on the concept of "biomass fusion hybrid" proposed by our laboratory, which could produce liquied fuels by gasifying biomass with fusion heat energy. In his research, Mr. Takeda successfully showeed that a large carbon dioxide reduction effect can be obtained through this concept.



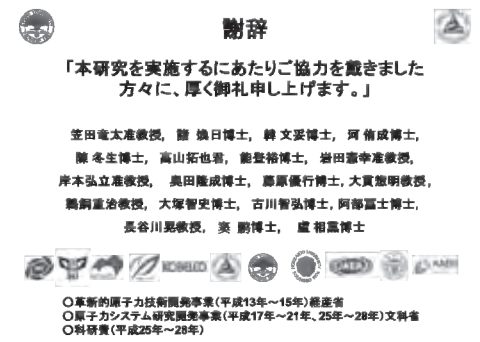
The 14th Japan Institute of Metals and Materials Distinguished Achievement Award

Advanced Energy Structural Materials Research Section
Akihiko Kimura (Professor)

Japan Institute of Metals and Materials (JIM) awards a prize to the sciences about metallurgy or the materials engineering or technological change development.

His title of the awarding talk is “Deformation and Fracture Mechanisms in High Purity Iron and Steels” where his research achievements on the strengthening mechanisms, deformation behavior and fracture mechanisms of iron and steels were introduced.

Materials degradation including hydrogen embrittlement, thermal aging embrittlement and irradiation embrittlement under operation of energy systems is now crucial problem for long time aged structural materials. Hydrogen embrittlement is well known as a phenomenon in which hydrogen causes a reduction of Peielrs stress of screw dislocations and a reduction of lattice decohesion. Aging embrittlement and irradiation embrittlement in tensile tests are less significant in oxide dispersion strengthened steels (ODSS) than in conventional steels with similar chemical compositions. He introduced a suppression mechanism based on the microstructural examination in nano-scale.



(Sep. 22, 2016)

The 8th Encouragement Award for Young Researcher of Atomic Energy Society of Japan in 2016

Advanced Energy Structural Materials Research Section
Zhexian Zhang (Researcher)

The Atomic Energy Society of Japan (AESJ) en-ergetically pursues human welfare and sustainable development while conserving global and local en-vironments through the atomic energy research, de-velopment, utilization, and education, under the prin-ciple of information disclosure with maintaining a harmonious relationship with society and securing nuclear safety.

This award was offered for the comprehensive study on irradiation hardening and maicrostructural evolution of tungsten under ion-irradiation, utilizung DuET/MUSTER facility.

His research title for the award is “Research on radiation damage mechanism in recrystallized tungsten under ion-irradiation”. Understanding not only the mechanical properties on engineering but also the fundamental material irradiation effects under irradiation is necessary. So far, the investigations on tungsten are still insufficient, especially the details of (1) microstructure evolution and their relation to irradiation hardening and (2) the material irradiation response at high temperature (>800°C). Dr. Zhang performed ion-irradiation experiments to understand the hardening and microstructure evolution at different temperatures including 1000°C, and the helium effect on the above issues, and found many new aspects of radiation damage structures in pure tungsten.

(Sep. 8th, 2016)

Best Presentation Award in The 13th China-Japan Symposium on Materials for Advanced Energy Systems and Fission and Fusion Engineering

Advanced Energy Structural Materials Research Section
Zhexian Zhang (Researcher)

The 13th China-Japan Symposium on Materials for Advanced Energy Systems and Fission and Fusion Engineering is an international symposium on nuclear materials and fuels held in Hefei. There were almost 300 participants from China, Japan, Korea and India. He made a nice oral presentation on “Microstructure stratification in pure tungsten after ion-irradiation at different temperatures” and awarded as a best presenter in the symposium.

In his presentation, irradiation hardening measurements nano-indentation method was introduced. An equation to evaluate the hardness of irradiated thin area near specimen surface was proposed simply based on the assumption that geometrically necessary dislocations (GND) density at an indentation depth was same before and after irradiation. The results showed a constant hardness depth area in the range from 200 nm to 300 nm. The hardness of this area was defined as the hardness of the irradiation layer.

He showed the hardening of tungsten irradiated at 300 °C was significantly lower than those at the other higher temperatures. In the case of single-ion beam irradiation, recrystallized W exhibited a higher hardening than as-received one at all the temperatures. The effect of helium on the irradiation hardening was dependent on the material condition: as-received W showed an additional hardening by helium at all the temperatures, while in recrystallized W the hardening was not affected by helium below 700°C.

He also found the self-ordering loop lattice structure in the tungsten irradiated at 1000 °C. It has been over 40 years for the finding of “void” lattice in tungsten. It is the first time the loop lattice was observed in BCC materials under irradiation.

(Sep. 28, 2016)

Student Session Outstanding Achievement Award in the Japan Society of Maintenology

Advanced Energy Structural Materials Research Section
Xiaoyong Ruan (D2)

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

Mr. Xiaoyong Ruan made an oral and poster presentation at the 2016 Annual Meeting. He was given the Student Session Award because his research fit engineering practice and besides he made a good presentation.

Poster Session Outstanding Achievement Award in the Irradiation Materials Meeting 2016

Advanced Energy Structural Materials Research Section
Xiaoyong Ruan (D2)

Irradiation Materials Meeting is organized as an appropriate meeting at which irradiation materials researchers in Japan may discuss the fundamental questions and concerns in radiation effects on nuclear materials. This year this meeting was held on October, at which Mr. Xiaoyong Ruan made a poster presentation and was given the poster Session Award because his research was useful in the nuclear power engineering.

Poster Session Outstanding Achievement Award in the Irradiation Materials Meeting 2016

Advanced Energy Structural Materials Research Section
Toshiki Nakasuji (D2)

Irradiation Materials Meeting is an appropriate meeting at which irradiation materials researchers in Japan may discuss the fundamental questions and concerns in radiation effects on nuclear materials. This meeting was supported by the "Joint Usage/Research Program on Zero-Emission Energy Research, Institute of Advanced Energy, Kyoto University" and held at October, 2016.

Mr. Nakasuji made a good presentation on their effort on “Rate Theory Modeling of Formation Process of Radiation Induced Precipitation in RPV steels”, and received the Poster Session Award for their valuable unique ideas. His future success is greatly anticipated.

AESJ 2017 Spring Annual Meeting Student Poster Session: Best Presentation Award

Advanced Energy Structural Materials Research Section
Xiaoyong Ruan (D2)

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

Mr. Xiaoyong Ruan is a Ph.D. student in Kyoto University, Kyoto, Japan. His current research interest lies in the deterministic and probabilistic fracture analysis of nuclear components and structures using finite element method and computational fluid dynamics.

He made oral and poster presentation at the AESJ 2017 Spring Annual Meeting. He was given the AESJ 2017 Spring Annual Meeting Student Poster Session: Best Presentation Award because he made an outstanding presentation, and his research be useful for a study on the structural integrity of nuclear reactor pressure vessel.

Encouragement award of Atomic Energy CSJ Presentation Award 2016 for Industries in 96th The Chemical Society of Japan (CSJ) annual meeting

Molecular Nanotechnology Research Section
Takahiro Nakae (Assistant Professor)

The Chemical Society of Japan (CSJ) was founded in 1878. It has contributed and circulated the results of chemical research to chemists and industry throughout the world. The CSJ holds the national meeting annually in spring, which covers all academic fields in Chemistry. Over 6,000 attractive presentations provide professionals in Chemistry with opportunities for meaningful discussions and deep insights for future research.
In the 96th annual meeting, I presented a work on synthesis of acene-type graphene nanoribbon using a surface transformable molecule, and its mechanism of polymerization and dehydrogenation. Newly designed Z-shape monomer was used for graphene nanoribbon synthesis by two-zone chemical vapor deposition method. Surface homochiral polymerization was proceeded by induction of special conformation of the precursor on surface. Selforganized homochiral polymer array can effectively converted to graphene nanoribbon by stepwise dehydrogenation, which supposed to proceed a novel conformation assisted mechanism.


優秀講演賞(産業)

京都大学　エネルギー理工学研究所
中江　隆博　殿

講演題名
「新規アセン型グラフェンナノリボンを
与える表面変型分子の設計と重合・
脱水素環環構築」

貴殿が日本化学会第96春季年会（2016）に
発表された上記の研究発表は，産学交流委員会
の選考の結果，特に優秀と認められましたので
ここに表彰します。

2016年4月12日

公益社団法人　日本化学会
会長　柳井　毅

Young Researcher Award in Symposium on Surface Science and Nanotechnology 25th Anniversary of the Surface Science Society of Japan Kansai

Molecular Nanotechnology Research Section
Shaotang Song (D3)

The Surface Science Society of Japan was established in 1979 by active researchers who shared surface science but had a variety of backgrounds, physics and applied physics, chemistry and chemical engineering, vacuum science, materials science, electrical and mechanical engineering, bioscience, etc. SSSJ has grown as a unique society that covers very interdisciplinary science and technology, and now about 1700 researchers from academia, national and public institute and industry come together to exchange their research.
In the 25th Kansai annual meeting, I presented a work on the synthesis graphene nanoribbon (GNR) with a new edge geometry via our newly developed 2-zone chemical vapor deposition system. A new concept of "conformation-controlled surface catalysis" was demonstrated during the growth of GNR from a "Z-bar-linkage" precursor. The obtained GNR was successfully transferred to an insulating substrate, and a field-effect transistor was fabricated based on it, which exhibited excellent semiconductor property.


SSSJ-Kansai
Young Researcher Award
to
Shaotang SONG
Kyoto University
"Fabrication of Acene-type Graphene Nanoribbons on Au(111)"
at
Symposium on
Surface Science and Nanotechnology
-25th Anniversary of SSSJ Kansai-
January 25, 2017, Kyoto, JAPAN

CSJ Award for Creative Works

Biofunctional Chemistry Research Section
Takashi Morii (Professor)

The chemical society of Japan (CSJ) was founded in 1878 to advance research in chemistry, has a history encompassing 130 years, with a current membership exceeding 34,000, and is one of the most affluent academic societies in Japan, covering most areas of pure and applied chemistry. The Chemical Society of Japan holds the national meeting annually in Spring, which covers all academic fields in Chemistry. Over 6,000 attractive presentations provide professionals in Chemistry with opportunities for meaningful discussions and deep insights for future research.

In the 97th Annual Meeting at Hiyoshi Campus, Keio University, I gave an award lecture entitled "A Bioorganic Chemistry Approach to Understanding Molecular Recognition in Protein-Nucleic Acid Complexes" to discuss a combination of synthetic, organic, and biochemical approaches to study how the proteins and nucleic acids assemblies modulate the affinity, specificity and cooperativity of protein-nucleic acids interactions. These strategies enabled formation of noncovalent peptide dimers on specific DNA sequences, and design of a new framework from RNA and peptide into a stable complex of ribonucleopeptide (RNP) to construct receptors and the fluorescent sensors for biologically relevant molecules. These challenges to design novel DNA-binding peptides, RNP receptors and sensors are ultimate test for our understanding of the principle of molecular recognition associated with the protein–nucleic acids interactions.

Professor Hisashi Yamamoto (*Right*, President of CSJ)

Best Presentation Award in 10th Bio-related Chemistry Symposium

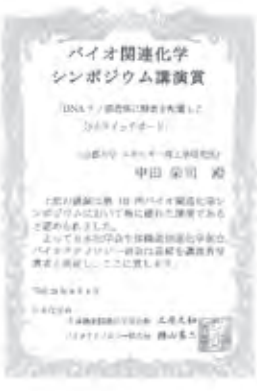
Biofunctional Chemistry Research Section
Eiji Nakata (Junior Associate Professor)

On 8th September 2016, Dr. Eiji Nakata wins best presentation award in 10th Bio-related chemistry symposium, which belongs The Chemical Society of JAPAN.

In the symposium, he presented the recent their research topics by following title, “Construction of molecular switchboard to assemble enzymes on DNA scaffold”.

In the natural living system, multi-enzyme synthetic pathways regulate the cellular activities. Understanding the effect of spatial organization on the efficiency of multi-enzyme systems is very important not only for revealing a principle that associates with the function of multi-enzymatic cascade but also for constructing an effective material conversion system in vitro. DNA nanostructure have been applied as scaffolds for the spatial organization of enzymes to form artificial enzyme cascades with which the efficient transport of reaction intermediates can be modelled. The definable nature of DNA nanostructures allows for the construction of a variety of spatially constrained enzyme assemblies. We have developed methods to use sequence-specific DNA binding proteins as adaptors to stably locate the enzymes at specific positions on DNA scaffold. Their protein adaptor based method successfully assembled the recombinant enzymes in high loading yield with control of the number of enzyme molecules and maintenance of the catalytic activities of enzymes. They have reported the construction of an artificial enzyme cascade based on XR-XDH pathway from the D-Xylose metabolic pathway.

The presentation was well received, discussed, and even garnered a presentation award.



The New Chemical Technology Research Encouragement Award from JACI

Biofunctional Chemistry Research Section
Eiji Nakata (Junior Associate Professor)

On 27th May 2016, Dr. Eiji Nakata wins The New Chemical Technology Research Encouragement Award from JACI (Japan Association for Chemical Innovation).

JACI, a public interest incorporated association, is composed of members from the chemical industry, user industries, academia, and leading national research institutions. This public interest corporation carries out activities with the aim of promoting various projects with highly public nature concerning chemical technology innovation. To support the activities of young researchers engaged in researching new chemistry at universities, public institutions and elsewhere, the committee from JACI selects the recipient of the New Chemical Technology Research Encouragement Award. The committee plans to invite public participation each fiscal year for each field by selecting a specific subject or the like. In his case, he selected from the working group for life sciences-Materials.


賞状
新化学技術研究奨励賞
中田 栄司 殿
公益社団法人 新化学技術推進協会
会長 高橋 恭平

Award for Researches on Chemical and Biological Materials from JBA

Biofunctional Chemistry Research Section
Eiji Nakata (Junior Associate Professor)

On 12th October 2016, Dr. Eiji Nakata wins Award for Researches on Chemical and Biological Materials from JBA (Japan Bioindustry Association).

JBA is a non-profit organization established in 1987. The organization is planning for sound development in bioscience-related industries and is dedicated to solving problems on a global scale through advances in bioscience. JBA is contributing to society in various areas from the development of advanced technology to the development of industry. The organization is planning for sound development in bioscience-related industries and is dedicated to solving problems on a global scale through advances in bioscience. JBA is contributing to society in various areas from the development of advanced technology to the development of industry.

In BioJapan2016, which comprises exhibitions, seminars for academia and industry, and business to business matching, he presented the related research topics by following title, “Construction of DNA nanoreactor for effiective material conversion”.


化学・生物素材研究開発奨励賞
中田栄司殿
貴殿は化学または生物の素材に関する基礎・応用研究及び利用技術開発に携わる有望な研究者として選考委員会において選ばれましたここに貴殿の研究の更なる飛躍を期待して研究奨励賞を授与致します
清水 [illegible]

Outstanding Poster Award in The 43rd International Symposium on Nucleic Acids Chemistry (ISNAC)

Structural Energy Bioscience Research Section
Yudai Yamaoki (Researcher)

International Symposium on Nucleic Acids Chemistry started in 1973 as an annual domestic meeting of nucleic acid chemists in Japan, and became an international symposium in 2005 having invited nucleic acid chemists from all over the world. ISNAC covers diverse aspects of genetic technology, molecular biology, nanobiotechnology, and therapeutic and diagnostic applications of these fields as well as nucleic acid chemistry. The 43th International Symposium on Nucleic Acids Chemistry was held in Kumamoto, Japan.

In this symposium, I presented our latest work entitled "Invention of K^+-responsive Tat-binding RNA aptamer and hammerhead ribozyme, and in-cell NMR of nucleic acids". An RNA R11, r$(GGA)_3GG$, forms a compact quadruplex under high K^+ concentrations. We replaced a part of the sequences of a Tat-binding RNA aptamer and hammerhead ribozyme by R11. Upon addition of K^+, the quadruplex formation of R11 sequence brings the 5'- and 3'-domains of each designed molecules closely together. Therefore, the new molecules fold into an active structure and exhibits Tat-binding and target RNA cleavage activity, respectively. Since, the concentration of K^+ is low outside the cell but high inside the cell, we expect that they are silent outside the cell, but turn on their activity upon entering the cell. Additionally, we performed in-cell NMR measurements of nucleic acids in living human cells. The imino-proton NMR signals of DNA and RNA inside the HeLa cells were successfully observed. The in-cell NMR technique may visualize the structural transition of functional RNAs inside the cell.

The 4th one from the left is author.

Student presentation award of the 54th Annual Meeting of the Biophysical Society of Japan (BSJ), 2016

Structural Energy Bioscience Research Section
Li Wan (D3)

The Biophysical Society of Japan (BSJ) was established on December 10th, 1960. Now BSJ is one of the members of International Union of Pure and Applied Biophysics (IUPAB). The 54th Annual Meeting of BSJ was held in Tsukuba, Japan.

In this annual meeting, Wan made a short oral presentation about the deamination characterization of human APOBEC3B, an enzyme that causes kinds of cancers once it is expressed abnormally. Wan also showed his studies via poster presentation and communicated a lot with many researches and exchanged their comments and suggestions. Wan received the student presentation award of this annual meeting. The following photograph is the certification that I received from BSJ-2016.

日本生物物理学会
学生発表賞

万　里　殿

演題：Characterization of the Deamination Activity of APOBEC3B by Real-Time NMR, Which is Distinct From That of APOBEC3G

発表者：Li Wan, Takashi Nagata, Ryo Morishita, Akifumi Takaori, Masato Katahira

あなたは、第54回日本生物物理学会年会において、大変優れた発表を行いました。ここに、第1回日本生物物理学会学生発表賞を授与します。

平成28年11月27日

一般社団法人日本生物物理学会

会長　中村　春木

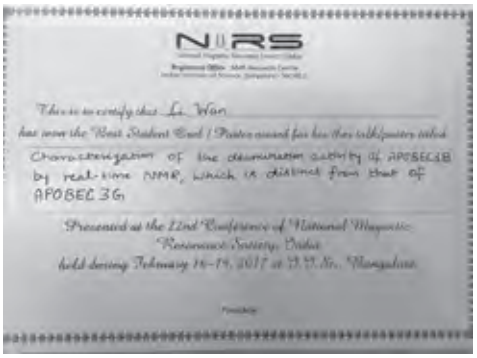
Photograph of the certification of the Student

The Best student Oral/Poster award of the 7th Asia-Pacific NMR Symposium (APNMR)

Structural Energy Bioscience Research Section
Li Wan (D3)

The Asia-Pacific NMR Symposium (APNMR) is an international forum for showcasing the advanced developments in all aspects of magnetic resonance in but not limited the Asia-Pacific region. The 1st APNMR was held in Japan in 2005, then Taiwan, South Korea, China, Australia, and Hong Kong. APNMR was held every two years and the 7th APNMR was held in Bangalore, India in 2017.

Wan was awarded the Best Student Oral/Poster Award for his excellent poster presentation in the conference. During the presentation, Wan introduced his research about the biochemical properties and scanning styles of APOBEC3B (A3B), which is quite different from those of APOBEC3G, another popular anti-HIV-1 enzyme belonging to the same protein family with A3B. Wan was one of the six students who received this award and he was highly encouraged for his research activities.



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 7th International Symposium

Many researchers have participated in this program. In FY2016, Joint Usage/Research collaborations of total 92 subjects (including one workshop) on Zero-Emission Energy were performed with more than 170 visiting participants from 43 all-Japan Universities and Institutions including graduate/undergraduate students. The results of these collaborations are summarized in a report "IAE Joint Usage/Research Program on Zero-Emission Energy 2016. Some of them were reported and discussed in a Research Summary Meeting of FY2016 held at Uji Campus on March 6, 2017. 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 7th International Symposium of Advanced Energy Science ~ Frontiers of Zero-Emission Energy ~" on September 5 – 7, 2016 at Clock Tower Centennial Hall and Uji Obaku Plaza, Kyoto University, in conjunction with International Workshop on Energy-Science Education by Graduate School of Energy Science, Kyoto University (Fig.1). This symposium consists of oral and poster sessions, panel discussion, parallel seminars and satellite meeting. About 300 scientists and students including four foreign and five domestic invited speakers were participated in the symposium. In addition, several informal seminars and/or internship on Zero-Emission Energy were also organized.(http://www.iae.kyoto-u.ac.jp/zero_emission/calendar/)

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

List of Zero-Emission Energy Joint Usage/Research Subjects in FY 2016

(Subject, Principal Researcher, IAE Key Person)

Damage Formation Mechanism of Tungsten under Repetitive and Pulsed High-Heat Load Conditions (Part 5)
K. Ezato, A. Kimura

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

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

Characterization and application of biomass originated from indigenous bacteria of activated sludge
M. Takeda, M. Katahira

Study on Dynamic Precipitation Behavior of Oxide Particles in Model Alloy Powders of ODS Ferritic Steels
N. Iwata, A. Kimura

Dynamics of Self-Organization to Helical-Axis Reversed-Field Pinch and Its Control for Plasma Performance Improvement
S. Masamune, T. Mizuuchi

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

Selective phonon-mode excitation in perovskite functional materials for energy conversion by mid-infrared free-electron laser
K. Hachiya, H. Ohgaki

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

Microbial Transformation and Dissolution Processes of Fine Particulate Organic Matter (FPOM) in Lake Biwa
Y. Shimizu, M. Katahira

Development of Radiation Measurement Method for the Detection of harzardous materials with IEC Device
T. Misawa, K. Masuda

Development of Refining Process of Silicon Utilizing Volatile Metal Flux for the Production of Solar-grade Silicon
K. Yasuda, T. Nohira

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

Development of Organic-Inorganic Hybrid Film toward High-Performance Organic Thin-Film Solar Cells
T. Akiyama, H. Sakaguchi

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

Hydrogen isotope permeation behavior of ceramic coatings irradiated by heavy ions under higher temperature
T. Chikada, K. Yabuuchi

He and Heavy ion synergism on hydrogen isotope behavior in tungsten at higher temperature
Y. Oya, T. Hinoki

Mechanical properties of fusion reactor materials, tungsten and reduced activation ferritic/martensitic steels (F82H), under high strain rate loading.
H. Lee, R. Kasada

Hydrogen isotope behavior in tungsten under plasma and neutron irradiation environment in fusion reactors
Y. Ueda, A. Kimura

Computational design and study of novel two-dimensional materials
S. Okada, K. Matsuda

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

Mechanism of Radiation Resistance of Advanced Tungsten Alloys
A. Hasegawa, A. Kimura

Irradiation embrittlement mechanism of plasma facing materials in fusion reactors based on micromechanics
M. Fukuda, R. Kasada

Characterization of Oxide Dispersion Strengthened Reduced Activation Ferritic/Martensitic Steel for DEMO Fusion Reactor
M. Ando, A. Kimura

Chemical state analysis of light elements in advanced neutron multiplier for fusion reactor blanket
M. Nakamichi, R. Kasada

Influence of high temperature irradiation on hydrogen isotope retention and permeation in first wall and divertor materials for fusion reactors
Y. Hatano, T. Hinoki

Study of interaction between dislocation and irradiation deffects for evaluation of material degradation in nuclear structural materials
K. Fukumoto, A. Kimura

Photo-Energy Conversion System Based on DNA and Photoresposible Dye Conjugation
K. Yamana, T. Morii

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

Relationship between cell wall structure and lignin structure for advanced biomass utilization
K. Fukushima, M. Katahira

A study of potential distribution formed inside the cathode region in IEC device
M. Utsumi, K. Masuda

Structural analysis of lignin and lignin-carbohydrate complex by ultra-high sensitivity NMR for biorefinery
T. Watanabe, M. Katahira

Study on Li vaporization property of high performance tritium breeding material by EPMA-SXES
K. Sasaki, R. Kasada

A Study on Mechanical Property Evaluation of Silicon for MEMS by Nanoindentation
T. Nakata, R. Kasada

Development of a small molecule that has affinity to RNA G-quadruplex
Y. Katsuda, T. Morii

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

Radiation effects on properties of plasma facing materials in fusion reactor
K. Tokunaga, A. Kimura

Rural Electrification by Renewable Energy in Sarawak, Malaysia
H.W. Ping, H. Ohgaki

Modeling and simulation study on radiation damage of reduced activation ferritc/martensitic steel for fusion application
Y. Watanabe, K. Morishita

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

Study of liquid metal embrittlement on SiC materials for high efficiency heat exchanger
C. PARK, S. Konishi

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

Development of in-situ physical property measurements of SiC CMCs at elevated temperatures
K. Shimoda, T. Hinoki

Study on causal relation between non-diffusive plasma heat transport and turbulence propagation using beam emission spectroscopy
S. Kobayashi, S. Kobayashi

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

Towards the development of rare metal and toxic metal recovery system: Development of a protein chip with integrated metal binding proteins
R. Sakaguchi, T. Morii

Nanoindentation of cellulose nanofiber / resin composite materials prepared with polymer dispersants
Y. Tsujii, R. Kasada

Development of a carbon electrode for energy storage devices by highly-efficient electropolymerization in porous silicon caused by surface-induced phase transition
K. Fukami, M. Kinoshita

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

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

Big data analysis of dynamic behavior of plasma measured with microwave reflectometry
S. Inagaki, K. Nagasaki

Analysis of radiation indudced nano-clustesr in Fe based structural alloys
H. Watanabe, A. Kimura

Flow analysis from a nozzle for SMBI
N. Nishino, T. Mizuuchi

Development of novel aptamers that confer stable guanine-quadruplex structures.
M. Hagihara, T. Morii

Development of an algorithm for tomographic reconstruction of HeI radiation distribution in Heliotron J
H. Kawazome, T. Mizuuchi

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

Effect of Hydrogen on Mechanical Properties in Tungsten
K. Sato, A. Kimura

Theoretical study on atomistic modeling for interactions between hydrogen/oxygen atoms and additive elements in zirconium alloys
Y. Kaneta, K. Morishita

Improvement of Fatigue Test Technology for Ceramics Matrix Composites
S. Nogami, T. Hinoki

Theoretical Analysis on Natural Convection Heat Transfer from Vertical Rod Bundles in Liquid Sodium (Part 2)
K. Hata, T. Mizuuchi

Development of artificial RNA and artificial peptide to control gene expression by using NMR
T. Sakamoto, T. Nagata

Pedestal Plasma fluctuation Diagnostics with High Spectral Resolution Digital Imaging Technique
M. Irie, T. Mizuuchi

Influence of permeation, diffusion and retention behavior of hydrogen isotopes in the fusion wall materials to the fusion reactor system designs
K. Ibano, S. Konishi

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

Development of ultrasound-enhanced cell-internalization method
A. Harada, E. Nakata

Application of atmospheric pressure plasma jet in food industry
H. Matsuura, S. Kado

Formation of high performance plasmas using high-energy neutral beam injection in three-dimensional magnetic configuration
Y. Nakashima, S. Kobayashi

Molecular Roles of Novel Protein PEP70 in Electron Transport System in Mitochondria
Y. Aizawa, T. Morii

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

Development of the zero-emission energy oriented boron neutron capture agents having tumor-selectivity and diagnosability.
Y. Uto, E. Nakata

Development of the site-directed RNA mutagenesis for regulating an energy production in the cell
M. Fukuda, T. Morii

Low-cost production of artificial immobilized multi-domain enzymes using GRP-tag affinity system
M. Horiuchi, T. Nagata

Evaluation of compatibility of Ni-ODS superalloys with nuclear reactors
S. Ukai, A. Kimura

Dielectric constant change of glass substrate after ion irradiation and SPR measurements by STEM/EELS
T. Shibayama, T. Hinoki

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

Infrared light fluctuation to electric power conversion by Seebeck ratchet
N. Yonekura, T. Nakashima

Correlation measurements of electron cyclotron emission signals at two toroidal and poloidal positions in torus plasmas
Y. Yoshimura, K. Nagasaki

Developing Social Decision-making System for Renewable energy and Nuclear Power Generation.
H. Iwakiri, K. Morishita

Heavy irradiation effect of Fe-based composite materials with a high thermal conductivity
N. Hashimoto, A. Kimura

Probing the intrinsic electrical and optical properties of high-quality atomic layers with microscopic spectroscopy
R. Kitaura, K. Matsuda

Direct demonstration of mode-selective phonon excitation by two photon excitation
K. Yoshida, H. Ohgaki

Boundary diagnostics using field corresponding double probe and rf heating in Heliotron J II
K. Uehara, T. Mizuuchi

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

Nanoablation on solid surfaces with 7-fs laser pulses
G. Miyaji, K. Matsuda

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

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

Evaluation of mechanical properties of electrodeposited Al-W alloy films
M. Miyake, R. Kasada

Study of Deuterium Retention Property of Heavy Ions Beam Irradiated Tungsten Using Compact Divertor Plasma Simulator for Hot Laboratory
M. Yajima, T. Hinoki

Atomic-level analysis of oxidation-inuduced amorphization of Nb precipitates in Zr-Nb nuclear fuel cladding subjected to corrosion
Y. Matsukawa, A. Kimura

Relaxation Measurements on the Electrochemically Lithium Inserted gamma-Fe2O3 by Means of NMR
S. Takai, T. Morii

Detoxification of endocrine disruptors by microbial enzymes.
T. Hara, T. Morii

A new era of high energy particle irradiation research towards development of radiation tolerant nuclear structural materials (Zero-emission energy workshop)
Y. Nagai, T. Morii

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 processes of energy production, conversion and application. Resource and energy problems as well as global warming problems become very serious in recent years. We have to concentrate all our knowledge and wisdom to find solutions to these problems. From such a viewpoint, the research targets of the laboratory should be focused on two specific fields, (i) "advanced studies of science and technology on plasma energy and quantum energy" and (ii) "innovative studies of nano-bio functional materials for power generation". Therefore, two sections (A2 and A3 mentioned below) are founded. In addition, a section of promotion for international collaborative research arranges and promotes international and domestic research collaborations.

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

A1 Section of Promotion for International Collaborative Research

This section promotes international collaborative research on advanced energy to lead the field of energy science and technology as an international pioneer. Collaborative researches between the institute and domestic/international organizations are supported towards realization of advanced energy systems as practical applications with contributions to human society. This section also promotes personal exchange, cooperative research activities and multi-lateral collaborative research with industries. Establishment of infrastructure and human resource development are supported for execution of collaborative R&D activities on advanced energy.

A2 Section of Promotion for Advanced Plasma and Quantum Energy

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

A3 Section of Promotion for Photon and Energy Nano-Science Research

This section promotes studies on photon and energy nano-science for realizing next generation soft (renewable) energy system. In particular, functional nano- and bio-materials to utilize solar energy and bio-energy are studied by unifying laser science, nano-technology, 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 (a mid-infrared range free electron laser), NMRs and so on.

B Cooperative use of facilities and equipment

Facilities and equipment of the laboratory are provided to researches cooperated for the scientists in the university.

2. The cooperative research program

A brief summary of the cooperative research subjects carried out in FY2016 are shown next pages, which were proposed by researchers of IAE and selected by the program committee of the Laboratory.

The collaboration works in the Laboratory for Complex Energy Processes are consist of two categories of “Kiban (基盤)” and “Shorei, Kikaku-Chosa (奨励, 企画・調査)” cooperative researches. The former means a program to promote leading research themes of the institute projects, which are proposed by the each chair of the research sections of the Laboratory. The latter means a program to promote seeds research with respect to the institute projects and to promote the organization of seminar or symposium. Every researcher of IAE can make proposal to this category.

As a result, the research themes of 25 were applied and applications of 25 were accepted. The number of research subjects is listed in Table 1 according to the project categories.

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

The whole sum 25

		category A			B	total
		A1	A2	A3		
Kiban	inside	1	1	1	0	3
	outside	0	0	0	0	0
Shorei/Kikaku-Chosa	inside	4	11	7	0	22
	outside	0	0	0	0	0

"inside" or "outside" : Number

The individual research subjects are as follows

Kiban A1

"International Collaborative Research on Advanced Energy Science"

- H. Ohgaki and Staff Researcher of IAE (Kyoto Univ.)
- J. Qika (Univ. Sci. Tech. China)
- P. Kaung (Univ. Yangon)
- Y.U. Jeong (Korea Atom. Energy Res. Inst.)
- D. Wang (Shanghai Inst. App. Phy.)
- M. Abdrahim (Univ. Malaya)
- B. Funtamasan (King Mongkuts Univ. Tech. Thanburi)
- P. Pinpathomrat (Rajamangala Univ. Tech. Thanyaburi)
- H. Saptadi (Univ. Gaja Mada)

Kiban A2

"Development of Advanced Plasma and Quantum Energy Studies"

- K. Nagasaki, R. Kasada, S. Ohshima, K. Yabuuchi, S. Konishi, A. Kimura, T. Minami, H. Okada, S. Kobayashi, S. Yamamoto, T. Mizuuchi, S. Konoshima (Inst. Adv. Energy, Kyoto Univ.)
- Y. Nakamura, Y. Ohtani, L. Xiangun (Grad. Sch. of Energy Sci., Kyoto Univ.)

Kiban A3

"Research on establishment of Photo-Energy Nano Science"

- H. Sakaguchi and Researchers of Photo-Energy Nano-Science (Inst. Adv. Energy, Kyoto Univ.)

Shorei/Kikaku-Chosa A1

"US-Japan Collaborative Research Ion-irradiation Effects on Materials"

- A. Kimura, K. Morishita, T. Hinoki, R. Kasada, K. Yabuuchi, W. Han, S. Kondo
- G. Was, G. Jiao, S. Taller (Univ. Michigan, USA)
- S. Maloy (LANL. USA)
- B. Weber (Univ. Tennessee, USA)
- S. Tumey (LLNL, USA)
- M. Toloczko (PNNL, USA)
- T. Shibayama, N. Hashimoto (Hokkaido Univ.)
- A. Hasegawa, K. Nagai (Tohoku Univ.)
- N. Sekimura (Univ. Tokyo)
- T. Muroga (National Inst. Fusion Sci.)
- H. Watanabe (Res. Inst. App. Mech. Kyushu Univ.)
- H. Tanigawa (JAEA)

"**International Collaboration Research on Plasma Production Using Microwaves**"

- K. Nagasaki, S. Yamamoto, K. Masuda, S. Ohshima, K. Sakamoto, T. Mizuuchi, T. Minami, H. Okada, S. Kado, S. Kobayashi, S. Konoshima (Inst. Ad. Energy, Kyoto Univ.)
- T. Stange, N. Marushchenko, H. Laqua (Max Plank Inst., Germany)
- E. Ascasibar, A. Cappa (CIEMAT, Spain)
- F. Volpe (Columbia University, USA)
- Y. Yoshimura (National Inst. Fusion Sci.)
- Y. Nakamura, (Grad. Sch. of Energy Sci., Kyoto Univ.)

"Investigation of spatiotemporal structure of density fluctuation in high density H-mode plasmas"

- S. Kobayashi, S. Ohshima, T. Mizuuchi, S. Yamamoto, H. Okada, T. Minami, K. Nagasaki, S. Konoshima (Inst. Adv. Energy, Kyoto Univ.)
- C. Deng, D.T. Anderson (Univ. Wisconsin-Madison, USA)
- G. Weir (JSPS)
- S. Torsten (Max-Plank Institute for Plasma Physics)
- L. Hyunyong (Korea Adv. Inst. Sci. Tech.)
- T. Kobayashi, Y. Suzuki, K. Nagaoka, T. Ohishi, S. Okamura, K. Mukai (National Inst. Fusion Sci.)
- Y. Nakashima (Univ. Tsukuba)
- S. Murakami (Dep. Nucl. Eng., Kyoto Univ.)

・Y. Nakamura (Grad. Sch. Energy Sci., Kyoto Univ.)

"Development of a highly efficient bioethanol production yeast by genetic engineering"
・T. Kodaki (Inst. Adv. Energy, Kyoto Univ.)
・S.M.R. Khattab (Microbial Biotech. at Botany and Microbiology Dep., Al Azhar Univ., Assiut Branch)

Shorei/Kikaku-Chosa A2

"Effects of irradiation-induced defects on the SiC hot-water corrosion and underlying mechanism"
・S. Kondo, T. Hinoki, (Inst. Adv. Energy, Kyoto Univ.)

"Risk assessment and management of unclear waste disposal"
・K. Morishita, R. Xiaoyong (Inst. Adv. Energy, Kyoto Univ.)
・H. Nakamura, D. Kato (National Inst. Fusion Sci.)
・M. Miyamoto (Interdisciplinary Faculty of Sci. Eng., Shimane Univ.)
・H. Iwakiri (Dep. Education, Univ. Ryukyu)
・Y. Kaneta (Akita National Coll. Tech.)
・Y. Watanabe (JAEA)
・X. Qui (Kyoto Univ. Res. Reactor Inst.)
・T. Nakasuji (Grad. Sch. Energy Sci., Kyoto Univ.)

"**Developing Innovative Method for Safety Assessment of Nuclear Energy System by the Systemic Accident Mode**l".
・K. Morishita, R. Xiaoyong (Inst. Adv. Energy, Kyoto Univ.)
・M. Miyamoto (Interdisciplinary Faculty of Sci.(JAEA)
・H. Iwakiri (Dep. Education, Univ. Ryukyu)
・Y. Yamamoto (Inst. of nuclear Safety System)
・N. Murayoshi (Grad. Sch. Energy Sci., Kyoto Univ.)

"Study of plasma fluctuation measurement using background light in Thomson scattering diagnostic"
・T. Minami, T. Mizuuchi, S. Kado, H. Okada, S, Kobayashi, S. Yamamoto, S. Ohshima, S. Konoshima (Inst. Adv. Energy, Kyoto Univ.)
・K. Tanaka, N. Kenmochi (National Inst. Fusion Sci.)

"Production of bulk size Cr(Fe) based (bo ro)carbide towards evaluation of irradiation resistance of advanced quantum energy structural materials"
・R. Kasada, S. Konishi, T. Hinoki, S. Kondo (Inst. Adv. Energy, Kyoto Univ.)

"Development of computational techniques for the interaction between radiation defects and dislocations"
・K. Yabuuchi, A. Kimura (Inst. Adv. Energy, Kyoto Univ.)

"Studies on fast ion loss by using scintillator type lost fast ion probe in Heliotron J"
・S. Yamamoto, K. Nagasaki, S. Kobayashi, T. Mizuuchi, H. Okada, S. Kado, T. Minami, S. Ohshima, S. Konoshima (Inst. Adv. Energy, Kyoto Univ.)

"Measurement of the impurity line spectra in Heliotron J for the plasma diagnostics"
・S. Kado, H. Okada, S. Yamamoto, T. Mizuuchi, K. Nagasaki, T. Minami, S. Ohshima, S. Kobayashi, S. Konoshima (Inst. Adv. Energy, Kyoto Univ.)
・Y. Nakamura (Grad. Sch. Energy Sci., Kyoto Univ.)

"Fast Ion Generation by Combination Heating of ICRF and NBI in Heliotron J"
・H. Okada, S. Kobayashi, S. Yamamoto, S. Kado S. Ohshima, T. Minami, T. Mizuuchi, K. Nagasaki, S. Konoshima (Inst. Adv. Energy, Kyoto Univ.)
・Y. Nakamura (Grad. Sch. Energy Sci., Kyoto Univ.)
・H. Kasahara (National Inst. Fusion Sci.)
・Y. Nakashima (Tsukuba Univ.)
・N. Nishino (Hiroshima Univ.)

"Study on Quantitative Analysis of B-10 for BNCT Pharmacokinetic Evaluation"
・K. Masuda, E. Nakata (Inst. Adv. Energy, Kyoto Univ.),
・Y. Uto (Grad. Sch. Tokushima Univ.)
・M. Nakamura (Grad. Sch. Yamaguchi Univ.)
・Y. Takahashi (Res. reactor Inst. Kyoto Univ.)

"Suppression of fringe jump using analytic signal on interferometry"
・S. Ohshima, T. Mizuuchi, S. Kobayashi, H. Okada, K. Nagasaki, S. Yamamoto, S. Kado, S. Konoshima, (Inst. Adv. Energy, Kyoto Univ.)

Shorei/Kikaku-Chosa A3

"Toward better utilization of woody biomass: Study of structure-function relationships on wood degrading enzymes"
・T. Nagata, M. Katahira, T. Morii, T. Kodaki, E. Nakata (Inst. Adv. Energy, Kyoto Univ.)

“Development of Compact THz-FEL System”

- H. Ohgaki, K. Masuda, T. Kii, H. Zen (Inst. Adv. Energy, Kyoto Univ.)
- S. Suphakul (Grad. Sch. Energy Sci., Kyoto Univ.)

“Development of the Methodology to Construct the High-efficient Material Conversion System on DNA Nanostructure”

- E. Nakata, T. Morii, T. Kodaki, M. Saimura S. Nakano, A. Rajendran (Inst. Adv. Energy, Kyoto Univ.)

“Mechanistic investigation on the topoisomerase enzymes and screening of their inhibitors”

- A. Rajendran, T. Morii, E. Nakata, S. Nakano, M. Saimura (Inst. Adv. Energy, Kyoto Univ.)

“Evaluation of the clustering effect of receptors by using DNA nanostructure scaffold”

- S. Nakano, T. Morii, E. Nakata, A. Rajendran, M. Saimura (Inst. Adv. Energy, Kyoto Univ.)

“Pulse Duration Measurement of ps-Photocathode Drive Laser”

- H. Zen, T. Nakajima, H. Ohgaki, K. Masuda, T. Kii (Inst. Adv. Energy, Kyoto Univ.)

“Detection and control of structural change in conductive polymer films using KU-FEL”

- T. Nakajima, H. Ohgaki, T. Kii, H. Zen (Inst. Adv. Energy, Kyoto Univ.)
- Y. Uto (Grad. Sch. Energy Sci., Kyoto Univ.)
- N. Yonekura (The University of Ryukyu)

THE LABORATORY SEMINARS

Laboratory Seminars

The Laboratory promotes topical academic seminars in order to strengthen the research activities in each research section and to enhance the mutual cooperation among a lot of academic fields. The Laboratory also had a symposium on April 7, 2017 for discussions of the cooperative research results in FY2016.

In FY2016 seminars were held with following themes.

1. Topical Seminars

(1) **July 7, 2016**

The laboratory seminar of the current year changed the taste slightly. Young and middle age researchers belonging to the center introduced their "Methods" in the seminar entitled "What I Can Do" as follows:
1) Associate Professor R. Kasada, "I can analyze the chemical state of complex materials by scanning electron microscope equipped with a soft X-ray emission spectroscopy".
2) Junior Associate Professor E. Nakata, "Our creative research and development".
3) Assistant Professor H. Zen, "Current status and future prospect of KU – FEL".
This kinds of communication on methods may accelerate new complex research themes.

6. PROJECTS WITH OTHER UNIVERSITIES AND ORGANIZATIONS

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

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

Efficient conversion of solar energy to electricity

Prof. Fukami aimed to utilize carbon dioxide in his research "Electrochemistry on nanoporous electrodes: Strategy for the photoreduction of CO_2." We experimentally detected the accumulation and acceleration of electrochemically active species originating from surface-induced phase transition in nanoporous electrodes. We have proposed a strategy for highly-efficient photoreduction of CO_2 by the effects in confined nanopores.

Prof. Sagawa's group studied the principle of polymer solar cells by his research entitled " Optimization of the thin-film making process for highly efficient and stable polymer solar cells with antimony sulfide." Sb2S3-based hybrid solar cells with electron transporting layer of TiO2 or ZnO nanoparticles in addition to poly(3-hexylthiophene)-2,5-diyl / (3, 4-ethylenedioxythiophene) : poly(styrene sulfonate), zinc phthalocyanine, or MoO3 for hole transporting layer were prepared and compared their photovoltaic properties with or without encapsulation by using glass and UV cut-off film.

Prof. Nohira's group developed new processes for the production of solar-grade silicon by molten salt electrolysis in the project " Electrodeposition of crystalline silicon films from molten salts." As a new method to prepare the crystalline silicon substrate for photovoltaics, we have investigated the electrodeposition of silicon in molten KF-KCl-K_2SiF_6 at 923-1023 K. We have clarified the optimum condition to obtain compact and smooth silicon deposits. We have also found that the crystallinity of silicon is much improved by the elevation of temperature from 923 K to 1023 K.

Prof. Ohgaki's group carried out a research on “Study on selective phonon excitation in energy materials by ps-laser and MIR-FEL" at Institute of Advanced Energy, Kyoto University. IR tunable coherent light source is quite useful tool to study molecular dynamics and material properties because such light can excite a specific stretching bands or a specific vibration mode. In this work, we demonstrated pump-probe spectroscopy of 6H-SiC using MIR-FEL (Free Electron Laser) and ps mode lock laser. Specific anti-Stokes Raman scattering lights synchronized with MIR-FEL were successfully obtained.

Prof. Nakajima's group developed a new method for the material analysis in the project " Discoveries in laser-irradiated nanoparticles and polymer films." Although the response of materials to laser is better understood by looking into their time-dependent behaviors, the commonly used techniques for the material analysis such as FTIR and XRD do not have time-resolution. We undertake the time-resolved in-situ detection of nanoparticles and crystalline polymer films by the optical methods, and find the number-density-dependent growth of nanobubbles and the time-varying temperature of polymer films.

Production of solar fuels

Prof. Morii's group studied on the artificial metabolic pathway in the project entitled "Spatially organized enzyme complexes". Multiple enzymes cooperate to catalyze the sequential steps of chemical transformations in the efficiency that artificial catalysts still cannot achieve. A clue for such efficient sequential processes comes from the assembly of multiple enzymes. To realize such an assembly of enzymes or biomacromolecules, we use DNA nanoarchitectures made by the DNA origami method as the molecular switchboard with defined addresses.

Prof. Sakaguchi's group studied development of a novel materials for light energy utilization in his research entitled " Carbon based nanoribbons for energy." They demonstrate a new concept of 'conformation-controlled surface catalysis'; the two-zone chemical vapor deposition of the 'Z-bar-linkage' precursor, which represents two terphenyl units are linked like a 'Z', exhibiting flexible geometry that allows it to adopt chiral conformations with height-asymmetry on an Au(111) surface, results in the efficient formation of acene-type graphene nanoribbons with a width of 1.45 nm through optimized cascade reactions.

Efficient conversion of biomasses to useful chemicals

Wood biomasses are produced by solar energy. Prof. Katahira's group works on new bio-refinery methods to contributes on exploring novel principles for highly efficient utilization of solar energy. Three major components of wood biomass are cellulose, hemicellulose and lignin. We elucidated the supramolecular structure of wood biomass, lignin-carbohydrate complex (LCC), by NMR on the basis of solid J connectivities. We also successfully monitored the stereo selective degradation reactions of lignin by enzymes derived from the marine bacterium in real-time by NMR.

NIFS Bilateral Collaboration Research Program on Heliotron J

Since 2004, 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 in Heliotron J through advanced helical-field control. Picked up in FY2016 are the following seven key-topics; (1) understanding plasma hear/particle transport phenomena with self-formation of plasma structure and its control by the magnetic field control in the advanced helical device, (2) development of high density plasma production scenario and investigation of high-beta plasma confinement, (3) instability control in the advanced helical configuration, (4) plasma current control and its application for plasma performance improvement, (5) sophistication of the diagnostic systems for local measurement of plasma parameters, (6) clarification of ECH/EBW heating scheme, (7) study of the boundary plasma physics in the advanced helical device.

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

Study of density control using pellet injection: The ice-pellet injection system has been developed [1] for a new fueling method in Heliotron J. This pellet injection technique is effective to supply particles deeply into the plasma core region. The conditions of the pellet injector are carefully selected for the plasma parameters of Heliotron J; injection speed is less than 300 m/s and the pellet diameter is less than 1 mm. After successful injection tests in FY2015, the injection experiment to NBI or ECH+NBI plasmas was done in FY2016. The density increase after pellet injection is very rapid and exceeds 5×10^{19} m^{-3} for NBI plasmas. Plasma stored energy decreases just after the injection, then, increases up to 3.4 kJ from 1 kJ (before the injection). The penetration length of the pellet is investigated using Hα detector array for ECH+NBI plasmas. The increase of the Hα line-emission is recognized from the edge sight-line (pellet injector side) to the central one. In some cases, however, the pellet penetrates through the entire plasmas, indicating the necessity of the optimization of the injection conditions.

H-mode transition in NBI plasma induced by high-intensity gas puffing (HIGP) [2]: The H-mode transition in high density NBI plasmas has been found in the low toroidicity (low-ε_t) magnetic configuration. Here, a pulse of high-intensity gas puffing (HIGP) is used to increase the plasma density. The relationship of H-mode transition to density fluctuation is investigated for NBI (~ 1 MW) plasma at B = 1.3 T. The plasma stored energy decreases just after the HIGP pulse, but it recovers and increases much over the level before HIGP. During HIGP the bursting fluctuation (~ 5 - 30 kHz) in the density is observed by using the beam emission spectroscopy measurement. The toroidal mode number of this fluctuation should be two, evaluated from the magnetic measurement. The ow-frequency modulation (~ 0.3 - 3 kHz) of this mode is observed and its toroidal mode is supposed to be zero. This fluctuation is considered to cause the particle pumping-out since the fluctuation diffuses outwards.

The isotope effect on long-range correlation and the nonlinear coupling with turbulences [3]: The plasma turbulence is studied from simultaneously measured floating potential (V_f) at different toroidal positions by using three sets of electrostatic probes. The low frequency (< 4 kHz) V_f fluctuation with LRC in the toroidal direction is observed and is found to couple nonlinearly with the broadband fluctuations. The experiments with different deuterium-to-hydrogen ratio revealed that he fluctuation amplitude and the coherence is almost proportional to the deuterium ratio, and that the nonlinear coupling in the low frequency region is stronger for the deuterium, suggesting isotope effect for LRC.

References

[1] G. Motojima, et al., "Injection barrel with a tapered structure for a low speed and small size cryogenic hydrogen pellet in medium-sized plasma fusion devices", RSI **87**, (2016) 103503.

[2] S. Kobayashi, et al., "Study of H-mode transition triggered by high-intensity gas puffing in NBI plasmas of Heliotron J", 26th IAEA Fusion Energy Conference (FEC2016), Kyoto, Japan, 17-22 Oct., 2016, EX/P8-17.

[3] S. Ohshima, et al., "Isotope Effect on Long Range Correlation and the Nonlinear Coupling with Turbulence in Heliotron J", ibid., EX/P8-20.

Application of DuET and MUSTER for Industrial Research and Engineering (The ADMIRE Project)

1. Introduction

The ADMIRE at the Institute of Advanced Energy (IAE), Kyoto University is the project to provide private companies, universities and national institutes with utilization of experimental facilities and expertise of IAE, Kyoto University. The DuET Facility i.e. dual beam ion accelerator system with a dedicated specimen irradiation stage, and the MUSTER Facilities consisting of high-performance TEM, SEM, FIB, EPMA, Auger, etc. are included in this program. Technical guidance to operate experimental equipment and consulting on the experimental results is also offered to the users.

2. Project details

The ADMIRE Project was launched in 2006. The DuET and MUSTER are two of the representing facilities in the IAE dedicated for the research of energy science and technology, with the special emphasis on fusion and fission reactor materials R&Ds. The ADMIRE Project aims to provide the researchers with the research resources of IAE. Research topics accepted by the ADMIRE Project are NOT restricted to fission or fusion reactor materials, nor energy science and technology. We welcome proposals from a variety of fields all over the world.

3. How to use the facilities

The ADMIRE Project has three modes of facility use: a) Charged use mode-X (exclusive use of data), b) Charged use mode-N (non-exclusive use of data), and c) Collaborative use.

a) Charged use mode-X (exclusive use of data)

This mode is programmed for those users who have strong interests on the intellectual property rights to be obtained through the ADMIRE utilization. There is no obligation to submit reports, etc. to the ADMIRE. The subject title and the name of the user may be kept undisclosed if the user so requests.

b) Charged use mode-N (non-exclusive use of data)

This mode is similar to the mode-X but is different only in that submission of a report is obligatory. The charge rate for facility use is lower compared to the mode-X.

DuET, the dual-ion beam irradiation facility

c) Collaborative use

This mode is similar to the standard collaborative research conducted jointly by private companies and university staff under a contract to which both parties agreed. This is not just utilization of the facility but full collaboration on specific subjects.

4. Benefits for companies

- Rapid progress of products development by use of high performance equipment
- Reduction of expenditure for equipment
- Rapid exploration of new idea
- Training of equipment operation and consulting on experimental results are available

for details, please visit our website at:
http://admire.iae.kyoto-u.ac.jp/

7. HOW TO GET TO THE IAE