ISSN 1342−3177

IAE−AR−2015

Institute of Advanced Energy
Kyoto University

ANNUAL REPORT

2014

京都大学エネルギー理工学研究所

Institute of Advanced Energy, Kyoto University

ANNUAL REPORT

2014

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Kyoto University

Gokasho, Uji, Kyoto 611-0011
Japan

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FOREWORD

Since it was launched in May 1996, the Institute of Advanced Energy (IAE) has pursued research aimed at the development of energy science and the creation of advanced technology that drives it. This work, which is outstanding both in terms of environmental harmony and social acceptance, is conducted by 3 divisions and 14 research sections (including two with guest researchers) that engage in research on energy generation, conversion, and utilization, as well as the Laboratory for Complex Energy Processes, which specializes in highly project-oriented cross-disciplinary R&D. Under the new university operation guidelines that took effect when the institute became a National University Corporation in 2004, IAE pursued its first six-year medium-term plan (2004-2009) and associated goals. In the current academic year (2013) IAE is entering the second half of its second medium-term plan and goals (2010-2015).

IAE is leveraging its track record and strengths as a research institute to focus on “advanced plasma and quantum energy” and “photon and energy nano-science” as fields of vital importance. It is devoted to R&D on nuclear fusion and advanced atomic energy, for which these disciplines serve as a scientific foundation, on distributed energy sources, typified by sunlight and biological systems, and on the advanced materials and effective energy utilization systems that support these technologies.

Since AY2011, IAE has been recognized by the Ministry of Education, Culture, Sports, Science and Technology as a Joint Usage/Research Center for Zero-Emission Energy Research (2011-2015). In the AY2013, the center was received an interim assessment and this research center was evaluated as “increasing its research performance in a wide range of fields, from scientific fundamentals to technological application in advanced energy.” Encouraged by this assessment, we have continued our efforts in the areas of zero-emission energy research and community formation toward the AY2015, which is the last year to complete the current 5 year program.

In AY2013, IAE was also approved for the development of “innovative strategy for highly efficient utilization of solar energy” (by the Ministry of Education, Culture, Sports, Science and Technology: 2013-2018) with the expectation of advancing energy research based on new bio, optical, and nano-technologies. The project has been aggressively advanced and produced several key results. The bidirectional collaborative research program with the National Institute for Fusion Science and also the promotion program of cooperation between industries and universities/national institutes by using advanced facilities have been progressed in pursuing research on boosting the performance of nuclear fusion plasma and on technology for the recovery and utilization of various advanced energy.

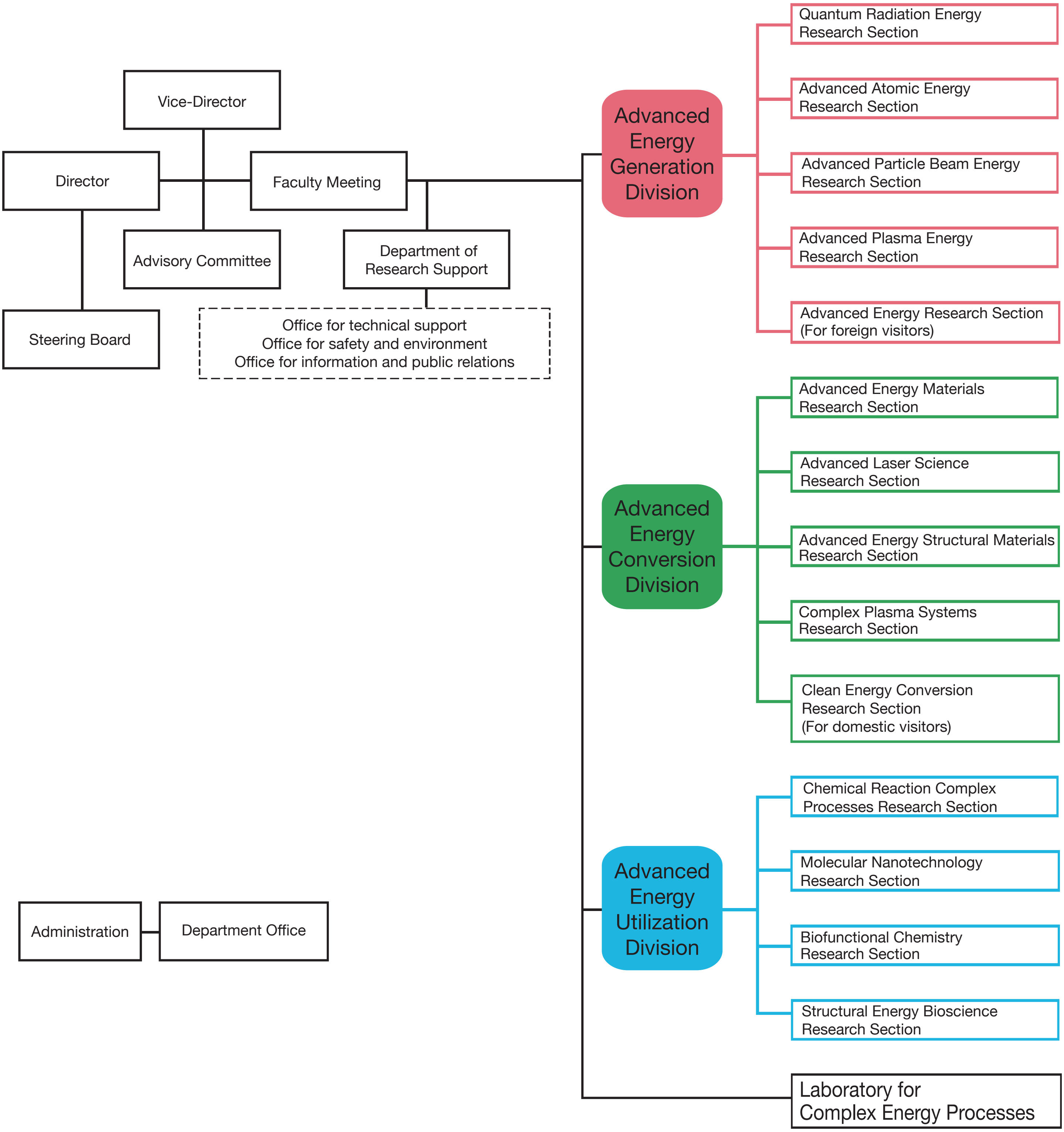
This year’s report summarizes the IAE’s research findings for the year. Four years have now passed since the Great East Japan Earthquake of March 2011, and amidst the persistent effort toward recovery by the Japanese government and people, the role and responsibility of universities have become even more important. Recognizing this, Kyoto University is working hard on a variety of fronts, to redefine its mission as a university, to formulate educational reforms and innovations, and to promote greater internationalization. In view of this, IAE feels a strong sense of social responsibility, to keep striving, harder than ever, as a key organization for energy research.

Y. Kishimoto

March 2015

Yasuaki KISHIMOTO
Director
Institute of Advanced Energy
Kyoto University

2. ORGANIZATION CHART



3. RESEARCH ACTIVITIES

3-1. TOPICS

Integration of Statistical Mechanics of Liquids and Structural Biology: Binding of an RNA Aptamer and a Partial Peptide of a Prion Protein

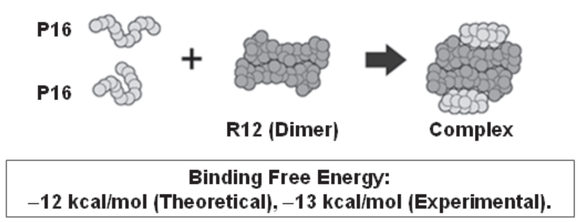
M. Kinoshita, Professor (Complex Energy Processes Research Section)
M. Katahira, Professor (Structural Energy Bioscience Research Section)

We have theoretically investigated the binding of R12 and P16 as an important example of the new type of molecular recognition accompanying a global structural change of a molecule upon binding to its targets. Changes in thermodynamic quantities upon binding are calculated using the molecular mechanics, hybrid method in which the angle-dependent integral equation theory is combined with the morphometric approach, and 3-dimensional reference interaction site model theory. Molecular models are employed for water.

The energy decrease due to the gain of R12-P16 attractive (i.e., van der Waals and electrostatic) interactions is almost cancelled out by the energy increase originating from the energetic dehydration effect (i.e., by the energy increase caused by the loss of R12-water and P16-water attractive interactions plus the energy lowering arising from the structural reorganization of water). The binding is driven by the water-entropy gain that predominates over the conformational-entropy loss upon the global structural change of P16. The water-entropy gain originates primarily from the overlap of excluded volumes of R12 and P16 followed by the increase in the total volume available to the translational displacement of water molecules in the system by the overlapped volume. Here, the excluded volume is the volume of the space which the centers of water molecules cannot enter. It is important to assure the gain of R12-P16 attractive interactions during the binding process though the gain itself is not a driving force. This is why stacking of flat moieties, specific hydrogen bonding, and electrostatic complementarity (i.e., contact of oppositely charged groups) are frequently observed in the complexes. Stacking of flat moieties leads to a gain of intermolecular van der Waals attractive interactions, and specific hydrogen bonding and electrostatic complementarity lead to gains of intermolecular electrostatic attractive interactions.

The geometric characteristics (overall shapes, sizes, and details of the polyatomic structures) of the solute molecules play crucially important roles in discussing the water-entropy gain. For instance, stacking of disc-shaped solutes brings a large decrease in the total excluded volume followed by a correspondingly large gain of the water entropy. The gain becomes larger as the solute size increases. These effects are enlarged when the interface atoms are closely packed. Further, it is obvious that the water-entropy gain becomes quite large when the shape complementarity occurs within the interface region. The most striking example is found in the lock-key binding. The induced-fit binding, in which the lock structure exhibits a slight structural change so as to acquire the shape complementarity, is also driven by a large gain of the water entropy.

When a solute molecule is not sufficiently large, the water-entropy gain is often incapable of surpassing the energetic dehydration and conformational-entropy effects with the result that the solute molecule takes a rather extended, flexible structure. Even for a large solute molecule like a protein, when its overall close packing is not achievable, only the portions that can closely be packed are preferentially packed: The other portions cannot participate in the close packing and therefore become disordered and flexible. (The water-entropy gain brought by such preferential close packing is considerably larger than that resulting from an overall loose packing.) These solute molecules can be referred to as “a soft molecule” and “a molecule possessing a soft portion”, respectively. By contrast, a solute molecule possessing a structure in which overall close packing of the constituent atoms is successfully achieved is “rigid” because even a slight change of its structure gives rise to an unacceptably significant loss of the water entropy. It is possible even for a soft molecule or a soft portion of a molecule to construct a structure with overall close packing if the construction is made in concert with another molecule as a partner. In particular, when the partner is rigid, the soft molecule or the soft portion may bind to the partner by changing its structure in accordance with the partner structure, leading to the formation of a stable complex. Of course, there are not significantly many partners realizing such formation: Only those which can realize it is successfully recognized.



T. Hayashi, H. Oshima, T. Mashima, T. Nagata, M. Katahira, and M. Kinoshita, Nucleic Acids Res. **42**, 6861 (2014): Impact Factor=8.81.

This has been chosen by “Faculty of 1000 Biology” as one of the most important articles in biology.

3-2. RESEARCH ACTIVITIES IN 2014

Quantum Radiation Energy Research Section

H. Ohgaki, Professor
T. Kii, Associate Professor
H. Zen, Assistant Professor
(T. Hori, Specially Appointed Professor)
(K. Miura, Specially Appointed Professor)
(Izuru Daito, Researcher)
(Janewit Wannapeera, 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 energy recovering system, 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 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 5 to 20 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 this fiscal year, we have achieved FEL lasing with photo-electron beam generated from LaB_6 cathode. Further study will be conducted in the next fiscal year.

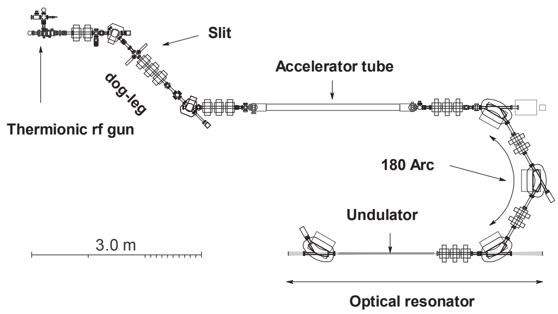


Fig. 1 Schematic drawing of the KU-FEL

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. A mid-infrared (MIR) pulse laser is suggested as a tool for MSPE. To demonstrate MSPE, anti-Stokes Raman scattering spectroscopy was applied on a silicon carbid. However, the S/N ratio of the observed signal was very low. Therefore, it is required to enhance the S/N ratio for precise measurement. To enhance the S/N ration of the observed signal, the introduction of a pico-second laser was planned. By using the pico-second laser, the noise in signal will be reduced. It induces the enhancement of S/N ratio. In addition, the investigation of the decay time of a particular phonon mode excited by MSPE will be available by pump-probe experiment with pico-second laser. By using the new equipment, further investigation of MSPE will be conducted in next year.

2.3 Compact seeded THz-FEL Amplifier

We are developing a new compact terahertz radiation source located in the same accelerator room with KU-FEL. The new system consist of a 1.6 cell BNL type photocathode RF-gun, a focusing solenoid magnet, a 4-dipole magnetic chicane bunch compressor, a triplet quadrupole magnet and a planar Halbach type undulator, a photocahode laser system and a seeded laser system. The target wavelength is from 400 to 800 μm. The system is designed to be simple, economic and compact with the total length less than 5 m. Schematic view of the proposed system is shown in fig 3.

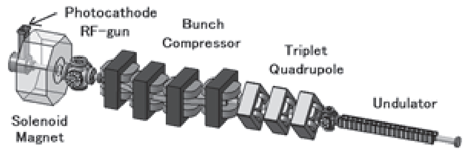


Fig. 3 Schematic view of the compact seeded THz-FEL amplifier.

In the first stage of the development, we will operate and investigate the performances of the system by without the seeded lasers. The photocathode RF-gun is driven by 10 MW klystron, which is commonly used with KU-FEL, and provides the beam energy about 5.5 MeV. The magnetic chicane compress the electron bunch until the final bunch length is in a picosecond order. The triplet quadrupoles are used for matching the beam profile respected to the undulator focusing characteristic. The ultra-short and high brightness beams are injected to the short undulator with the number of periods of 10 and the period length of 7 cm. The undulator generate a high power THz radiation by a "Coherent Synchrotron Radiation" process. We expect to complete the construction and start the commissioning of the first stage system in 2016.

3. Bulk HTSC Staggered Array Undulator

An undulator or a wiggler with strong magnetic field will play an important role in future synchrotron light sources and free electron lasers. We proposed the bulk high critical temperature superconductor staggered array undulator (Bulk HTSC SAU) in order to generate a strong periodic field. The Bulk HTSC SAU consists of stacked bulk high-Tc superconductors (HTSs) and a solenoid magnet which is used to magnetize the bulk HTSs as shown in fig.4. We have constructed the prototype of the undulator which consists of 12 pieces of GdBaCuO bulk superconductor and a superconducting solenoid. At the condition of λ_u = 10 mm, gap = 4 mm, and $T_{operation}$ = 6 K, the undulator field B_0 of 0.85 T have been achieved. The demonstrated field strength is stronger than the limit of the conventional undulator using permanent magnet.

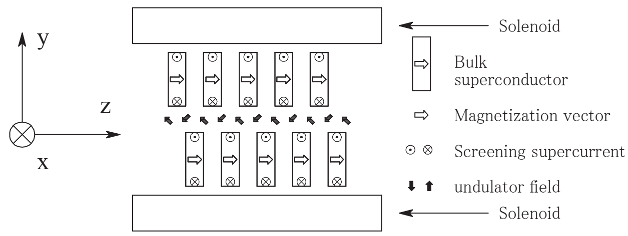


Fig. 4 Conceptual drawing of the bulk HTSC SAU and generation principle of the periodic undulator field using an induced current.

4. Non-destructive Isotope Detection using NRF

A Nuclear Resonance Fluorescence (NRF) measurement is a powerful tool for investigation not only of the nuclear physics, but also of isotope detection for the nuclear security such as the detection of special nuclear materials (SNMs) hidden in the ship cargo. We have developed the standard Monte Carlo code, GEANT4, for a radiation detection system to take into account the physical process of the NRF and successfully reproduced experimental data of ^{238}U target. By using developed code, we carried out a large scale simulation for the cargo screening system by NRF method. Figure 5 shows an example of energy spectrum from the scintillation detector array of the nondestructive detection system of ^{238}U hidden in the 20' cargo container.

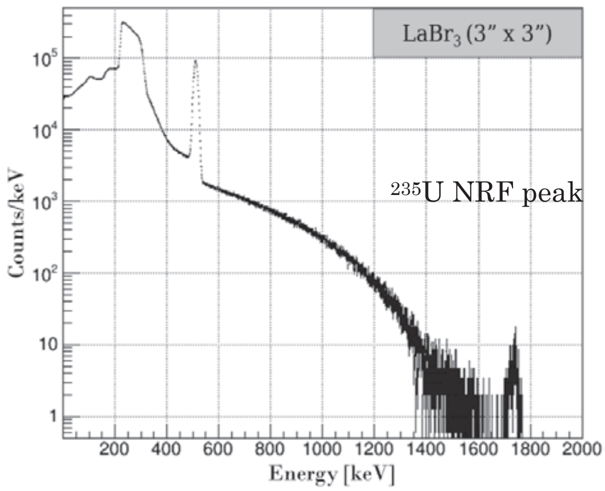


Fig. 5 Simulated energy spectrum from the 3"x3" $LaBr_3$(Ce) scintillator array detector.

Acknowledgment

These works were partially supported by the Grant-in-Aid for Scientific Research B, the Grant-in-Aid for challenging Exploratory Research by MEXT, Strategic Funds for the Promotion of Science and Technology, Kyoto University Global COE program, Collaboration Program of the Laboratory for Complex Energy Processes, IAE, Kyoto University and Grant-in-Aid for JSPS Fellows Grant Number 254954.

Collaboration Works

日本原子力研究開発機構量子ビーム応用研究部門，レーザー逆コンプトンガンマ線による模擬核物質探査実験，大垣英明

兵庫県立大学高度産業科学技術研究所，LSC ガンマ線を用いた核共鳴蛍光の研究，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，射出方向・エネルギー・エネルギー広がり可変の高輝度Ｘ線・ガンマ線ビーム発生法

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

吉田恭平，特別研究員奨励費，中赤外自由電子レーザーによる選択的格子振動励起の検証と電子状態への影響

2. Others

大垣英明，研究拠点形成費等補助金（博士課程教育リーディングプログラム），京都大学大学院思修館

大垣英明，政府開発援助ユネスコ活動費補助金，ミャンマーにおける持続可能な発展のためのエネルギー科学教育の推進

大垣英明，先導的創造科学技術開発費補助金，安全・安心な社会のための犯罪・テロ対策技術等実用化プログラムガンマ線による核物質非破壊検知システム

大垣英明，大学等連携支援事業（高エネ事業），光陰極高周波電子銃を用いた THz-FEL 開発とこれによる大学院学生の加速器教育

紀井俊輝，研究大学強化促進費補助金（SPIRITS），軌道角運動量をもつ自由電子とヘリカル磁場を用いた新しい物性研究手法の開拓

三浦孝一，（独）科学技術振興機構，低品位炭とバイオマスのタイ国におけるクリーンで効率的な利用法を目指した溶剤改質法の開発

三浦孝一，（独）国際協力機構，低品位炭とバイオマスのタイ国におけるクリーンで効率的な利用法を目指した溶剤改質法の開発プロジェクト

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Advanced Atomic Energy Research Section

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

1. Introduction

Future energy could not be discussed without zero-emission sources such as renewables. 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 generation, but also consideration on conversion and utilization systems. The attractiveness of the total energy system was evaluated by the socio-economic analysis, and their features in the 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 in 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 endo-thermic reaction to generate hydrogen and liquid fuel,
(4) Design and analysis of DC microgrid system for zero-emission electricity system,
(5) Development of compact neutron beam using newly developed cylindrical discharge device,
(6) Analysis of radioactive impact of nuclides from fusion plants, and
(7) Materials R&D for the above-mentioned issues.

2. High-performance divertor system design for advanced fusion reactor

Target surface of divertor of fusion reactor takes high heat flux from plasma, high energy particles and radiation. In the case of ITER divertor, assumed heat flux to the target surface is postulated to be average of 10 MW/m^2, and peak of 20 MW/m^2 as design criteria. However, transient high heat flux with 100 MW/m^2 order is anticipated to the target surface at a few milliseconds intervals by edge localized modes (ELMs). Tungsten is expected to minimize sputtering damage due to tungsten's higher sputtering threshold energy compared to that of carbon, as well as good heat tolerance. This study considers transient response of plasma facing materials (PFMs) of divertor particularly tungsten. Although the averaged heat load may not exceed the design criteria, ELMs could cause melting, recrystallization, thermal stress and thermal fatigue in localized area of tungsten armor, and they lead to the fracture of tungsten armor. The heat-structural response of divertor under dynamic heat load like ELMs was analyzed and evaluated by Finite Element Method (FEM) code.

When 100 MW/m^2–10 ms of heat flux was applied, the maximum temperature and temperature fluctuation on tungsten surface could be reduced by introduction of composite enhanced with carbon fiber. Amplitude of temperature fluctuation of tungsten surface depends on thermal conductivity of the divertor target material. With the thermal conductivity of 415 W/mK that is possible with composite, temperature fluctuation on tungsten surface could be controlled. Temperature gradient of tungsten armor causes thermal stress of tungsten, and the analytical results suggest that would exceeds the allowable limit. Thickness of tungsten armor is required to be reduced within 0.6 mm, when 100 MW/m^2–10 ms of heat flux is applied in order to avoid such a stress due to the temperature gradient.

[H. Gwon, Y. Takeuchi, R. Kasada, S. Konishi, Fusion Engineering and Design 89 (2014) 1003-1008.]

3. Compatibility of Ni and F82H with liquid Pb-Li under rotating flow

The present study reports the compatibility of a reduced-activation ferritic steel F82H and Ni with liquid Pb–Li under rotating flow conditions at 600 °C. Cross-sectional observation of Ni using field emission electron probe micro-analyzer (FE-EPMA) after exposure for 100 h revealed that severe grain boundary penetration of Pb into Ni occurred up to approximately a depth of 700 µm, causing liquid metal embrittlement (LME). In contrast, the results for F82H after exposure for 500 h showed the formation of pitting holes and a

Cr-depleted layer at the surface with an approximate maximum depth of 10 μm. Oxide particles were also found in the Pb–Li region in the F82H specimen after exposure. The radio-frequency glow discharge spectrometers successfully detected Li and indicated Li oxide formation at the surface.

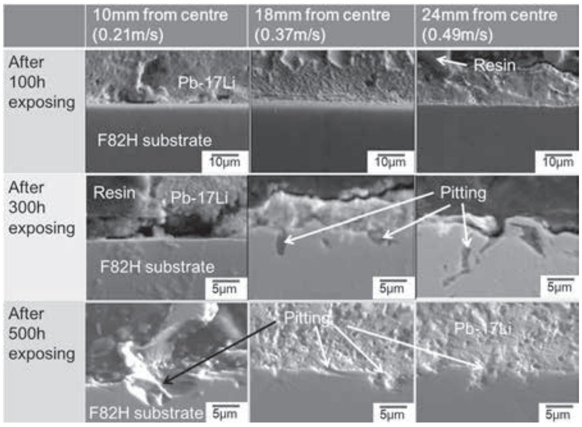

Fig. 1 Cross-sectional SEM images of F82H after immersing in Pb-Li at 600C for 100, 300, and 500 hrs.

[A. Kanai, C. Park, K. Noborio, R. Kasada, S. Konishi, T. Hirose, T. Nozawa, H. Tanigawa, Fusion Engineering and Design 89 (2014) 1653-1657.]

4. Underwater explosive welding of tungsten to reduced-activation ferritic steel F82H

The present study reports the underwater explosive welding of commercial pure tungsten onto the surface of a reduced-activation ferritic steel F82H plate. Cross-sectional observation revealed the formation of a wave-like interface, consisting of a thin mixed layer of W and F82H. The results of nanoindentation hardness testing identified a gradual progressive change in the interface, with no hardened or brittle layer being observed. Small punch tests on the welded specimens resulted in cracking at the center of the tungsten, followed by crack propagation toward both the tungsten surface and the tungsten/steel interface.

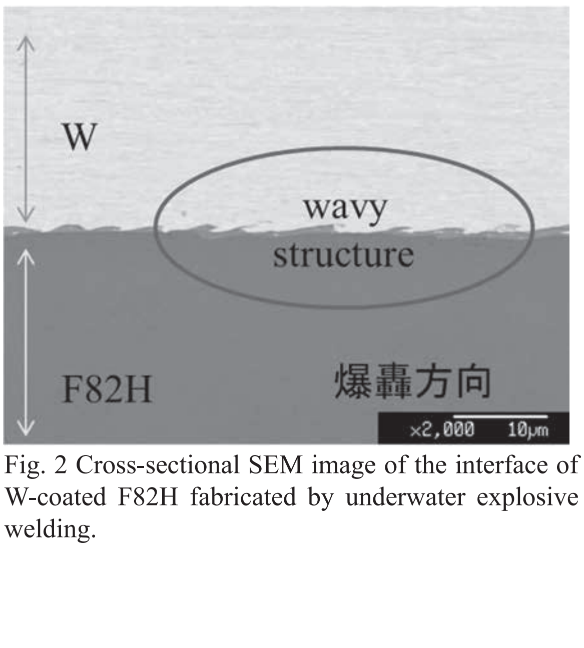

Fig. 2 Cross-sectional SEM image of the interface of W-coated F82H fabricated by underwater explosive welding.

[D. Mori, R. Kasada, S. Konishi, Y. Morizono, K. Hokamoto, Fusion Engineering and Design 89 (2014) 1086-1090.]

5. Nanoindentation hardness of reduced-activation ferritic steel after ion-irradiation

The ion-irradiation techniques using MeV self-ion (ex. Fe ion for steels) beam are of great use in experimentally simulating neutron irradiation environment in fusion reactors as well as in advanced fission systems because of their advantages: the high damage rate, no induced-radioactivity, widely controllable irradiation conditions, and co-implantation with helium and/or hydrogen. To investigate the mechanical properties of ion-irradiated materials, nanoindentation has been used to measure the hardness of materials in the surface up to a few micro-meters since the pioneer works of nanoindentation methodology. However it has been believed that the nanoindentation hardness of ion-irradiated materials has difficulty to be compared with the bulk mechanical properties including Vickers hardness of the neutron-irradiated materials.

Kasada suggested a useful model to evaluate bulk-equivalent hardness for the ion-irradiated materials. The newly developed model is based on a combination of the Nix–Gao model for the indentation size effect (ISE) and a composite hardness model for the softer substrate effect (SSE) of the non-irradiated region beyond the irradiation range. The model was successfully applied not only for the simple model alloys but also for the F82H reduced-activation ferritic steels. However the damage-gradient effect (DGE) due to the damage profile in these ion-irradiated materials is not considered in the model. The present study investigated the irradiation hardening behavior of F82H reduced-activation ferritic steels after MeV Fe-ion beam irradiation experiments followed by a nanoindentation test. Two sets of ion-irradiation experiments were conducted at 270 °C with 10.5 MeV Fe^{3+} ions up to 5 dpa at a 1000 nm depth at TIARA facility and at 290 °C with 6.4 MeV Fe^{3+} ions up to 3 dpa at a 600 nm depth at DuET facility, respectively. The measured nanoindentation hardness was converted to the depth-dependent bulk-equivalent hardness based on the new model to explain the indentation size effect and the film/substrate model to explain the damage gradient effect in the ion-irradiated region and softer substrate effect of the non-irradiated region beyond the irradiated depth range.

[R. Kasada, S. Konishi, K. Yabuuchi, S. Nogami, M. Ando, D. Hamaguchi, H. Tanigawa, Fusion Engineering and Design 89 (2014) 1637-1641.]

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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. Zero-dimensional model analysis of NBI plasma start-up with an assistance of 2.45 GHz microwaves

In stellarator/heliotron devices, plasma start-up using neutral beam injection (NBI) has been proposed to extend the operational range of magnetic field strength, which is useful for high β and toroidal magnetic field scaling experiments. In the Heliotron J device, plasma start-up by NBI has been realized with the assistance of non-resonant 2.45 GHz microwaves. The 2.45 GHz microwaves produce a seed plasma which is effective for ionizing the neutral beams. The high density plasma is built up after starting the NBI heating with an additional gas puff. This scheme is strongly dependent on the seed plasma condition and the timing of additional gas puff. The dependence of the electron density built up on the seed electron density is plotted in figure 1 as blue circles, which indicates the threshold of seed plasma density around 1–3 $\times 10^{17}$ m^{-3} for high-density plasma production in Heliotron J.

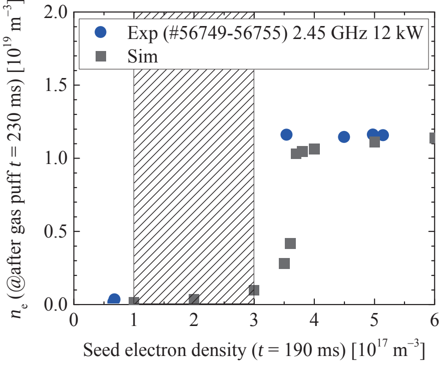

Fig. 1 Dependence of electron density after gas puff on seed electron density.

A zero-dimensional (0-D) model was developed to investigate the physical processes of the NBI plasma start-up in Heliotron J. The 0-D model comprises of four sets of time dependent equation: equations for fast hydrogen ion density, equations for bulk ion density (hydrogen and deuterium), energy density equations for electrons and ions, and equations for neutral atom density (hydrogen and deuterium). The results of the model calculation are also shown in Fig. 1 as red closed squares, which successfully reproduce the threshold of seed plasma density and agree well with the experimental results. The 0-D model analysis clarified that fast hydrogen ion density remains low due to insufficient beam ionization in the case of low seed plasma density ($n_e = 2.0 \times 10^{17}$ m^{-3}), resulting in unsuccessful plasma start-up. On the other hand, in the case of successful plasma start up, fast ions are produced enough and heat the plasma through the Coulomb collision. This leads to the increase in electrons contributing to the ionization process. In order for successful plasma start-up, electron temperature is required to be high enough to ionize the additional gas puff.

3. Pulsed operation of glow-discharge-driven inertial electrostatic confinement fusion device

Inertial Electrostatic Confinement (IEC) fusion is recognized as a useful scheme of neutron source. While most of IEC devices have been operated using DC power supplies, pulsed IEC neutron source are being developed to extend their application. One of the urgent applications using the pulsed IEC devices is active interrogation of U-235 to block smuggling. An issue to be coped with in pulsing the neutron yield in an IEC is that, in an earlier work, the rise in glow-discharge current was seen to be delayed considerably. It is important to study the delay time dependence on operating parameters for designing pulse forming circuits for IEC.

In this study, we experimentally investigated the dependence of the delay time on operating gas pressure and applied voltage. We then examined a method to reduce the pulse rise time by modifying the pulse

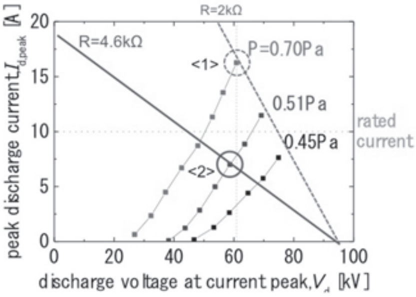

Fig.2 I-V curves of glow discharge at different gas condition.

forming circuit. Figure 2 shows the operating points of pulsed IEC device which are determined by an intersection point between a line given by the external circuit and an I-V curve for glow discharge. The delay time at <1>-point is the shortest in this study because of the highest operating gas pressure and applied voltage, but the pulse discharge current is higher than the rated current of pulse generator in this system. By changing the current-limiting resistance R from 2 kΩ to 4.6 kΩ, it is expected that the discharge current can be suppressed at the same discharge voltage (point <2>), and higher voltage operation can be expected.

4. Numerical Study about 0 Mode in Photocathode RF Gun

As repetition frequency of the laser pulse to drive a photocathode has been recently improved, the photocathode RF gun is considered to be utilized as an electron source for Free Electron Lasers. One of the concerns in such RF guns is 0 mode excitation caused by beam-loading, which leads to the degradation of beam properties.

A new equivalent circuit (Fig. 3) model, which takes the beam-loading effect into account and can describe 0 mode excitation, has been developed in this study. This consists of power source and GLC resonance circuit of π mode and 0 mode. The contribution of beam-loading is described as a current source (beam-loading current) and it has influences on voltages of both modes. The circuit constants are based on an eigenmode analysis and experimental result. The voltage of π mode and calculated voltage of 0 mode are obtained by solving circuit equation. The beam-loading current and beam properties are simulated by a 2-D particle-in-cell simulation code, KUBLAI. Then, the voltage of 0 mode is obtained again using the calculated beam-loading current. This process is iterated until the voltage of 0 mode is converged.

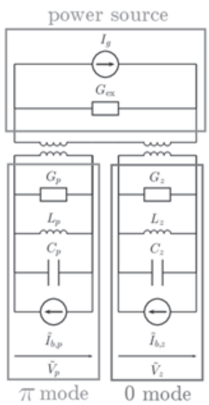

Fig. 3 Equivalent circuit.

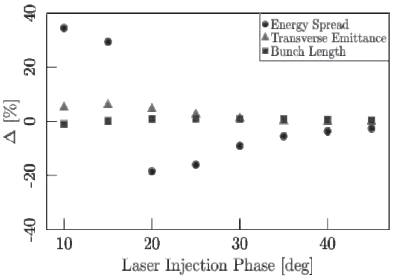

Fig.4 Influence of 0 mode on beam properties.

Figure 4 shows the simulation result of beam property degradation by the 0 mode, for energy spread, emittance, and bunch length. This figure suggests that the influence on beam properties is acceptable in practical use. .

5. Study of isotope effect on local turbulence in Heliotron J

Isotope effects on plasma confinement is an urgent issue in the study of magnetic confinement fusion. One of the hypothesis to explain the effects is that zonal flows driven by turbulence suppress the turbulence and improves the confinement in deuterium plasmas. An experiment to investigate isotope effects has been conducted in Heliotron J by changing the hydrogen and deuterium (H/D) ratio shot by shot. Two Langmuir probes at different toroidal sections, #8.5 section and #11.5 section, are utilized to measure measured floating potential of the edge plasma.

Figure 5 (a) and (b) shows the wave number spectra in different H/D ratio at each section. No clear difference is observed at #8.5 section, while the wave number increases at #11.5 section as the H/D ratio increase. The scale size of local turbulence should be proportional to ion mass, and hence this observation is not simply explained by conventional theory. One of the possibilities is that the three-dimensional magnetic structure has influence on turbulence and zonal flow in Heliotron J, and another is toroidal asymmetry of fueling or wall-recycling although further analyses are required. In any cases, this result indicates multi point measurement are indispensable to study isotope effect on turbulence and zonal flow, especially in helical devices.

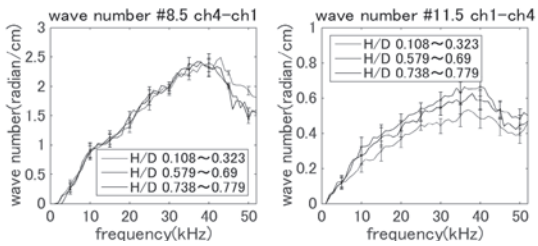

Fig.5 Wave number spectra at (a) #8.5 and (b) #11.5 sections.

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，佐野史道，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、佐野史道

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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、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、佐野史道、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、佐野史道

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核融合科学研究所, ヘリオトロンJ装置における機械振動自己補正型干渉計の設計検討，水内亨、大島慎介、岡田浩之、佐野史道、門信一郎、長﨑百伸、小林進二、南貴司

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Financial Support

1. Grant-in-Aid for Scientific Research

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2. Others

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Advanced Plasma Energy Research Section

T. Mizuuchi Professor
T. Minami, Associate Professor
S. Kobayashi, Assistant Professor

1. Introduction

The objectives of the advanced plasma energy section are to study the nuclear fusion physics of high temperature plasmas in order to control and improve the plasma energy confinement. The experimental and theoretical investigations for the optimization of the helical-axis heliotron configuration are in progress under the collaboration with universities/institutes under the auspices of the Collaborative Program of the Complex Energy Processes on IAE, and the Collaborative Research Program of NIFS (National Institute for Fusion Science).

In FY2014, following remarkable achievements (1) Electron internal transport barrier (eITB) is successfully formed on the Heliotron J plasma and (2) observation of poloidal flow reversal due to additional heating of electron cyclotron resonance heating (ECH) in Heliotron J were accomplished in the Heliotron J experimental study.

2. Electron internal transport barrier formation on Heliotron J

The eITB of helical devices plays an important role on plasma confinement. This barrier is known to be formed due to the radial electric field and the electric field shear is created by the bifurcation of radial electric field with the electron cyclotron (EC) heating. The transition is caused by the 'electron-root' solution of the ambipolarity condition for the radial electric field. Recently, the phenomena that have similar characteristics as the eITB have been observed on Heliotron J.

Figure 1 shows a typical electron temperature and density profile that has eITB. The profiles are measured with the Nd:YAG Thomson scattering system. The plasma is heated by the EC of ~330kW and $N_{//}$=0.0. The resonance zone of the EC is precisely located at the plasma center. When the line averaged density is smaller than the threshold value of ~1.2x10^{19}m^{-3}, the steep electron temperature gradient has been observed in the core region (r/a<0.3). In contrast, when the line averaged density is larger than the threshold value, the plasma has no steep gradient. The temperature gradient in the outside of the core region in both profiles has the almost same value. The result shows the possibility of the transport improvement in the core region by the EC heating.

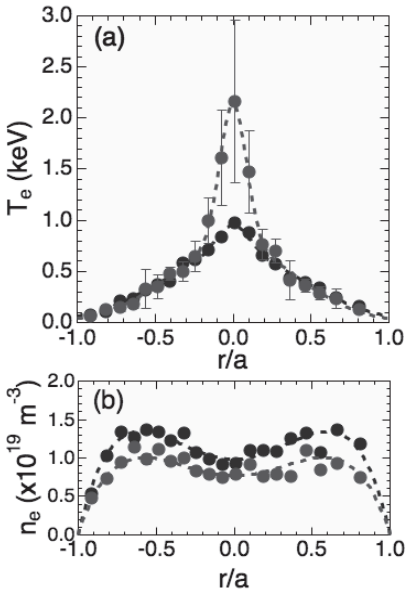

Fig. 1 Typical electron temperature (a) and density (b) profiles with and without the eITB. The plasma density is slightly different in both plasmas. The profiles are measured with Nd:YAG Thomson scattering system.

Comparative study of the phenomena is carried out between CHS and Heliotron J. Figure 2 shows the density dependence on the temperature gradient in the core region and on the outside of the core [1]. In both plasmas, when the line averaged density is lower than the threshold value, the temperature gradient in the core region increases, though the temperature gradient in the outside region maintains almost the same value. The similarity of the density dependence in both experiments suggests the possibility of the same barrier formation in Heliotron J plasma as CHS plasma. However, the threshold value is different between both plasmas. In CHS, the threshold value is ~ 0.5 x10^{19}m^{-3}, which is smaller than the Heliotron J value.

There are two possibilities of the cause of the threshold value difference. One possibility is that the magnetic configuration is different between Heliotron J and CHS. The other possibility is that the heating power is different for both experiments. In CHS experiment, the injected EC power is 130kW – 150kW. Both factors affect to the electron root transition of the radial electric field, which is related to the barrier formation. However, the further study is required to clear which factors are important to the threshold value difference.

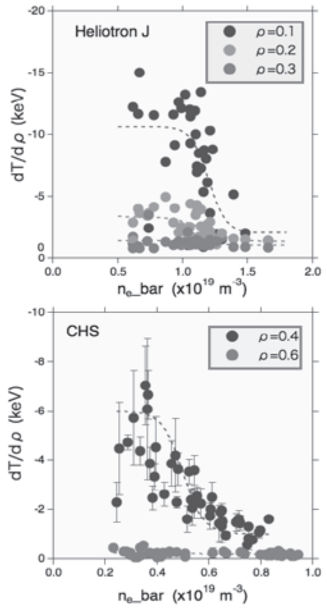

Fig. 2 Density dependence on the temperature gradient in the core region and the outside of the steep temperature gradient for Heliotron J and CHS plasmas.

3. Observation of the poloidal flow reversal in ECH plasmas of Heliotron J [2]

It is important subject to measure the radial structure of toroidal/poloidal flow velocity and to evaluate the radial electric field, since the radial electric field sear has been recognized to contribute an improvement of plasma confinement such as internal transport barrier or high confinement mode. Recently, a new Charge-eXchange Recombination Spectroscopy (CXRS) system has been installed to measure the poloidal flow velocity. In this section, we present the results of the radial profile and the time evolution of the poloidal flow velocity of carbon impurity ion.

Figure 3(a) and 3(b) show the time evolutions of line averaged electron density ($\bar{n}_e$) and stored energy (W_p) in the Neutral Beam Injection (NBI) plasmas (ctr-injection, P_{NBI}=400 kW) with and without the additional heating by ECH (P_{ECH}=331 kW, $N_{//}$=0.4). The time evolutions and the radial profiles of poloidal flow velocity (v_θ) are shown in Figure X(c) and X(d), respectively. In this experiment, the time resolutions of the poloidal CXRS was 10 ms. The poloidal flow near the plasma core is changed from the electron diamagnetic direction to the ion diamagnetic direction when the additional (2nd) ECH is applied to the NBI plasma. In this case, the electron temperature increases up to 1.5 keV with significant increase in the temperature gradient in the core region. The electron density profile becomes hollow from a peaked shape when the 2nd ECH is turned on, while slightly decrease in the ion temperature profile is observed as seen in Figure 3(e)-3(g), respectively.

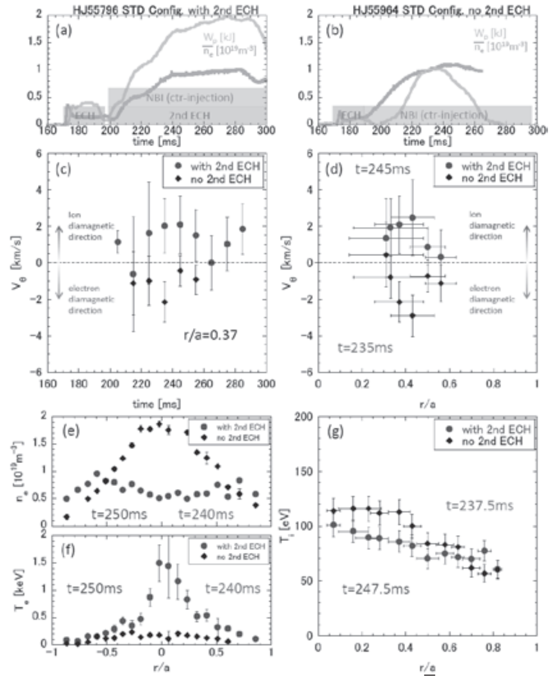

Fig. 3 (a) and (b); time evolutions of $\bar{n}_e$ and W_p in the case of with and without 2nd ECH plasmas. (c) and (d); time evolution and radial profile of $v\theta$, (e) and (f); radial profiles of electron density and temperature and (g) radial profile of ion temperature in the case of with and without 2nd ECH plasmas.

These phenomena indicate the change in the radial electric field from positive (ion root) to negative (electron root) by applying 2nd ECH. Neoclassical transport analysis is required to understand the phenomenon.

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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，佐野史道，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、佐野史道、水内亨、岡田浩之、南貴司、小林進二、山本聡

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Advanced Energy Research Section

Jia Qika, Foreign Visiting Professor
(National Synchrotron Radiation Laboratory, University of Science and Technology of China)

1. Summary

From April to June of 2014, as a guest professor I visited the Institute of Advanced Energy, Kyoto University. According the plan the cooperative studies on FELs especially on THz FEL have been carried out.

2. Activities in Institute of Advanced Energy

At the Institute of Advanced Energy, a new compact terahertz radiation source is under the development. It consist of a 1.6-cell S-band BNL-type photocathode RF-gun, a focusing solenoid magnet, a magnetic chicane bunch compressor, quadrupole magnets, and an undulator. By using an ultra-short electron pulse (the length of electron bunch is shorter than the radiation wavelength $\lambda_b<\lambda_s$) the system will generate the THz (100 to 300 μm) coherent radiation for scientific researches or industrial applications.

I studied the superradiant in 1-D theory and give the radiation power formula:

$$P_{sr} = (4\pi \frac{l_b}{\lambda_s} b_0)^2 \rho^3 P_e = (\frac{l_b}{\sqrt{3}L_c} b_0)^2 \rho P_e \quad (1)$$

where ρ is the FEL parameter, P_e is the power of electron beam, $b = \int e^{ik_s z} f(z)dz$ is the bunching factor, f is the electron density distribution. For a Gaussian distribution of electron pulse $b \approx \exp[-2\pi^2(\sigma_z/\lambda_s)^2]$, and a rectangle distribution, $b \approx \sin c(\pi l_b/\lambda_s)$.

The diffraction effect is investigated and the correction factor is given as follow

$$f_d = Arsh^2(x)/x^2 \quad (2)$$

where $x = \min(Z, l_b\lambda_u/\lambda_s)/Z_R$, λ_u is the period of undulator, Z_R is the Rayleigh length. The diffraction correction factor is shown in Fig.1.

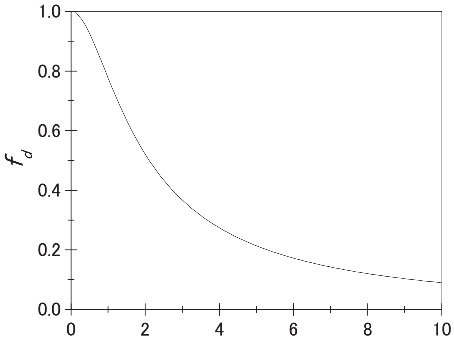

Fig.1 the diffraction correction factor

It is needed to check above result with the simulation, but the current simulation code such as Genesis can't simulate the radiation process of ultrashort election pulse. Therefore the check is made indirectly:

1), By using the same method, the diffraction effect is analyzed for the exponential gain, the result is compared with that from the diffraction correction on the gain length by Xie Ming's experience formula. They are in agreement when the Rayleigh length is smaller than the gain length (Fig.2).

2), The radiation power formula (Eq.1) is extended to including the pre-bunched e-beam ($\lambda_b>\lambda_s$) case:

$$P_{sr} = (4\pi \frac{b}{\lambda_s})^2 \rho^3 P_e \min{}^2(S, l_b)$$

$S<4L_c \quad (L_c = (\lambda_s/\lambda_u) L_g) \quad (3)$

where $S = \lambda_s z/\lambda_u$ is the slippage distance. Then the comparison with the simulation by using Genesis are made, it is shown that the result of the formula agree with that of the simulation in the initial stage (Fig 3).

In the cooperative studies on THz FEL, I also provide help to Mr. Suphakul Sikharin in his study on the design. The research work on the superradiant is still going on and to be studied in more depth.

I also have made an analysis for harmonic SASE(the liner harmonic generation case), a potential way for compact high gain FEL, and give the expressions for the gain length, the saturation power and the bandwidth, respectively:

$$L_{gn} \approx L_{g1} * (\frac{[JJ]_1^2}{n[JJ]_n^2})^{\frac{1}{3}} > L_{g1} \quad ,$$

$$\frac{P_{sn}}{P_{s1}} \sim (\frac{[JJ]_n^2}{n^2[JJ]_1^2})^{\frac{1}{3}} \quad ,$$

$$\frac{\Delta\lambda_{sn}}{\lambda_{sn}} \approx (\sqrt{n}\frac{[JJ]_n}{[JJ]_1})^{\frac{1}{3}}\frac{\Delta\lambda_{s1}}{n\lambda_{s1}}$$

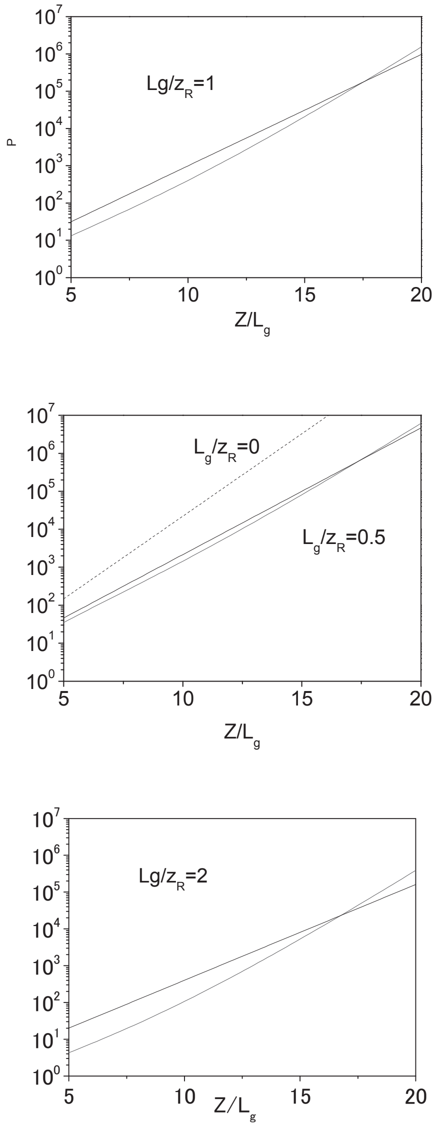

Fig.2. The diffraction effect on exponential gain for different ratio of gain length and Rayleigh length. The red line: our numerical result; The black line: the result from the diffraction correction on the gain length by Xie Ming's experience formula.

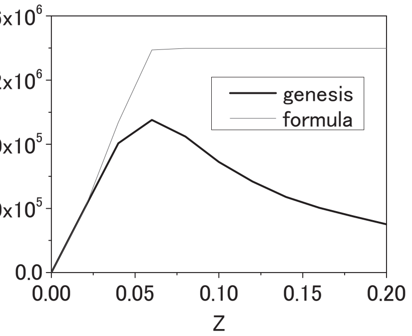

Fig.3 the radiation power of pre-bunched e- beam, $l_b \approx 4\lambda_s$, b_0=0.86. The red line: the result of the formula (3); The black line: the result of Genesis simulation.

Comparing with the nonliner harmonic generation case, the power of the liner harmonic generation is more large, the wave bandwidth is narrower than the fundamental, but the gain length of the harmonic is longer than the fundamental instead of shorter as in the nonliner harmonic generation case (Fig 4).

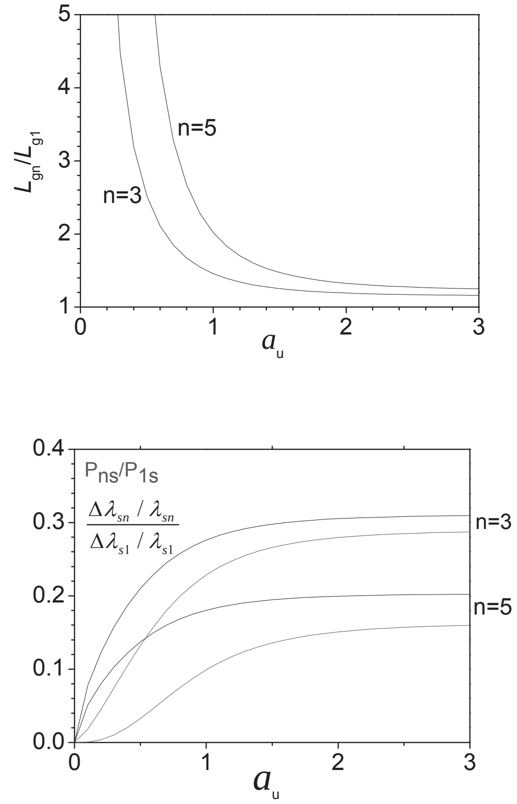

Fig.4, Gain length, the saturation power and the bandwidth of the liner harmonic with the undulator parameter.

Advanced Energy Research Section

Zhengying Cui, Foreign Visiting Researcher
(Professor in Southwestern Institute of Physics,
No 5, Huangjing Road, Shuangliu County,
Chengdu, Sichuan 610225, China)

1. Summary

The author spent three months (Nov. 1, 2014-Jan. 31, 2015) as a guest professor at the Uji campus of Kyoto University, hosted by the Heliotron J group.

Here the author reports about an investigation on edge impurity transport based on the visible spectroscopy in Heliotron J.

2. Introduction

The role of impurities played in magnetically confined fusion devices has been extensively studied so far, since the impurity strongly affects the performance of high-temperature plasmas through power balance and dilution of fuel ions. In particular, the edge impurity transport is extremely important because a quantitative understanding on the particle recycling and impurity source in the vicinity of first wall and divertor plates is necessary for the steady state operation of high-performance plasmas. On the other hand, the edge impurity transport in the tokamak configuration is generally dominated by the parallel transport, whereas both the parallel and cross-field transports become important in the stellarator configuration [1]. The edge impurity screening in the tokamak is much sensitive to the impurity source location [2]. Recent studies show that a strong screening effect appears with increasing density against the divertor impurity source but no screening effect appears for the impurity released from the first wall [3]. However, a strong impurity screening can be expected for impurity released from both divertor and first wall in LHD [2]. Therefore, it is interesting to investigate the edge impurity behaviour in the Heliotron J for comparison.

Since the charge state of impurities increases with electron temperature, impurity ions are distributed along radial locations according to the ionization energy, E_i. The line radiation from impurity ions in certain ionization state forms an emission contour as a function of the geometry of magnetic surfaces. The electron temperature in Heliotron J is generally higher with ECH than that with NBI heating. C^{2+} (E_i=48eV) and O^{4+} (E_i=114eV), which respect to CIII and OV line emission, are located in the SOL and near the last closed flux surface (LCFS), respectively. Based on the measurement of CIII (4647Å) and OV (2781Å) in the visible wavelength region the edge impurity transport can be studied with relation to different plasma performances in Heliotron J.

In general, the emissivity of the spectral line is expressed as follows:

$$I^{Z}\left(T_e, n_e\right) = n_e n_{\mathrm{imp}}^{Z}\ L^{Z}\left(T\right)\ , \qquad (1)$$

where n_e is the local electron density, n_{imp}^{Z} is the density of impurity ions with ionization state of Z and $L^z(T)$ is the emission coefficient. Since the emissivity of CIII (977Å) is almost constant against the temperature when $T_e \geq$ 10eV CIII/n_e can simply express its ion density behaviour [3]. So does OV if its emissivity is also not strongly dependent on T_e for the typical Heliotron J plasmas. The value of CIII/n_e and OV/n_e can be then used to characterize the edge impurity transport at Heliotron J.

3. Experimental observations

(1). Effect of magnetic configuration

In order to focus on the effect of magnetic configuration on CIII/n_e and OV/n_e the NBI heated plasmas are taken into account. The result is plotted in Fig. 1.

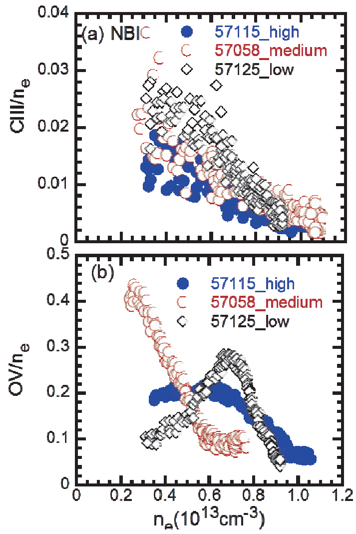

Fig. 1, Plot of (a) CIII/n_e and (b) OV/n_e as a function of n_e with different magnetic configurations.

In general, the density gradient along the magnetic field in the SOL region transfers impurity ions downstream to the low T_e region. A strong impurity screening effect can be expected when the electron density increases. The result shows that the n_e dependence of CIII/n_e and OV/n_e in the low ε_b magnetic configuration is quite different from other two cases. This may be caused by a significant shrinkage of plasma cross-section in the low ε_b case when compared to the high and medium ε_b cases. The result in Fig. 2(a) suggests that the impurity screening seems more efficient in the medium ε_b case than that in the high ε_b case if C^{2+} is located around the LCFS. In Fig. 2(b) for the low ε_b configuration, the increase of OV/n_e in the low n_e range of $n_e < 0.7\times10^{13}$cm^{-3} is mainly due to the fact that T_e is low. The effect of T_e on OV intensity is strong. Simulation with the local plasma parameters, such as the input power, T_e and n_e, the position of the LCFS and magnetic connection length is necessary to understand the density dependence of CIII/n_e and OV/n_e.

(2). Effect of heating regime

Since the temperature with NBI is generally lower than that with ECH, the OV/n_e sometimes is strongly affected by T_e at the beginning of discharge with NBI. Therefore, the value of OV/n_e in the discharge with NBI at the low n_e region is absent. A series of discharges have been checked in this study.

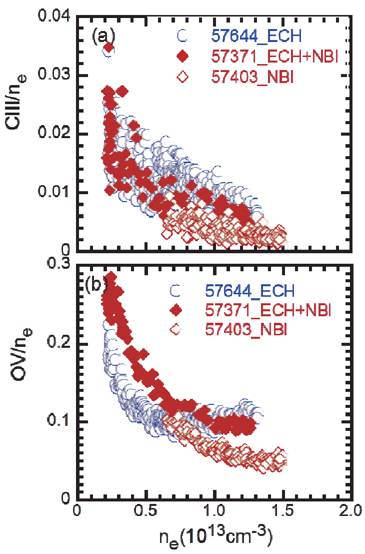

Fig. 2, Plot of (a) CIII/n_e and (b) OV/n_e as a function of n_e with different heating regimes.

For the ECH plasma T_e is high. Both CIII and OV are located near the LCFS. The result indicates that OV/n_e decreases quickly with ECH when n_e is low, shown in Fig. 2(b). This may suggest that a strong impurity screening appears with ECH. This could be caused by the increase of n_e at edge with the particle pump-out by ECH. When $n_e > 0.5\times10^{13}$cm^{-3} OV/n_e is saturated with ECH but it continuously decreases with NBI. The detail comparison of edge T_e and n_e between the ECH and NBI plasmas is necessary before making any solid conclusion. Asymmetric profile of T_e was sometimes observed with NBI heating. The effect of the local T_e and n_e on the CIII/n_e and OV/n_e should be taken into account. Plasma rotation with relation to different turbulent mode ITG or TEM could play a role on the edge impurity transport when the heating regime is different. The tendency of CIII/n_e and OV/n_e in the discharge with NBI heating is similar with that of ECH+NBI but it is different from that in the discharge with ECH only. Note also that the CIII/n_e with ECH is more scattering than that with NBI and ECH+NBI. The reason is unclear. Further study is needed.

(3). Effect of plasma isotope

In this study the plasmas with combined ECH and NBI heating are adopted.

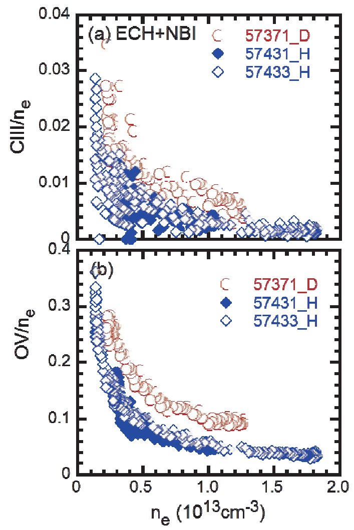

Fig. 3, Plot of (a) CIII/n_e and (b) OV/n_e as a function of n_e with relation to H and D plasmas.

A series of discharges were checked. The result indicates that the density dependence of CIII/n_e is similar in the H and D plasmas but OV/n_e decreases quickly with n_e in the H plasma than in the D plasma. The value of CIII/n_e and OV/n_e are obviously higher in the D plasma by a factor of 2 than in the H plasma. The careful check of the heating power as well as n_e and T_e at edge between the D and H plasma are necessary.

Edge impurity behaviour has been studied based on the visible spectroscopy in Heliotron J. Preliminary result showed that clear change of the edge impurity behavior can been observed with relation to the effect of magnetic configuration, heating regime and plasma isotope on CIII/n_e and OV/n_e. Simulation combined with plasma parameters is important to understand the observations. Other carbon line emissions, such as CIV, CV, CVI and the value of CIV/CIII, CV/CIV and (CVI+CVI)/(CIV+CIII) are needed also.

[1]. Feng Y. et al 2011 Plasma Phys. Control. Fusion **53** 024009

[2]. Kobayashi M. et al 2013 Nucl. Fusion **53** 033011

[3]. Cui Z. Y. et al 2014 Proc. 25th Int. Conf. on Fusion Energy

Advanced Energy Research Section

Pattrick Calderoni, Foreign Visiting Professor
(Technical Project Officer,
The European Joint Undertaking for ITER and the Development of Fusion Energy (F4E))

1. Summary

The overview of the study of the tritium recovery technology for fusion breeding blanket with liquid metal blanket is given. The author has jointly worked with the research team of the Advanced Atomic Energy Section and proposes an attractive technical option as the results of the collaboration for the European blanket concept for ITER/TBM and future DEMO. He also suggested the necessity of planning a concrete strategy for the blanket technology to experimentally evaluated its engineering feasibility toward the fusion energy, and emphasizes the validation of the performance of the blankets.

2. Introduction

The author, Dr. Calderoni have involved in the study of fusion breeding blanket based on liquid lead lithium (LiPb) breeder, and in particular the related tritium recovery process in the present responsibility in the Fusion for Energy in Barcelona. He stayed in the Institute of Advanced Energy from January to March of 2015 for three months, and jointly involved in the collaboration on the research of tritium recovery technology from liquid metal blankets. In our institute, dedicated liquid facilities are equipped and we have shown a successful proof of principle experiment of the newly developed innovative concept, Vacuum Sieve Tray. Under the collaboration, we have evaluated this process for feasibility and applicability to the Test Blanket Module Program for ITER (ITER/TBM) by Europe, and the future fusion DEMO concept, both based on liquid LiPb as breeder. Dr. Calderoni is managing design and research activities for the EU TBM program for the development of the Helium Cooled Lead Lithium (HCLL) and Helium Cooled Pebble Bed (HCPB) Test Blanket Systems for ITER. Main areas include:

- Design and supporting research activities for the HCLL and HCPB ancillary systems, specifically: Helium Cooling System (HCS), Coolant Purification System (CPS), Tritium Extraction System (TES) and liquid metal system (PbLi loop).
- Development of HCLL and HCPB TBS Instrumentation and Control system.
- Development of modelling tools for the design of solid and liquid metal fusion blanket.

He has further developed our concept and promoted our research and development from his expertise, while both of us expect it would also contribute to his professional development and to the mission of the F4E TBM project.

3. Tritium Extraction Process for European TBM

European party (EU) plan to install two types of TBMs for ITER, and the liquid option is Helium Cooled Lithium Lead (HCLL) concept. Figure 1 (a) and (b) respectively show the blanket structure and its supporting systems.

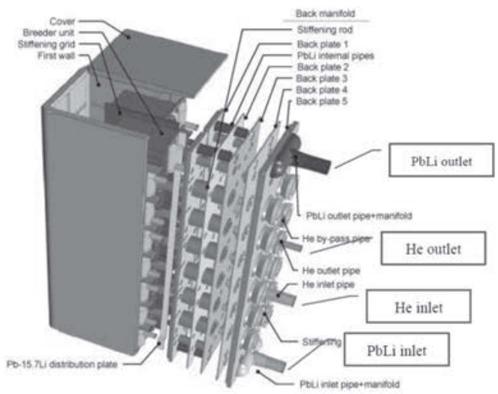

Fig. 1. (a) A schematic of the European HCLL TBM

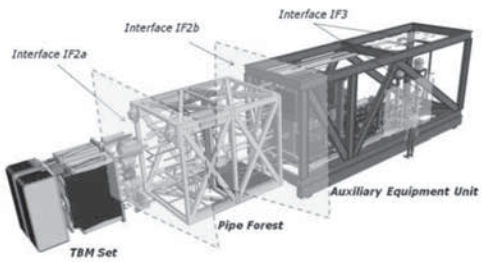

Fig. 1. (b) TBM system for HCLL.

Blanket module is a rectangular box with breeder filled in it. The HCLL uses liquid LiPb mostly for tritium breeding purpose, and generated tritium is transferred with the slow circulation. Nuclear heat is removed with high pressure helium. Because of the slow flow speed, MHD pressure drop due to the electromagnetic force is kept minimal. The TBM is backed with supporting systems for tritium recovery and heat transfer behind it, and installed in the Port Cell of the ITER tokamak. Both tritium and heat is removed from the closed loops and transferred to the ITER tritium plant and heat rejection system, respectively. Because of the function of the closed loop, required recovery efficiency is not extremely high, but the space limitation is critical.

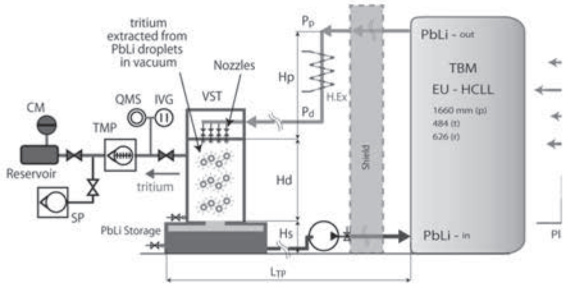

Fig. 2. Vacuum Sieve Tray for HCLL TBM

The design analysis of a tritium extraction system based on Vacuum Sieve Tray (VST) technology for the Helium Cooled Lithium Lead (HCLL) Test Blanket System for ITER was performed. Figure 2 shows the schematic of the HCLL TBM with VST. This is a process developed by the authors, and hydrogen isotope is released and recovered from the falling liquid PbLi droplets in a vacuum. The rate of this process is limited by the transport of hydrogen dissolved in the liquid metal droplet. We found that its mass transport coefficiency is approximately two orders of magnitude faster than that by static diffusion. Because of this enhancement of transport, tritium recovery efficiency expected to this process is extremely high with short free fall height of the droplets. This is the main advantages with respect to the reference design, gas-liquid contactor by EU. Because this process apply vacuum to the fresh surface of the metal droplets, avoiding surface recombination resistance due to the possible impurity effects by the ambient gas is another advantage. The analysis of the parametric dependence of the system efficiency from the main operative parameters of the PbLi loop (on which the component is mounted) as well as its main geometrical features, such as droplet size and number of nozzles, is considered. Typically, tritium production ratio is 0.6μg /s m^3 and flow speed of LiPb is 5.7 mm /s . Total inventory of the liquid LiPb is assumed to be 1.0 m^3, but strongly dependent on the process design, because majority of the volume is in the process piping.

The performance of the VST tritium extraction process was evaluated based on the previously measured diffusion coefficient of hydrogen in the droplets.

Figure 3 shows the estimated extraction efficiency as the function of the nozzle size. As seen in the figure, the efficiency is dependent on the diameter of the droplets, that is expressed as d_d in the following diffusion equation.

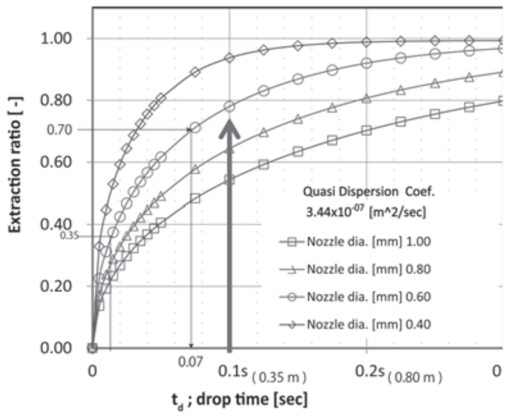

Fig. 3. Estimated extraction efficiency as the function of nozzle size for droplet formation.

$$\varepsilon = 1 - \frac{6}{\pi^2}\sum_{n=1}^{\infty}\frac{1}{n^2}\exp\left[\frac{-\mathbf{D}_{qua}\, n^2\pi^2 t_d}{\left(d_d/2\right)^2}\right]$$

The required extraction efficiency is approximately 0.7 that keeps tritium concentration within the closed loop within the acceptable inventory limit, while bred tritium can be returned to the plasma as the fuel. The size of the droplet is easy to control with the designated nozzle diameter.

Required height of free fall is 0.35m, that provides sufficient time of 0.1 second for tritium extraction from each droplets. The total head height is 1.1m for pumping LiPb, that is shorter than the height of TBM, and is expected to fit within the space limitation.

4. Conclusion and future plan

It is concluded that the VST developed by the Kyoto University is technically applicable for the European HCLL TBM for ITER, and resolve the present problem with the current reference design. This concept is also attractive for European DEMO design that requires better performance. The collaboration yielded a fruitful conceptual design, and further joint development will be planned based on the present results.

Advanced Energy Materials Research Section

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

1. Introduction

We are investigating the scientific principle and applications of new materials including nano-materials for advanced energy science. In Advanced Energy Material Research section, the physical properties of nano-carbon and atomically thin layered materials (carbon nanotube, and graphene) by advanced optical spectroscopy and compositional ceramics (SiC) materials by multi-scale experiments for the material properties (MUSTER) are studied. Followings are main research achievements in the year of 2014.

1. Drastic Improvement of Photovoltaic Performance of Carbon-nanotube Based Solar Cells using Metal Oxide Multifunctional Layers

Recently, photovoltaic devices using nanoscale materials, such as semiconductor quantum dots, nanowires and so on, have been extensively studied. Carbon nanotubes with cylinder-like, one-dimensional structures have attracted much interest for photovoltaic applications because of their electronic and optical properties, including the ability to tune their band gaps over a wide wavelength range, high carrier mobilities along their one-dimensional axes and high optical transparency values with low-resistivity. Indeed, a variety of photovoltaic devices using carbon nanotubes such as carbon nanotube-based organic solar cells, photoelectrochemical cells, dye-sensitized solar cells and carbon nanotube/Si solar cells have been reported. Furthermore, the importance of carbon nanotubes as photovoltaic materials is continually increasing. However, several crucial issues remain to be solved for further improvement of the carbon nanotube photovoltaic device performance and to enable the shift from the fundamental research to the technological applications development. First, a high Schottky barrier at the interface of the carbon nanotubes and the metal electrode limits the performance in carbon nanotubebased photovoltaic devices. Control of the Schottky barrier using an efficient carrier transport layer should enable the delivery of a high current without the carrier recombination loss. Second, more efficient carrier doping for the carbon nanotubes is required to reduce the series resistance loss and increase the power conversion efficiency. Third, solar light management within the device structure of the carbon nanotube solar cells is required to enhance the photocarrier generation efficiency.

We report on the improvement in the photovoltaic performance of the carbon nanotube-based solar cells containing environmentally friendly, durable and inexpensive MoO_x and ZnO metal oxide layers. The MoO_x and ZnO layers play multiple roles as antireflection, carrier doping and efficient carrier transport layers in the carbon nanotube-based solar cells. The photovoltaic performance of the single-walled carbon nanotube (SWNT)/Si hybrid solar cells is improved using these multifunctional MoO_x and ZnO layers, with high power conversion efficiencies (PCE) of 17.0 (Figure 1) and 4.0% achieved for *p*-SWNT/*n*-Si and *n*-SWNT/*p*-Si devices, respectively. The 17.0% PCE value is the highest yet reported for the PCE of *p*-SWNT and the 4.0% PCE value is also quite high compared to the *n*-SWNT hybrid solar cells reported in the literature.

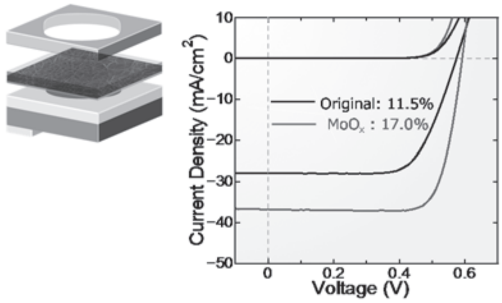

Figure 1: Photovoltaic performance of carbon nanotube solar cells using metal oxide layers.

2. Photocarrier Relaxation Pathway in Two-dimensional Semiconducting Transition Metal Dichalcogenides

Atomically thin transition-metal dichalcogenides (TMDs) have attracted a great deal of attention from the viewpoints of fundamental physics and various applications. TMDs have potential applications as novel two-dimensional direct-band gap semiconductors in various opto-electronic devices, such as low-electricity consumption transistors, light-emitting devices, and solar cells.

Individual layers of TMDs are excellent light absorbers despite being atomically thin. Absorption spectra of MX_2 (M=Mo, W and X=S, Se) consist of characteristic peaks due to excitonic resonance and interband transitions. Recent *ab initio* studies have attributed the strong light-matter interaction to "band nesting", which gives rise to singularity features in the joint density of states (JDOS). In the nesting region of the band structure, the conduction and valence bands are parallel to each other. The JDOS diverges for the resonance energy, resulting in giant enhancement in the corresponding optical conductivity. Since absorption is highly efficient in the resonance conditions, understanding the resulting photocarrier relaxation dynamics is crucial in implementing these materials into light-harvesting devices. Photocarriers generated in the band-nesting region are of particular interest as the electrons and holes are expected to relax at the same rate, but with opposite momentum.

We examined the relaxation processes of photoexcited carriers in mono- and bilayer MX_2 using photoluminescence excitation (PLE) spectroscopy and *ab initio* density functional theory (DFT) calculation. The giant absorption reaching several-tenth percentage was experimentally observed in the atomically thin monolayer MX_2, due to the characteristic band nesting. We showed that the relaxation channel of the photoexcited carriers is strongly dependent on the excitation energy by PLE, and the spontaneous electron-hole separation at the momentum space occurs in MX_2. Our findings reveal the unique implication of 2D band structure and the characteristic photocarrier relaxation.

3. Irradiation Effect on SiC

Silicon carbide (SiC) is one of very attractive engineering ceramics in particular for high temperature use and nuclear application due to high temperature strength, oxidation resistance, chemical stability, low activation, radiation resistance and so on. Silicon carbide composites have pseudo ductile behavior by debonding and sliding at fiber/matrix interphase. Fundamental mechanical properties of highly crystalline nuclear grade SiC composites are stable following neutron irradiation. Silicon carbide composites are promising materials for accident tolerant fuel. However highly crystalline nuclear grade SiC composites are different from high purity SiC like CVD SiC. Liquid phase sintered (LPS) SiC has highly crystalline microstructure. However it also has remained sintering additives as impurities. Those impurities are concerns in particular for corrosion behavior by high temperature water and high temperature steam.

No significant degradation of mechanical properties have been reported for high purity SiC/SiC composites reinforced with high purity fibers following neutron irradiation at up to 1300 °C. To evaluate irradiation effects in addition to neutron irradiation to obtain systematic data, ion irradiation was carried out on high purity SiC using the DuET facility, Kyoto University. It is possible to ion-irradiate at over 1500 °C with precise temperature control at the DuET facility. Swelling behavior and mechanical properties of constituents following irradiation are keys to estimate the performance of the composites under neutron irradiation. Ion irradiation effects on swelling behavior and mechanical properties of high purity SiC fabricated by CVD were evaluated up to 1600 °C.

Figure 2 shows the swelling of CVD SiC and LPS SiC at 3 dpa plotted as a function of irradiation temperature. Basically swelling behavior of SiC is affected by impurities. If the data includes various kinds of SiC, it causes large scattering of data. The material was selected to the high purity CVD SiC and the LPS SiC fabricated from the same batch. The LPS SiC was fabricated with the amount of 9w% of sintering additives. It should be reasonable to regard swelling values at 3 dpa as saturated ones, since the amount of swelling basically saturated at around 1 dpa above 200 °C. The amount of swelling was determined by means of a precision surface profilometry following irradiation through molybdenum meshes. One of the concerns for high temperature use of SiC under neutron irradiation was the large void swelling at more than 1000 °C. However the amount of swelling was very limited to low levels even at 1600 °C.

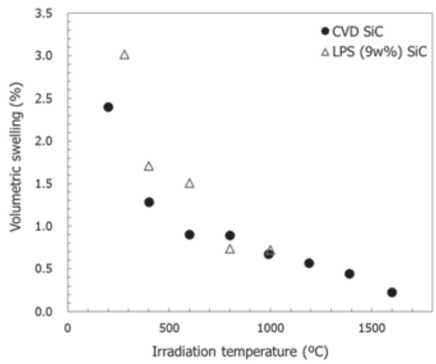

Figure 2: Irradiation effect on swelling of CVD- and LPS-SiC.

The LPS SiC shows relatively larger swelling than CVD SiC in particular for low temperature region. Even in that case, the LPS composites consisting with highly crystalline fibers and matrix showed stable mechanical properties following neutron irradiation due to reduct

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

Idaho National Laboratory（米国）、Idaho National Laboratory（米国）、Oak Ridge National Laboratory（米国）, Accident Tolerant Fuels for LWRs Research and Development（CNWG），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

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

Financial Support

1. Grant-in-Aid for Scientific Research

松田一成，新学術領域研究，ナノグラフェン・遷移金属カルコゲナイドにける新規光物性の開拓

松田一成，挑戦的萌芽研究，グラフェン量子ドットの創生と光電子変換機能の開拓

宮内雄平，若手研究（A），革新的光電デバイス応用に向けたカーボンナノチューブ量子多体効果の学理の開拓

毛利真一郎，基盤研究（C），単原子層物質の励起子光物性の解明とその制御

2. Others

松田一成，（財）キャノン財団，革新的光電変換機能をもつオールナノカーボン太陽電池の開発

松田一成，日立造船（株），CNT 太陽電池の開発
檜木達也，（株）東芝，安全性を追求した革新的炉心材料利用技術に関する研究開発＜試料の作製・検査およびイオン照射試験＞

檜木達也，（独）日本原子力研究開発機構, 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，（株）近畿レントゲン工業社，タングステン・SiC 繊維複合化技術によるフィラメントの開発

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Advanced Laser Science Research Section

T. Nakajima, Associate Professor
K. Hata, Assistant Professor

1. Introduction

The main objective of our research is to carry out the theoretical as well as experimental study on the various kinds of laser-matter interactions in a time-dependent manner so that the obtained knowledge and know-how can be applied to energy science. The laser wavelength can be in the mid-infrared, near-infrared, visible, ultraviolet, extreme ultraviolet, or even x-ray regions, while the target can be atoms/molecules, nanoparticles, thin films, etc.

2. Coherent population trapping in negatively charged self-assembled quantum dots using a train of femtosecond pulses

Quantum dot (QD) is often called "artificial atom", and many phenomena which have been realized in atoms can also be realized in QDs. One of the difficulties in QDs, however, is its inhomogeneity: None of them can be made exactly identical. This means that the realization of delicate nonlinear optical phenomena such as electromagnetically induced transparency (EIT) or coherent population tapping (CPT) in a single QD does not guarantee that the similar can be realized in an ensemble of QDs. In this work we have theoretically demonstrated CPT in a single as well as an ensemble of negatively charged QDs using a pulse train.

In Fig. 1(a), we depict the four-level QD system and the corresponding selection rules. Under the externally applied magnetic field in the Voigt geometry, the electron spin and trion states are split by the Zeeman frequencies. The linearly polarized transitions $|X\pm\rangle \leftrightarrow |T\pm\rangle$ are labeled as V and H. These transitions are referred as vertically (V) and horizontally (H) polarized with respect to the polarization axis of QDs. In Fig. 1(b) we show the change of coherence in an ensemble of QDs as a function of the number of irradiated pulses. Maximum coherence (~0.5) is established after ~25 pulses if the pulse area is $\Theta=\pi/5$, which means that coherent electron spin can be generated within 100ns. This is much shorter than the decoherence time (10μs) of QDs at the cryo-temperature, and it implies that the preparation of coherent electron spin described in this work may be applied for the quantum information processing.

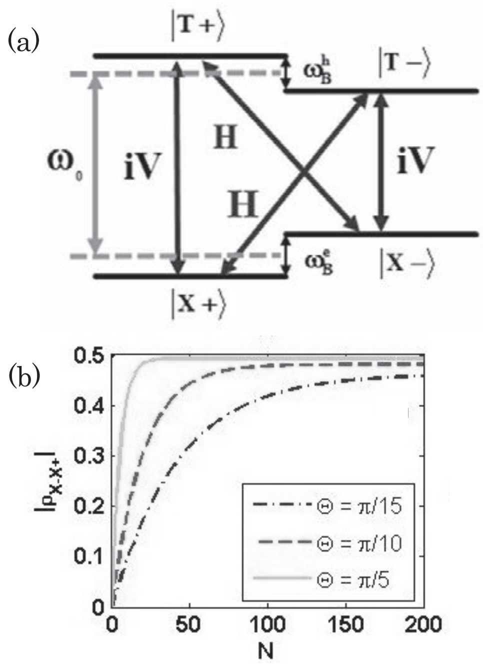

Fig. 1 (a) Four-level model of a negatively charged quantum dot and (b) accumulation of coherence in an ensemble of QDs for the different values of pulse area as a function of irradiated pulse number.

3. Detuning-induced stimulated Raman adiabatic passage in atoms with hyperfine structure

Coherence generated in a few-level system plays a very important role in many applications such as EIT, CPT, etc. In reality, however, it is not necessarily easy to find an appropriate scheme due to the presence of undesired fine as well as hyperfine structures, and to clarify the similarities as well as the differences between the ideal two-level (three-level) and quasi two-level (three-level) systems would be important. We have performed a study for quasi two-level systems (Fig. 2(a)) in terms of detuning-induced stimulated Raman adiabatic passage (D-STIRAP), a variant of ordinary STIRAP, which has many interesting applications in quantum optics and quantum computing. Attained coherence is plotted in Fig. 2(b) as a function of time. Although it cannot be the possible maximum value (0.5) due to the hyperfine structure we find that coherence can

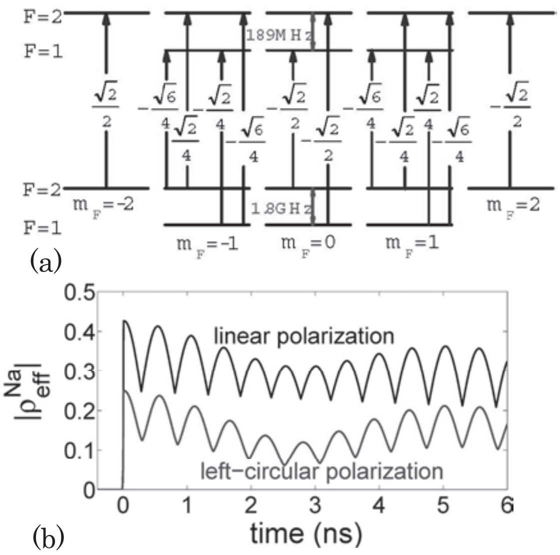

Fig. 2 (a) Scheme. (b) Time evolution of the degree of coherence for the linearly and circularly polarized pump pulse.

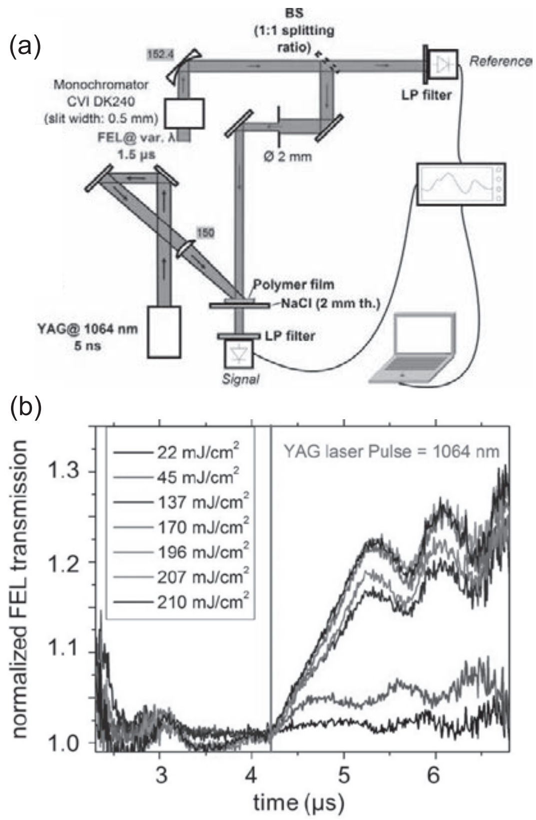

Fig. 3 (a) Experimental setup. (b) Temporal change of transmission of the FEL pulse at 13.7 μm as a function of YAG laser fluence.

still be quite high if a linearly polarized pulse is employed.

4. Observation of phase change in a dye-doped polyethylene film using KU-FEL

Some of the organic polymers have crystalline structures, while others have amorphous structures. For a crystalline organic polymer such as polyethylene it is known that some absorption lines are sensitive to its structure, and hence we can say whether it is in the crystalline or amorphous phase from the absorption spectra. We have carried out the time-resolved spectroscopy of a polyethylene (PE) film for the time-resolve detection of phase change from the initial crystalline to amorphous, and then back to the crystalline structure. The experimental setup is shown in Fig. 3(a). We prepare a dye-doped PE film by dropping dye(IR165)- and PE-dissolved dichlorobenzene solution onto a 2mm NaCl crystal (preheated to 100 degrees Celsius). The dye-doped PE film is irradiated by a single YAG laser pulse (5ns) with a sufficient fluence, and we probe the transmission change of the laser pulse at 13.7 μm from KU-FEL. The results are shown in Fig. 3(b). This demonstrates that we have successfully induced the structural change in the PE film by the laser heating, and detected the phase-change in a time-resolved manner, which is not possible by the standard technique such as the FTIR analysis.

5. Natural Convection Heat Transfer from Vertical Rod Bundles in Liquid Sodium

Natural convection heat transfer from vertical rod bundles in liquid sodium was numerically analyzed for three types of the bundle geometry (two parallel, equilateral triangle and equilateral square arrays). The unsteady laminar three dimensional basic equations for natural convection heat transfer caused by a step heat flux were numerically solved until the solution reaches a steady-state. The PHOENICS code was used for the calculation considering the temperature dependence of thermo-physical properties concerned. The 2 to 4 test rods for diameter (D=7.6 mm), heated length (L=200 mm) and L/d (=26.32) were used in this work. The surface heat fluxes for each cylinder were equally given for a modified Rayleigh number, $R_{f,L}$, ranging from 3.06×10^4 to 3.14×10^7 ($q=1\times10^4 \sim 7\times10^6$ W/m^2) in liquid temperature (T_L=673.15 K). The values of S/D for the rod bundle were ranged from 1.4 to 3 on each bundle geometry. The spatial distributions of local and average Nusselt numbers, $Nu_{\theta,z}$ and $(Nu_{av,B})_N$, on vertical rods of a bundle were clarified. The average values of Nusselt number, $(Nu_{av,B})_{N,S/D}$, for three types of the bundle geometry with various values of S/D were calculated to examine the effect of the bundle geometry, S/D and $R_{f,L}$ on heat transfer. The bundle geometry for the higher $(Nu_{av,B})_N$ value under the condition of S/D=constant was examined. The correlation for $(Nu_{av,B})_{N,S/D}$ for three types of bundle geometry above mentioned including the effects of $R_{f,L}$ and S/D were developed. The correlations can describe the theoretical values of $(Nu_{av,B})_{N,S/D}$ for three types of the bundle geometry for S/D ranging from 1.4 to 3 within -7.44 to 10.73 % difference.

Collaboration Works

宇宙科学研究所（ルーマニア），高強度超短パルスレーザーによって誘起される非摂動相互作用の理論研究，中嶋隆

中国計量学院（中華人民共和国），アト秒パルスのキャラクタリゼーション，中嶋隆

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Financial Support

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2. Others
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Advanced Energy Structural Materials Research Section

A. Kimura, Professor
K. Morishita, Associate Professor
K. Yabuuchi, Assistant Professor
W. Han, 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, such as development of fusion blanket structural materials and fuel claddings of Gen-IV nuclear systems. Current main researches are as follows:

(1) Development of structural materials for fusion systems: Materials R&D is essential for realization of fusion energy. Among the issues for materials R&D for fusion application, we have been focusing on the development of radiation tolerant structural materials, which include reduced activation ferritic (RAF) steels and oxide dispersion strengthened (ODS) steels for fusion blanket. R&D of high Cr ODS steels has been performed as a national program to develop an innovative material with radiation tolerance, corrosion-resistance and high-temperature strength for advanced nuclear fission and fusion systems.

(2) Tungsten diverter R&D: Evaluation of feasibility of tungsten (W) diverter has been performed along with joining technology development of W/ODS steel joints by means of transient liquid phase bonding method. The application of ODS steels as structural components of W-diverter has been considered to be effective to reduce the temperature gradient between plasma facing material and coolant constituents.

(3) Multi-scale modeling: Tungsten (W) is proposed as one of the candidates for the first wall protection in fusion power plants. In irradiated tungsten at temperatures where vacancies can move, voids (vacancy clusters) are experimentally observed by transmission electron microscopy (TEM). Voids induce swelling, which leads to the dimensional changes of the material.

(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. Irradiation effects on ODS steel

Irradiation damage management of structural material is important for safety and economically competitive energy source of nuclear fusion and fission systems. It is expected that recrystallization causes grain growth which results in a significant reduction of trapping site for irradiation damage structures in ODS steels. Unfortunately, however, the effect of recrystallization on irradiation performance of the steels was not investigated in detail, although many researches on the effect of oxide particle morphologies on irradiation behavior of ODS steels have been done.

Single-ion irradiations used 6.4 MeV Fe^{3+}. Dual-ion irradiation is used 6.4 MeV Fe^{3+} ions for displacement damage simultaneously with energy-degraded 1.0 MeV He^{+} ions. The value of nominal dose rate is 4×10^{-4} dpa/s. Fig. 1 shows the dislocation microstructure and He bubble with oxide particles after dual-ion irradiated at 470 °C to 30 dpa.

The dislocation is line-shape and no or very fine cavities exist in as-received material. The oxide particles are fine in as-received specimen, it is trapping site for He bubble formation and there is almost no cavities. The line-shape dislocations in un-irradiation area (above 2 μm) are primarily dislocations formed at

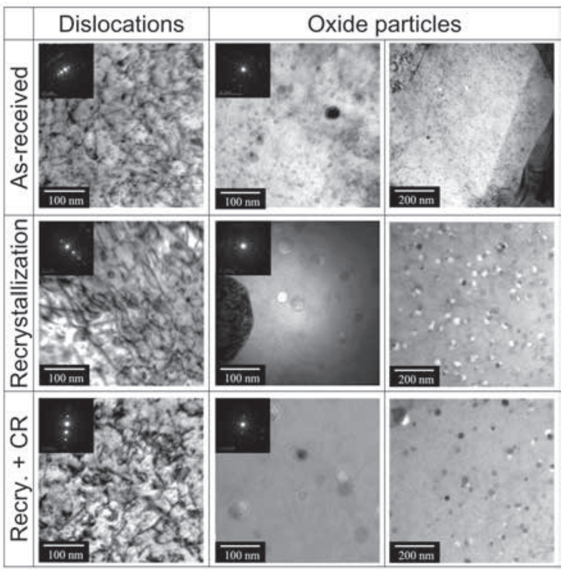

Fig. 1: Dispersion of oxide particles in ODS steel

470 °C. In contrast, many dislocations exist with loop type in a lower irradiation temperature. The grain boundaries also play a role as annihilation sites of irradiation damages which are vacancies and interstitial atoms. In case of recrystallized specimen, no grain boundary was observed. It is like a single crystal grain morphology because the grain is very big after recrystallization. Thus, the expected trapping or annihilation at grain boundaries is suppressed. Also, dislocation in high density and bubbles around precipitates are observed. There are not only bigger oxide particles but also abnormally coarse precipitates. This shows a significant difference between unirradiated and irradiated area. Furthermore, some of the large cavities have a spherical shape as well as faceted shapes as shown Fig. 1.

3. Development of methodology to optimize management of failed fuels in a light water reactor

Fuel cladding is one of the key components in a fission reactor that confines radioactive materials inside a fuel tube. During reactor operation, however, cladding is sometimes breached, and radioactive materials leak from the fuel pellet into the coolant water through the breach. The primary coolant water is therefore monitored so that any leak is quickly detected; coolant water is periodically sampled, and the concentration of radioactive iodine 131 (I-131), for example, is measured. Depending on the measured leakage concentration, the faulty fuel assembly with leaking rod is removed from the reactor and replaced immediately or at the next refueling. In the present study, an effort has been made to develop a methodology to optimize the management for replacement of faulty fuel assemblies due to cladding failures using measured leakage concentration.

A new attempt has been made to optimize the management for the replacement of faulty fuel assemblies, which is discussed in terms of the critical concentration of I-131 in the primary coolant water as well as the rate of water sampling to monitor I-131concentration. The usual methodology for probabilistic risk assessment (PRA) was uniquely applied to this issue of fuel management optimization. Additionally, a model numerical equation describing the time evolution of I-131 concentration in the coolant water was proposed and solved by the valuable Monte Carlo method.

Some calculation results were here obtained as example cases, where the frequency of immediate reactor shutdown is evaluated as a risk caused by variation in the severity of fuel failures (Fig. 2). An optimized management for the replacement of faulty fuel assemblies with leaking rod was then discussed.

The frequency of immediate reactor shutdown that is performed to cope with faulty fuel assemblies was ingeniously used here as an index indicating the optimized level of management and obtained as a function of operational parameters. From the calculation results, we have finally concluded that, to achieve the optimized management of failed fuels, high resolution to detect a small amount of I-131 is not necessarily required, but frequent sampling is favorable. This methodology developed here is very important to consider an optimized management to be performed so as to reduce total risks.

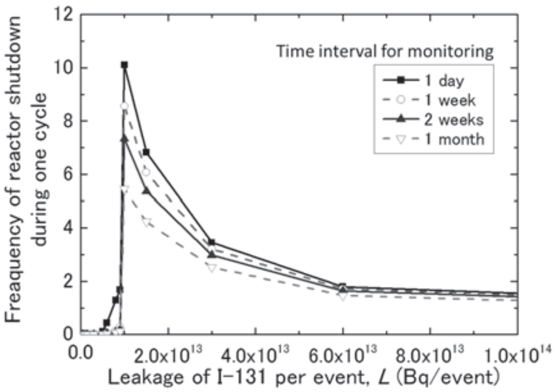

Fig. 2: Frequency of immediate reactor shutdown for a fixed value of the leak rate, when the time interval of intermittent monitoring is changed

4. Radiation damage mechanism

Particle irradiation leads to the formation of oversaturated interstitials and vacancies. The behavior of the point defects is responsible for the evolution of the microstructure, which may cause degradation, (or improvement), of the mechanical properties of the material. Hence, the elucidation of the behavior of point defects is essential for understanding the mechanisms responsible for the changes in mechanical properties. In our study, the microstructure evolution under particle irradiation has been investigated experimentally and computationally with use of the ion accelerator (DuET), electron microscopies, the first principle, MD, and so on. One of the recent results is the following.

We investigated the effect of Mn on the irradiation hardening of Fe after ion irradiation at 300°C up to 3 dpa using DuET, which showed that Mn addition enhanced irradiation hardening. In-situ TEM observations revealed that the significant irradiation hardening was due to the formation of small dislocation loops in high number density. It is considered that Mn solutes play a role of nucleation site for the interstitial dislocation loops by retarding one-dimensional motion of dislocation loops. This results in the formation of small dislocation loops in high number density, and consequently large irradiation hardening in Fe-Mn alloy.

Collaboration Works

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Complex Plasma Systems Research Section

F. Sano, Professor
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.

Recent results of this section in FY2014 are as follows:

2. Monitoring of wall conditioning with VUV spectroscopy

High-Z impurity in the plasma can release the stored energy through the collisional excitation followed by the line radiation. These line spectra exist mainly in the vacuum ultraviolet (VUV: 10 - 200 nm) region, so that an oblique incidence vacuum ultraviolet spectrometer has been applied in Heliotron J. Unequal spacing concave diffraction grating was adopted for the spectrometer. Measurable wavelength is 5 - 40 nm by moving the detection position. The reciprocal linear dispersions are 0.018 nm/ch around 18 nm and 0.026 nm/ch around 39 nm. The minimum time resolution is 5 ms.

Plasma facing components (PFCs) can be cleaned by main plasma discharges through ion bombardment (physical sputtering) and chemical reaction (chemical sputtering) by hydrogen ions. In order to monitor the long-term progress in the conditioning of the PFCs, we have conducted daily reference discharges under the same condition where plasma is initiated only by electron cyclotron heating (ECH) with the standard magnetic configuration, and the electron density is controlled around 0.6 x 10^{19} m^{-3} by controlling the gas injection. The results are shown in Fig. 1. Assuming coronal equilibrium for impurity ions, and assuming the spatial profile of the electron density was not significantly different for the daily reference discharges, the spectral intensity divided by the line-averaged electron density can be regarded as corresponding the impurity concentration.

One can see that the impurities adsorbed in early

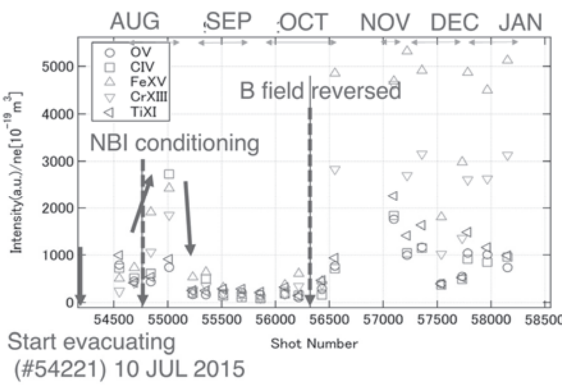

Fig. 1 Daily changes of the VUV spectral intensities.

phase of the neutral beam injection (NBI) conditioning, then they have gradually been reduced. However, the impurities increased after the magnetic field (B-filed) reversed for a certain experimental requirement. This observation indicated that the plasma-wall interaction (PWI) increased.

In order to clarify the impurity species that can enhance the radiation loss of the stored energy, we compared the spectral intensities with a radiation monitoring using an absolute UV silicon photodiodes detector (AXUV), as shown in Fig. 2.

Dominant radiators in the AXUV signals were found to be Fe and Cr, *i.e*. the alloys of stainless steel. It should be noted that dependence of VUV lines on AXUV was similar even before the B-field reversed, although both intensities were smaller.

In the next study, we are planning to compare the impurity contents with the plasma parameters to clarify the effect of impurity against the achievement of high performance plasmas.

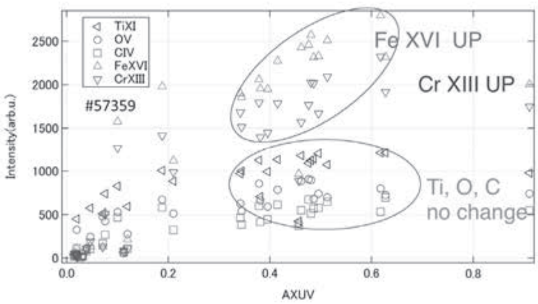

Fig. 2 Radiation loss monitor (AXUV) VS.

3. External Control of Energetic-ion-driven MHD Instabilities by ECH/ECDD

Energetic-ion-driven magnetohydrodynamis (MHD) instabilities such as Alfvén eigenmodes (AEs) and energetic particle modes (EPMs) enhance transport and induce the loss of energetic ions such as alpha particles in a Deuterium-Tritium fusion reactor. Since redistribution and exhaust of alpha particles lead to the reduction of fusion gain and damage of first wall, methods to control the energetic-ion-driven MHD instabilities are required, but they have not been established yet. ECH/electron cyclotron current drive (ECCD) may be an ideal tool to control the modes since they can provide highly localized EC waves with a known location and good controllability. We focus on the effect of continuum damping, which is related to the magnetic shear. Heliotron J has low magnetic shear in vacuum and, therefore, the magnetic shear can accurately be controlled by ECCD. We investigate the effect of continuum damping, whose rate is related to the magnetic shear, mainly on the observed EPMs. The continuum damping is also important damping mechanism of AEs in certain conditions.

We fixed the NBI power, line averaged electron density and plasma stored energy in the $N_{//}$ (refractive index along magnetic field line) scan experiments as much as possible. Therefore, electron and ion Landau damping, energetic ion beta were also fixed in these experiments. The plasma current I_p can be controlled in the range of $-2.0 < I_p < 2.5$ kA by ECCD by the combination of the changing $N_{//}$ from 0.0 to 0.5 and the changing direction of magnetic field B. The direction of EC driven plasma current does not depend upon the direction of magnetic field B_t. The change of direction of magnetic filed B means the change of sign of EC driven plasma current. The EC driven plasma current profile calculated by TRAVIS code indicates that EC driven plasma current locally flows at the plasma core ($\rho < 0.2$) and enhances the magnetic shear in whole plasma region. When we vary $N_{//}$ from 0 to 0.5, total plasma current increases as the increase of $N_{//}$ in the range of $N_{//}$ = 0.0 ~ 0.2 and saturates in the condition of $N_{//} \geq 0.2$ although profile of plasma current is slightly different for each $N_{//}$.

Figures 3 show that the dependence of amplitude of the observed EPMs on the plasma current. We successfully mitigated the EPMs amplitude by using ECCD in NBI-heated Heliotron J plasmas. Since NBI power and energy between experiments with $B > 0$ and < 0 are different, the characteristics of the observed EPMs such as observed frequency and mode structure are different from each case for $m = 4/n = 2$ EPMs. We independently show the dependence of EPM amplitude in different figures for $B > 0$ and < 0. It seems that same EPMs with same toroidal mode number $n = 1$ are observed in the plasma with both the positive and negative B. The amplitude of the observed EPMs with m=2/n=1 obviously decreased with an increasing absolute value of EC driven plasma current, as shown in Fig. 3. This corresponds to that the effect of magnetic shear on the mode did not depend on its sign as shown in Figs. 3 (a) and (b). Asymmetry dependence of m=2/n=1 EPMs amplitude on the plasma current can be explained that bootstrap current, of which direction does not depends on the magnetic field direction, modifies the rotational transform at plasma edge region. Observed m=4/n=2 EPMs shown in Figs. 3 (c) and (d) are different from each other because of different observation frequency.

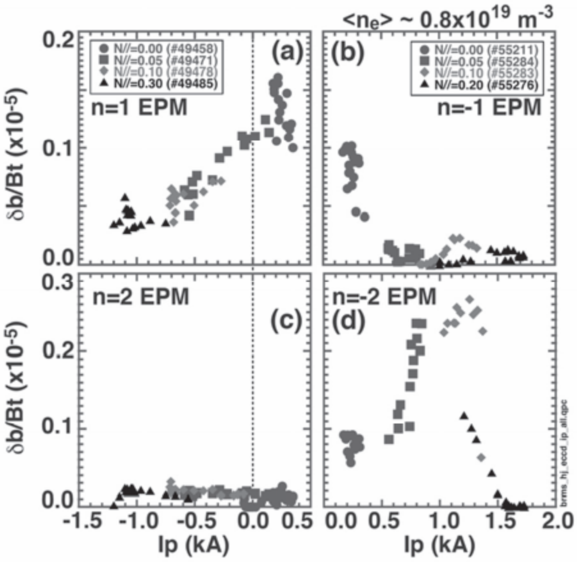

Fig. 3 Dependence of amplitude of observed EPM.

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，佐野史道，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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Clean Energy Conversion Research Section

Hiroyuki Hama, Visiting Professor
(Tohoku University)

1. Introduction

Chirality (or handedness) is one of fundamental aspects of the nature. Definition of the chiral object is that its mirror image is not identical, on the other hand achiral object's mirror image can be superposed. In the particle physics, chirality can be found in spin. Invariance under parity by Dirac fermion is chiral symmetry. However chiral symmetry breaking in QCD gives hadron's mass. For the classical electromagnetism, chirality is found as circular polarization. In chemistry, optical isomer of molecule is chiral object. It is well known the function of chiral isomer is sometimes much different from that of another object. There is a fundamental question why the most of amino acids are left-handed. In the bioscience, there is another interesting fact that most of coiled shellfishes on the earth are right-handed. An interesting hypothesis is the helicity of circular polarized light in the universe governs those chiral characteristics.

It has been proved that the radiation helicity can control the abundance of chiral isomer products in chemical reaction. Circular polarization can extract or prove the spin information of the molecular. In this sense control of helicity in the circular polarized radiation source is crucial for the chirality study in the chemistry and the bioscience.

2. THz superradiant

Radiation having the frequency from 0.1 To 10 THz is called THz radiation. It is very much closed to "far-infrared" radiation. Since there had been no powerful source of THz radiation, someone called "THz-gap" in radiation sources. However rapid progress of the laser and semiconductor physics has brought remarkable development of THz source. Since THz wave can excite vibrational and rotational states of heavy bio-molecular, it is useful for molecular spectroscopy in bioscience. Spin information can be derived by circular polarization with helicity switching. Variable polarized intense THz radiation seems to be attractive source for many scientific applications including the study of chirality problem. In order to provide helicity switchable polarized THz radiation, we have proposed variable polarization superradiant (superradiance) from crossed-undulator.

In 1954, R. H. Dicke described that supperradiance arises when a high degree of phase coherence exists between the radiation fields of the individual electron bunches, and manifests itself as a series of narrow spectral peaks at harmonics of the bunch frequency [1]. This article mentioned regarding radiation from molecules in gas. Although we know the coherent radiation from the bunched electrons, it is not completely identical with supperradiant because of transverse coherency. Superradiant should mostly satisfy three-dimensional coherence such as lasers.

Using the longitudinal form factor for the electron bunch, the radiation power from the bunched beam is described as

$$P(\lambda) = p(\lambda)\left[N + N(N-1)f(\sigma)\right] \ , \qquad (1)$$

where $p(\lambda)$, N and $f(\sigma)$ are single electron radiation power, number of the electrons and the bunch form factor. In case of the $f(\sigma)$ is the unity, the coherent radiation power is proportional to square of the number of electrons. The form factor of the Gaussian bunch is written as

$$f(\sigma) = \left| \exp\left(-2\pi^2 \frac{\sigma^2}{\lambda^2} \right) \right|^2 \ . \qquad (2)$$

Here σ is the bunch length and λ is the wavelength interested. Meanwhile the transverse coherence is resulted from the source emittance comparable to or less than the light intrinsic emittance, i.e. diffraction limited phase space of the photons

$$\sigma_r \sigma_{r'} \leq \frac{\lambda}{4\pi} \ , \qquad (3)$$

where σ_r and $\sigma_{r'}$ denote the source size and its angular spread. As one can see in Fig. 1, sufficiently large form factor is obtained at the bunch length shorter than one-tenth of the wavelength. Taking look at the wavelength of 300 μm (1 THz), the source emittance has to be less than 48 mm.mrad to reach

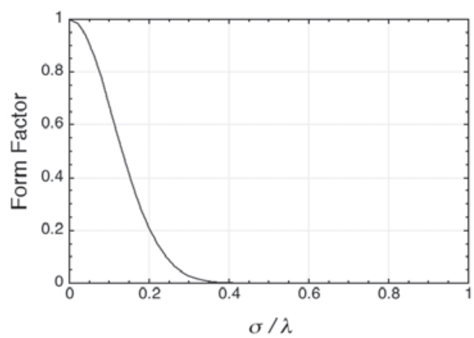

Fig.1: The form factor plotted as a function of bunch length relative to the wavelength concerned.

the supperradiance. Calculated temporal electric fields of radiation from a long-period (10 cm) undulator are shown in Fig. 2. The electron beam energy is 20 MeV, and a resonant wavelength with a peak magnetic field of 0.4 T is 300 μm.

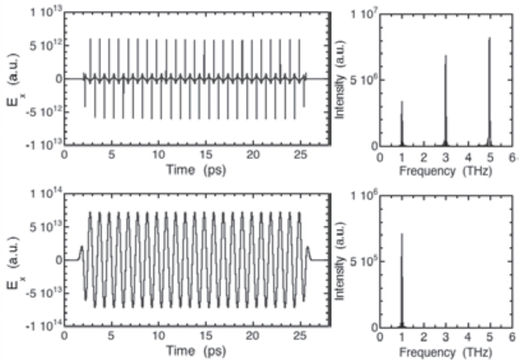

Fig.2: Upper figures show the radiation electric field and the spectrum from single electron. Lower shows those from the bunched electron whose rms bunch length is 200 fs. In the lower figure, it is clear the higher harmonics is suppressed due to bunch length dependence of the form factor.

3. Crossed-undulator configuration for variable polarization

Crossed-undulator scheme was initially proposed for polarization control in XFEL [2]. However, because of complicated lasing process in SASE, complete control of the polarization is pretty difficult. Using multi-undulator scheme, polarization switching was demonstrated at an oscillator FEL at Duke University [3]. Our proposed scheme is close to K.-J. Kim's one as shown in Fig. 3. There are two

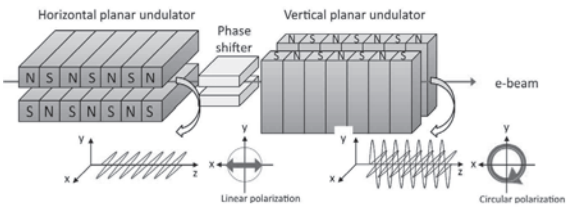

Fig.3: Proposed crossed-undultor configuration for variable polarized THz superradiant. Phase shifter delays the radiation so as to choose proper phase between two undualtor radiations.

planer undulators with perpendicular deflecting planes. Superradiant phase differences of 0.5 π (1.5 π) give right-handed (left-handed) circular polarizations. Elliptical polarization is certainly achievable arbitrarily. Radiation field simulated numerically is shown in Fig. 4. Note that the linear polarization can be obtained at the phase difference of $n\pi$ (n=0, 1, 2 ...), but it is tilted by 45 degree.

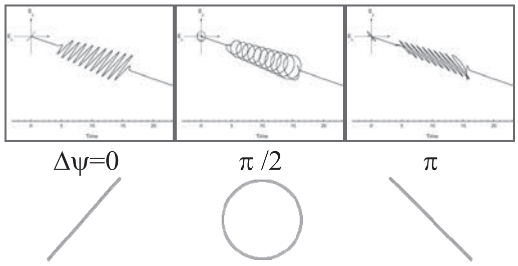

Fig.4: Radiation field and polarization for the phase differences of 0, π /2 and π.

4. Bunch compression

In order to produce femtosecond electron pulse, we have developed an independently tunable cells (ITC) RF gun, in which the longitudinal phase space of the extracted beam can be manipulated by changing relative field strength and phase between two cavities. In addition, velocity bunching in an accelerating structure has been studied as a compression technique [4]. Test experiments were performed already at our accelerator test facility t-ACTS [5]. We have thought the proof of principle of velocity bunching was well done by observing sub-picosecond bunch length. However the achieved bunch length was not confirmed precisely because of poor resolution of the bunch length measurement system employing a streak camera to observe optical transition radiation (OTR). Sufficient number of photons was not transported in to the streak camera, because OTR emitted from electrons with relatively lower energy is not brilliant and spreading widely.

5. Summary

Based on undulator superradiant with femtosecond electron bunch, we have proposed a THz radiation source for variable polarization. Velocity bunching method seems to be suitable to produced short electron bunch length. Although further study is required, the method was found to be effective. Design work of the crossed-undulator was almost completed. We are going to establish the experimental apparatus in near future.

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Clean Energy Conversion Research Section

Hideo Watanabe, Visiting Associate Professor
(RIAM, Kyushu University)

Radiation-induced embrittlement of reactor pressure vessel (RPV) steels during the use of thermal fission reactors is clearly of considerable importance to the safe operation of reactors and plays a major role in plant life extension considerations. The neutron irradiation of these steels leads to an increase in the ductile-to-brittle transition temperature (DBTT) with a decrease in the upper shelf energy [1-2]. Cu has a strong effect on such embrittlement phenomena, and Cu-rich precipitates have been thought to be responsible for embrittlement. On the other hand, mechanical property studies of steels with different Cu levels have shown that so-called matrix defects are dominant in the embrittlement of low Cu steels [3] and of high Cu steels at high fluences [4].

Furthermore, it is known that the nucleation and growth processes for dislocation loops during neutron irradiation are strongly controlled by various factors, including neutron flux, irradiation temperature, chemical composition, and applied stress [5,6]. On the other hand, the effects of dislocation loop formation on hardening are not clearly understood. In this study, therefore, to understand the effects of dislocation loop formation on radiation hardening in RPV steels, Fe ion irradiation was performed on steels with three different Cu contents. To compare the effects of the Cu content on the radiation-induced hardness during neutron irradiation, the UCSB irradiation variable program database [7] and the same A533B steels that were used in the previous IVAR program [7] were investigated. In a previous study, we showed that ion irradiation of A533B steels with a dose of 0.5 dpa did not result in the formation of any visible defect clusters using conventional transmission electron microscopy (TEM).

Three A533B steels with different Cu levels were used in this study. The A533B steels are referred to as A533B(LG) without Cu, A533B(LH) with a low Cu content (0.11 wt%), and A5333B(LI) with a high Cu content (0.20 wt%). The specimens for ion irradiation and in situ observation via HVEM were annealed (austenitized) at 900 °C for 1 h, air cooled, tempered at 664 °C for 4 h, air cooled, stress relieved at 600 °C for 40 h, and air cooled. Ion irradiation with 2.4 MeV Fe^{2+} was conducted in the temperature range from room temperature to 350 °C using the tandem accelerator at Kyushu University. Hardness tests were conducted at room temperature before and after ion irradiation using an Elionix ENT-1100 with a load of 1 gf. A triangular pyramidal diamond indenter (Berkovich type) with a semi-apex angle of 65° was used. The indenter load (L) and displacement (d) were continuously monitored using a computer system. L and d are given by

$$L/d = Ad + B, \qquad (1)$$

where A and B depend on the material but are independent of the load and indenter displacement. A is proportional to the Vickers hardness (Hv) and is given as follows:

$$A(\mathrm{GPa}) = 0.287\ \mathrm{Hv}. \qquad (2)$$

To understand the fundamental defect clustering processes resulting from irradiation, electron irradiation with in situ observations was performed using 1.0 MeV electrons and a high voltage electron microscope (JEM-1000) in the HVEM Laboratory at Kyushu University. Electron irradiation was conducted at 290 °C and 350 °C. To reduce the temperature rise due to electron beam heating during irradiation, a relatively low electron dose rate of 2.5×10^{-4} dpa/s (the same as the ion radiation) was selected. After electron irradiation, the solute enrichment around preexisting dislocations due to irradiation was analyzed via STEM (Hitachi HD-2700). For the LI (0.2 wt% Cu) sample, atom probe tomography (APT) was also conducted after irradiation. The irradiated regions were approximately 9 μm in diameter, and the specimens were approximately 200 nm in thickness. FIB machining was then employed to prepare APT samples from the irradiated regions. Both TEM and APT observations were carried out for the irradiated regions.

Ion irradiation with 2.4 MeV Fe^{2+} and electron irradiation using HVEM were performed on A533B steels with different Cu contents. The main results are summarized as follows.

1) The effect of Cu content on the irradiation-induced hardening of the steels was prominent at higher dose levels (1.0 dpa) at 290 °C. At lower dose levels (~0.1 dpa) and temperatures above 320 °C, nearly the same dose dependence of the hardness change was observed for all A533B steels with different Cu contents.

2) Log–log plots of the irradiation hardening at 290 °C, which were fit to the dose dependence of the irradiation hardening using $\Delta H \propto (\mathrm{dpa})^n$, revealed a higher value of 0.5 for doses of 0–0.1 dpa and became saturated. In addition, this study of the

radiation-induced hardness due to ion irradiation strongly demonstrated that the fundamental studies of materials during the early stage of irradiation (up to 0.1 dpa) are essential for evaluating radiation-induced phenomena in saturated regions.

3) Analysis of the microstructure resulting from electron irradiation revealed that the nucleation and growth of dislocation loops were prominent at the dose level where the saturation of the hardness occurred. At this dose, prominent radiation-induced solute segregation to dislocations and cluster formation were also detected using APT.

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Chemical Reaction Complex Processes Research Section

T. Nohira, Professor
T. Kodaki, Associate Professor
X. Yang, Program-Specific Assistant Professor

1. Introduction

In this research section, we studies 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

The global photovoltaic (PV) market has been growing rapidly in recent years. Up to now, the prevalent material for solar cells is silicon, particularly crystalline silicon. With the expansion of the PV market, the consumption of solar-grade silicon (SOG-Si; 6N purity) has also climbed dramatically. However, the conventional Siemens process has several disadvantages such as low productivity and high energy consumption. Thus, a novel, high-yielding and inexpensive process for SOG-Si production is required.

We have already demonstrated that solid SiO_2 can be directly reduced to solid Si by molten salt electrolysis. Using the contacting electrode method, SiO_2 is reduced to Si by electrolysis at the three-phase zone of SiO_2/molten salt/electrode via the reaction:

$$SiO_2\,(s) + 4e^- \rightarrow Si\,(s) + 2O^{2-} \qquad (1)$$

Accordingly, a new process for SOG-Si production was proposed by combining electrochemical reduction with the use of high-purity SiO_2 granules. In the present study, the mechanism and kinetics for reduction of SiO_2 granules in molten $CaCl_2$ at 1123 K were investigated, and the purity of the obtained Si was evaluated.

The molten salt reactor was assembled in a vertical electric furnace. An Al_2O_3 crucible charged with $CaCl_2$ was set inside a SiO_2 vessel and heated to 1123 K in a dry Ar atmosphere. The working electrode was consisted of an Al_2O_3 tube with a Si plate at the bottom. High-purity SiO_2 granules were charged in the Al_2O_3 tube. The potential of the working electrode was set at 0.5 V vs. Ca^{2+}/Ca for the potentiostatic electrolysis for 20 to 240 min. The post-electrolysis working electrode was vertically cut into two halves to observe the cross section. The amounts of reduced SiO_2 were calculated from the weight changes of the samples before and after the electrolysis. The mechanism and kinetics of electrochemical reduction were evaluated from these data. The impurity level of the recovered Si after washing by HF and water was analyzed by GD-MS.

Fig. 1 shows the cross section of the working electrode after electrolysis for 10, 30 and 120 min. A brown layer is observed above the Si plate, which grows up from the bottom as the electrolysis time increases. Formation of crystalline Si in this layer was confirmed by XRD. This result indicates that the reduction progresses from the SiO_2 granules near the conductor at the bottom to the top. Fig. 2 shows the time dependences of the reduction fraction and the calculated apparent current density. It is indicated that the reduction is fast at the initial stage of electrolysis, and gradually becomes slow. An apparent current density of 0.7 A cm^{-2} was achieved at the initial stage of electrolysis. Direct electrochemical reduction of SiO_2 in molten $CaCl_2$ is prospective to be applied in the commercial silicon production in terms of productivity.

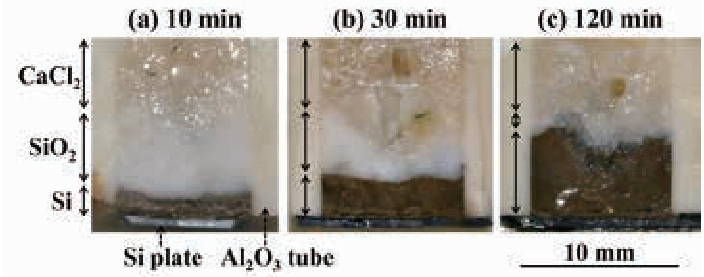

Fig. 1. Cross-section of the working electrode after electrolysis for 10, 30 and 120 min.

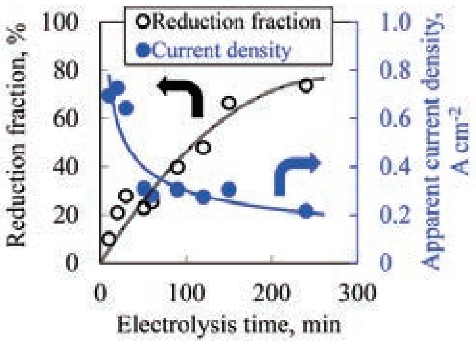

Fig. 2 Time dependences of the reduction fraction and the apparent current density during electrolysis.

3. Development of Highly Efficient Bioethanol Production Yeast Using Protein and Metabolic Engineering

Naturally occurring *Saccharomyces cerevisiae* strains have been used for industrial scale bioethanol production from hexose sugars. Furthermore, there is considerable research interest in the development of recombinant strains that can efficiently ferment both hexose and pentose sugars from lignocellulosic hydrolysates for effective bioethanol production. Lignocellulosic biomass is one of the major renewable substrates that can be used for ethanol production. Complete conversion and fermentation of cellulose and hemicellulose is essential for producing high ethanol yields. Since glucose and xylose are the two predominant sugars in the lignocellulosic hydrolysates, many previous studies have focused on developing recombinant strains that maximize ethanol production from xylose and glucose by eliminating byproducts through metabolic conversion. Construction of efficient xylose-fermenting yeast *S. cerevisiae* has been subjected to large number of trials for improving ethanol productivity from mixture of glucose and xylose that are widely distributed in lignocellulosic hydrolysates. Oxidative metabolism of xylose can be performed by using recombinant yeast *S. cerevisiae* strains expressing xylose-metabolizing enzymes. However, xylose metabolism by recombinant yeast strains can be affected by cofactor availability. Previous studies indicate that effective regeneration of cofactors by the introduced enzyme may increase the cofactor availability and prevent xylitol accumulation as a by-product of the fermentation process. In this study, the effects of overexpression of the genes involved in the non-oxidative pentose phosphate pathway (PPP) was investigated. In *S. cerevisiae*, PPP is really the only way by which xylulose can be introduced into glycolysis pathways and this occurs via two reactions that convert xylulose 5-phosphate to fructose 6-phosphate and glyceraldehyde 3-phosphate. The non-oxidative reactions of this pathway are reversible reactions of which are important for generating ribose 5-phosphate for nucleic acid synthesis as well as for catalyzing the interconversion of a variety of pentoses, hexoses and trioses. Both transaldolase and transketolase create a reversible link between two main metabolic pathways, the PPP and glycolysis, which allows the cell to adapt its NADPH and ribose 5-phosphate production to meet its' immediate needs. However, it is well known that, in *S. cerevisiae*, the flux through the PPP is insufficient compared to other yeast species, most likely resulting in lower rates of xylulose fermentation. Therefore, enhancement of the PPP in xylose-utilizing strains by the overproduction of non-oxidative PPP enzymes has been attempted to improve yeast growth on xylose as well as the rate of xylulose consumption. A recombinant xylose-fermenting yeast *S. cerevisiae* was transformed with a plasmid containing the genes for non-oxidative PPP enzymes including transaldolase (*TAL1*), transketolase (*TKL1*), ribulose-5-phosphate 3-epimerase (*RPE1*) and ribose-5-phosphate ketol-isomerase (*RKI1*). Eighteen colonies were randomly picked up and measured xylose consumption rate and ethanol production rate (Fig. 3). Several colonies showed both higher xylose consumption rate and higher ethanol production rate. These colonies will be investigated in more detail about ability of xylose fermentation and ethanol production.

These researches were partly supported by grants to T. N. from JST-CREST and MEXT (23246131), and to T. K. from NEDO, the Iwatani Foundation and MEXT (23603003).

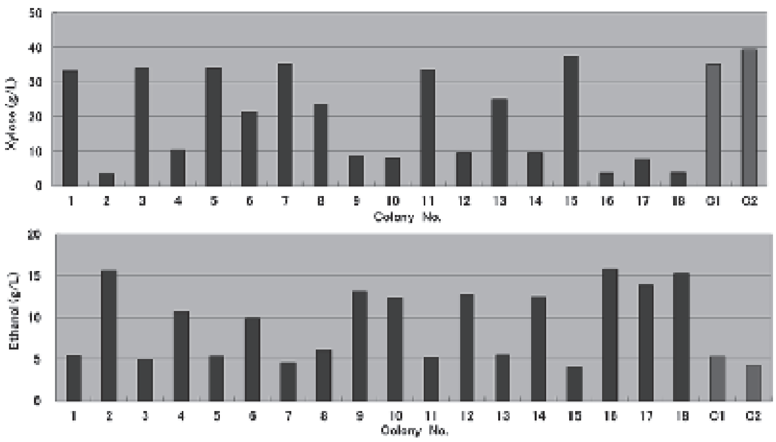

Fig. 3. Screening of strains of highly bioethanol production from xylose.

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Molecular Nanotechnology Research Section

H. Sakaguchi, Professor
T. Kojima, Assistant Professor
T. Nakae, Assistant Professor

1. Introduction

Nanotechnology is so important to produce the unprecedented materials for 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 developed 'Electrochemical Epitaxial Polymerization' and 'Radical-Polymerized Chemical Vapor Deposition' technique which are totally new molecular assembling techniques of molecular wires on metal surface from single molecules. By the use of these techniques, unprecedented materials for energy use will be developed. Organic electronic devices such as field effect transistors and solar cells will be studied. Followings are main research achievements in Molecular Nanotechnology Research section in the year of 2014.

2. Highly effective bottom-up synthesis of graphene nanoribbons by 2-zone radical-polymerized chemical vapor deposition

Graphene nanoribbon (GNR) is a promising organic electronic material. GNR can work as a semiconductor with an atomically thinness and a sub-nanometer width. Atomically precise synthesis of monolayer GNR was achieved under an ultra-high vacuum condition. GNR growth reaction is required bond formation between monomers and conjugation expansion between connected monomers. Ultra-high vacuum (UHV) condition is required, because of short life times of highly reactive aromatic biradical species.

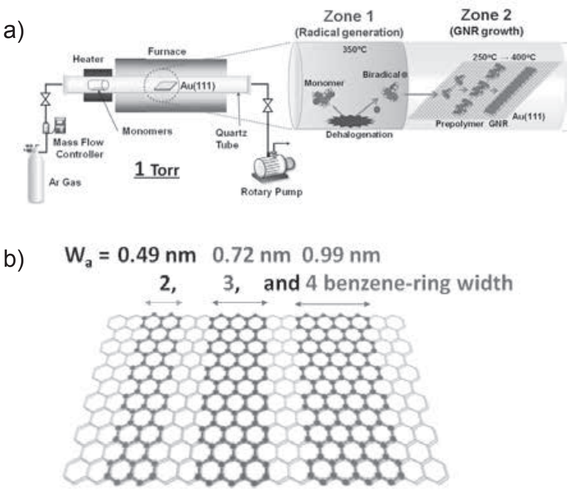

Fig. 1 Schematic illustrations of a) 2-zone RP-CVD instrument and b) synthesized graphene nanoribbons.

To develop GNR devices, atomically precise synthesis of "multilayer GNRs," isolation, and device fabrication are required. We have demonstrated bottom-up growth of multilayered GNR under low vacuum condition from halogenated polycyclic aromatic hydrocarbons by 2-zone radical polymerized chemical vapor deposition (Fig 1-a). Attractive features of this method originate from an independent temperature-control of radical-generation process (zone 1) and the growth process (zone 2) to produce the biradical source for polymerization efficiently, leading to a high yield of GNR. Au(111) on a glass substrate was placed in a quartz tube as a reactor heated by an electric furnace (zone 2). The system was evacuated using a rotary pump with Ar gas flow, resulting in pressure of 1 Torr. Solid monomers placed in a quartz boat were vaporized by heating at 200-250 °C, followed by collision with the hot wall of the quartz tube (zone 1) heated at a temperature to produce biradicals by dehalogenation, to supply on substrate as a first stage for 15 min, and to be radical-polymerized into prepolymers. Subsequently, the temperature was raised to 400 °C, and was maintained for 10 min as a second stage, for the prepolymers to be dehydrogenated into GNR.

We found two important parameters for massive GNR-growth by RP-CVD. Only when the condition meets these requirements, an intense Raman signal from GNR was observed. The first requirement is cleaning of a quartz tube by immersion in concentrated nitric acid after heating at 1000 °C. The Raman intensity was enhanced markedly by cleaning processes compared with that of untreated tube. A second requirement is the side (vertical position) of Au(111) substrate placed in the quartz tube. Facing Au(111) side to the nearest surface of quartz tube gave more intense Raman intensity than that to the gas side. Organic biradicals produced from gaseous aromatic dibromide by thermal activation at cleaned hot wall of the reaction tube. The concentration of organic biradicals was dense at the confined space from near the wall. An atomically flat Au (111) metal surface was placed at the optimized space in a reaction tube, GNR prepolymer propagated and converted into GNR efficiently despite extremely low-vacuum (1 Torr) conditions. The utilization of the high-density biradicals is a remarkable benefit of 2 zone RP-CVD method. In fact, RP-CVD is applicable to the other monomers to produce GNR of different widths. We synthesized different width of armchair-type GNRs (A-GNR) with 2,3, and 4 benzene-ring width (Fig 1-b). This is the first example of narrowest GNR.

In our process, GNR propagation reaction proceeded efficiently. We obtained first example of multilayered GNRs by bottom-up synthesis. A multilayered GNR film can be isolated from Au(111) surface. This is the first example of isolation of GNR material with an atomically well-ordered width prepared by bottom-up synthesis. GNR films could be transferred onto insulator surface. We achieved the first example of the measurement of nanogap electrode FET device of bottom-up synthesized GNR films by e-beam lithography technique.

3. STM studies of GNRs and their band gaps

GNR was characterized using STM measured in air (Fig. 2). STM images of poly (perianthracene) GNR produced by RP-CVD showed a multilayered high-density array of linear wires. An intense Raman signal from the same sample was confirmed to originate from the massively grown multilayered GNR. The monolayer height corresponds to 0.22 nm from cross-sectional analysis of STM image. The GNR length is analyzed as up to 20 nm of the longest. To examine the GNR growth mechanism, the STM image of RP-CVD-grown sample at the first stage was measured. It shows a zigzag chain with spacing of each side corresponding to 0.82 nm, which shows good agreement with that of 0.85 nm for the alternate anthracene-ring in poly(anthrylene). These data suggest the mechanism of RP-CVD to be based on radical polymerization and dehydrogenation, in which the intermediate at the first stage corresponds to the prepolymer (poly(anthrylene)), followed by conversion to the poly(perianthracene) GNR at the second stage.

In fact, RP-CVD is applicable to the other monomers to produce GNR of different widths. When using monomers of mixtures containing 3,9-dibromoperylene and 3,10-dibromoperylene, the multilayered linear wires of poly (perinaphthalene) GNR, produced by RP-CVD, appeared in the STM images. The monolayer height was analyzed as 0.27 nm using cross-sectional analysis. The length of poly (perinaphthalene) GNR is distributed up to 24 nm. Production of poly(perinaphthalene) GNR was also supported by Raman spectrum of the RP-CVD grown sample which showed identical peak-positions with those of the simulation. The GNR growth mechanism was evaluated by measuring STM at the first stage. It clearly shows the existence of prepolymer and poly (perylenylene). Spacing at each line of image (1.75 nm) agrees with alternate spacing (1.7 nm) of the perylene rings in poly (perylenylene). Based on these data, the growth mechanism of poly(perinaphthalene) GNR was confirmed as polymerization of biradicals generated from monomers followed by dehydrogenation. Poly(peritetracene) GNR with width of four benzene rings was produced when using 1,4-bis(4-bromophenyl)-2,3,6,11-tetraphenyltripheny lene as a monomer. The multilayered linear wires of poly(peritetracene) GNR, produced by RP-CVD, appeared in the STM images. The monolayer height was analyzed as 0.27 nm using cross-sectional analysis. The length of poly(peritetracene) GNR is distributed up to 7 nm from the STM image. Production of poly(peritetracene) GNR was also supported by the Raman spectrum of the RP-CVD grown sample, which showed identical peak-positions with those of the simulation.

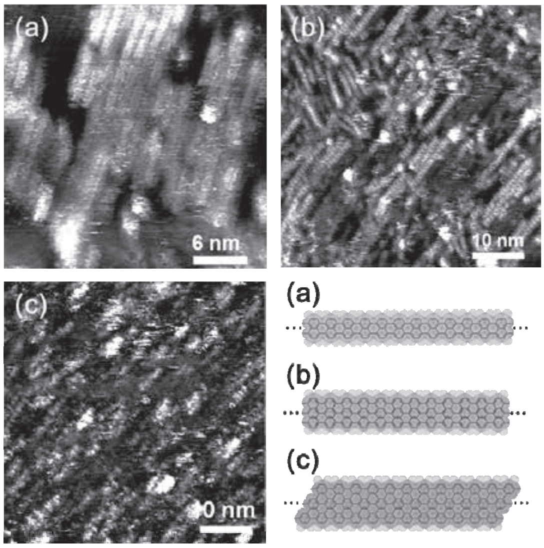

Fig. 2 STM images of (a) Poly(perinapththalene), (b) Poly(perianthracene), (c) Poly(peritetracene) .

The band gap of GNR is inferred to depend on the edge structure and width. Although there are some reports on the width dependence on the band gap, especially of armchair-edge type GNR, it has never been studied systematically. We measured the band gaps of our GNRs using scanning tunneling spectroscopy (STS). Present measurements experimentally established the band-gap value for the armchair-edged GNRs having sub-1 nm width. Experimental values of poly(perinapththalene), poly(perianthracene, and poly(peritetracene) were 0.4 eV, 1.5 eV and 1.3 eV, respectively.

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Biofunctional Chemistry Research Section

T. Morii, Professor
E. Nakata, Lecturer
S. Nakano, Assistant Professor

1. Introduction

The work in our research group takes synthetic, organic chemical, biochemical and biophysical approaches to understand the biological molecular recognition and chemical reactions. Rational design and functional evaluation of semi-synthetic miniature proteins, synthetic peptides and RNA/peptide assemblies enable precise recognition and fluorescence detection of biologically important molecules and in water, the solvent of life. Followings are main research achievements in fiscal year 2014.

2. Development of a modular zinc finger adaptor to locate proteins on DNA nanoscaffolds through the covalent linkage

DNA nanostructures are ideal scaffolds for arranging small molecules and nanomaterials at the single molecular level by taking advantage of their addressable nature. Among these, proteins are molecules of particular interest for assembly with nanoscale precision because of their wide functional variability range. For instance, spatially organized assemblies of multiple enzymes would realize natural or artificial multienzymatic pathways in vitro.

We have previously reported that sequence-specific DNA binding proteins act as ideal adaptors for locating a protein of interest (POI) at a specific address on the DNA nano-architecture. Adaptors derived from a zinc finger (ZF) protein, zif268, and a basic-leucine zipper protein, GCN4, are utilized for locating POIs in the monomeric and dimeric forms, respectively. The sequence-selective DNA binding characteristics of these adaptor proteins enable orthogonal arrangements of POIs on the DNA nanoarchitecture with fast binding kinetics, by simply constructing adaptor-fused proteins.

However, even with the high stability of the adaptor–DNA address complex, the reversible nature of the DNA–protein complexes causes difficulty in preserving the POI to that location during the assay procedures, as well as in loading the adaptor-fused POI with high efficiency, especially to closely located or sterically hindered addresses. Moreover, even when an ODN is specifically introduced into a POI, it is difficult to saturate the target addresses on a DNA origami scaffold with ODN-tethered proteins and with the ZF adaptor-fused POI. For the POIs that are noncovalently loaded onto the DNA nanoscaffold, it is necessary to maintain the appropriate concentration of the unbound POI, whether it binds the DNA nanoscaffold through DNA hybridization or protein–DNA interactions, to ensure stable complex formation.

A combination of the DNA binding protein adaptor and the self-ligating protein tag should afford a new class of covalent cross-linking adaptors that would facilitate efficient loading of POI on a DNA nanoscaffold with fast kinetics. We utilized one of self-ligating protein tags called SNAP-tag to construct a modular DNA-binding protein adaptor. The zif268 derived ZF adaptor was modified with the SNAP-tag, which reacts specifically with benzylguanine (BG) (Figure 1a), as the modular adaptor named ZF-SNAP. ODNs containing the zif268 binding sequence (ODN-zif) were designed to form a loop with four T nucleotides, and one of these T nucleotides was displaced by the BG-modified T derivative as the substrate for the SNAP-tag (ODN-zif-BG; Figure 1b).

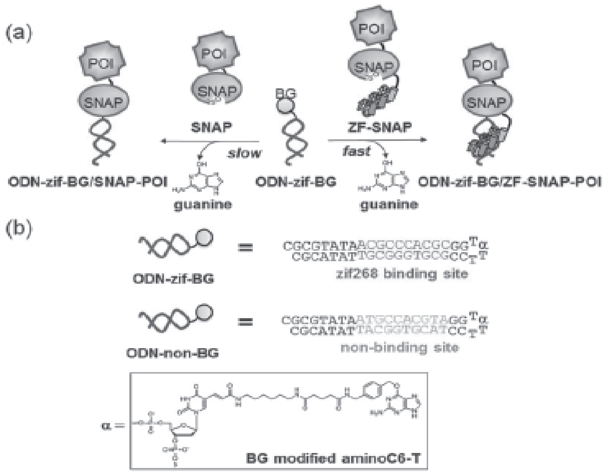

Figure 1. (a) Design of the zinc finger (ZF) adaptor and (b) the nucleotide sequence of ODN-zif-BG and ODN-non-BG, and chemical structure of BG-modified T (denoted as “α”).

Formation of a covalent linkage between ODN-zif-BG and ZF-SNAP was analyzed by denaturing polyacrylamide gel electrophoresis (PAGE). Formation of a covalent linkage between ZF-SNAP and ODN-zif-BG was confirmed as 90% yield after 30 min incubation at ambient temperature. Because no detectable amount of the crosslinking product was obtained for SNAP and ODN-zif-BG within the same reaction time, the results clearly demonstrated that the zif268 domain accelerated the formation of a covalent linkage at the SNAP moiety of the ZF-SNAP modular adaptor. The sequence selectivity of covalent linkage formation was also confirmed by comparing the reactions of ZF-SNAP with ODN-zif-BG and with ODN-non-BG, BG modified ODN containing a nonspecific DNA sequence to zif268 (Figure 1b). The efficient location of the modular adaptor-conjugated autofluorescent protein (ZF-SNAP-EGFP) as a model of POIs onto the programmed and BG-modified addresses on DNA nanoscaffolds by using the modular adaptor ZF-SNAP was confirmed by AFM analysis.

Formation of covalently linked assemblies of POIs through a modular protein adaptor is ideal for reducing the possible inactivation of POIs and as well as background reactions resulting from excess free POIs in the system for the study of the effect of proximity on reaction efficiency on DNA nano-scaffolds such as DNA origami.

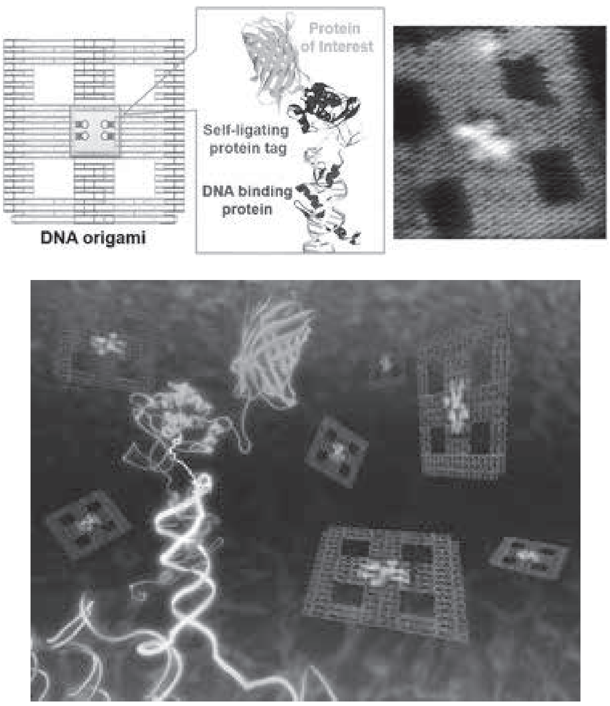

Figure 2. (top) The concept and AFM image of the covalent linkage between modular adopter (ZF-SNAP) modified POI (*e.g.* EGFP) and BG-modified DNA on DNA nanoscaffolds. (bottom) The conceptual illustration.

3. Regulation of fibrillation of an aggregation core peptide in the second repeat of microtubule-binding domain of human tau by phosphorylation

Amyloid-type aggregation has been extensively studied to clarify the mechanism of self-assembling by proteins and peptides, which is controlled by physicochemical parameters such as pH, temperature and ionic strength. Understanding the mechanism of the spontaneous formation of ordered biomolecular assemblies has been of great interests for its potential applications in the biomedical and bioengineering fields.

We focus on the aggregation properties of the hexapeptide VQIINK (PHF6*) located in the second repeat of human tau microtubule-binding domain. The aggregation properties of them were evaluated by using ThT fluorescence measurement, FTIR, CD measurement, and AFM and TEM observation. The PHF6* derivative peptides that contain the additional five amino acid residues including the putative tau phosphorylation site Ser285, either in the nonphosphorylated (PHF6*S) or in the phosphorylated (PHF6*pS) state, showed higher fibril formation tendency than PHF6* itself, possibly through assisting the proto-fibril formation. The flanking sequence of the aggregation core does contribute to the fibril stability. All the peptide fibrils possessed the typical cross-β structure, while the appended five amino acid residues likely formed non-β-sheet type structures. Most importantly, the phosphorylation and dephosphorylation of Ser sensitively controlled the stability of the fibrils in neutral and acidic conditions. Phosphorylation and dephosphorylation play key roles to the change of the aggregation property of the PHF6* derivative peptides as observed for the cases of the other hexapeptide VQIVYK (PHF6), which locates in the third repeat and PHF6 derivative peptides. The net charge and the positional effect of charged amino acids in the peptide are the critical factors to determine the stability of the fibrils.

PHF6* formed the amyloid-type fibrils with less stability than that formed by PHF6 peptide. A possible explanation for this phenomenon is the loss of hydrophobic interactions in the π-stacking between Tyr residues. The Tyr residue was found to be essential for the assembly of paired helical structures of the filament because the replacement of Tyr with Asn resulted in a morphological shift towards the formation of straight filaments.

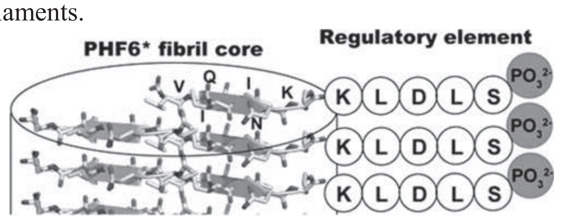

Figure 3. The regulatory element of the aggregation of PHF6* peptide and their phosphorylation

These research projects were partly supported by a Grant-in-aid for Scientific Research from Ministry of Education, Science, Sports and Culture, Japan (No. 25620131, 25248038 to T. M., 26620134, 26107710 to E. N. and 26810090 to S. N.).

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Structural Energy Bioscience Research Section

M. Katahira, Professor
T. Nagata, Associate Professor
T. Mashima, Program-Specific 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 components of wood biomass at atomic resolution. The analysis is usefule to develope 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 2014.

2. Direct identification of LCC in natural wood biomass by NMR

Three major components of wood biomass are cellulose, hemicellulose and lignin. Although bonding between lignin and sugar is assumed, precise information on the bonding has not been obtained for natural wood biomass. It is critical to get this information in order to efficiently utilize wood biomass for the production of bioenergy and various chemical materials. We have analyzed the lignin carbohydrate complex (LCC) of natural wood biomass by NMR (in collaboration with Prof. Watanabe and Dr. Nishimura of RISH, Kyoto Univ.). Combined use of HSQC, HMBC and HSQC-TOCSY spectra identified the ether bond between an α position of the lignin and the sugar. Further analysis with methylene-filtered HSQC indicated the involvement of a 6-position of a hexose sugar in the bond. Thus, we have directly identified the LCC structure of the natural wood biomass for the first time. This methodology with NMR is expected to be applied for the identification of other types of LCC structures.

3. Real-time NMR analysis of the substrate specificity of the antiviral factor APOBEC 3G

Human APOBEC3G protein (A3G), an anti-HIV-1 factor, is a highly sequence specific deaminase that converts CCC within single stranded DNA (ssDNA) into CCU. We investigated the nucleic acid determinants for deamination by A3G using a real-time NMR method in combination with a series of ssDNA substrates each carrying a nucleotide analog at a single or multiple positions. We showed that the sugar and base moieties of the consecutive 5 nucleotides, positioning the CCC hotspot at the center (Fig. 1) play an important role for A3G to exert its activity. We then showed that A3G can tolerate the introduction of either a 2'-OH substitution in the sugar moiety or the removal of the base in the consecutive poly-nucleotide to slide along an ssDNA and exert the 3'→5' polarity. This suggests that the electrostatic interaction between A3G and the phosphate backbone of an ssDNA is the key for sliding. This idea was confirmed by the fact that the 3'→5' polarity is dependent on the NaCl concentration. Altogether we have observed A3G's deamination reaction directly and unambiguously, and thus we have successfully showed that the combination of a real-time NMR method and a chemically modified nucleotide substrates is a powerful strategy for analyzing deamination activity.

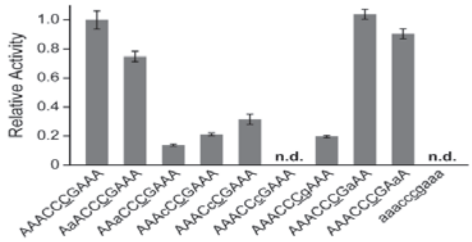

Fig. 1 The Effect of 2'-OH substitution on A3G's activity The activity of A3G reduces significantly when 2'-OH is introduced (lower case) within 5 nucleotide positioning the CCC hotspot at the center.

4. Development of Tat-binding aptamer whose activity switches on in response to K^+

The concentrations of K^+ is low (~ 5 mM) outside the cell and high (~ 100 mM) inside the cell. Therefore, a molecule that senses the K^+ concentration and switches the function may be utilized for a molecular tool that functions either inside or outside the cell. Since, an RNA, r(GGA)$_3$GG, named R11, changes from single-stranded elongated form into a compact quadruplex structure in response to K^+, it could be used as a K^+-switch. To challenge this idea, we have chimerized R11 and Tat aptamer. Tat aptamer is an RNA that specifically and strongly binds to HIV Tat protein. We split this Tat aptamer into two subunits and connected each to the 5'- and 3'-ends of R11 (named QTAp). We examined the binding of QTAp to Tat peptide (16-mer) derived from Tat that is labeled with FAM and TAMRA fluorescent dyes at the N- and C-termini, respectively. Tat peptide was mixed with QTAp. In the absence of K^+, fluorescence was not observed because of contact quenching, indicating that the Tat peptide remains un-stretched because QTAp is unstructured and exhibits no binding to the Tat peptide. However, upon addition of K^+, strong fluorescence was observed as a result of an efficient intramolecular FRET. This is due to the separation of TAMRA and FAM by the stretch of Tat peptide upon binding to QTAp, which reveals that aptamer activity was restored through the formation of quadruplex in QTAp in the presence of K^+. Additionally, we have shown that K^+ but not Na^+ can switch the activity of QTAp. Thus, we have demonstrated that R11 can be combined with aptamer and add K^+-switch to its function, which may be applied to a development of therapeutic drug and advanced drug delivery system.

5. Elucidation of the recognition mechanisms of telomeric DNA and TERRA by TLS

TLS is involved in gene expression, maintenance of genomic integrity, miRNA processing, and so on. TLS reportedly take parts in telomere shortening by recruiting the histone modifying enzyme via formation of ternary complex with G-quadruplexes, i.e. telomeric DNA and its transcriptional product, TERRA. To obtain interaction information at atomic resolution, we pursued a series of NMR titration experiments. We analyzed in particular the chemical shift perturbation of aromatic residues in TLS. F506 in TLS was similarly perturbed upon addition of either telomeric DNA or RNA, or both. On the other hand, the perturbation of Y479, Y484 and F494 in TLS upon addition of telomeric DNA was different to that upon addition of TERRA. Additionally, the chemical shifts of two tyrosines in the ternary complex were similar to those in TLS:TERRA binary complex. Accordingly, here we propose binding models for binary and ternary complexes (Fig. 2). In the cases of the TLS binary complexes, each with telomeric DNA and TERRA, four aromatic residues are involved in interaction. In contrast, in the ternary complex, Y479 and Y484 of TLS located at the interface with TERRA, whereas F506, and probably F494, too, recognizes telomeric DNA. Our findings add information to understand a molecular insight into how TLS recognizes telomeric DNA or TERRA, and forms the ternary complex to regulate telomere shortening.

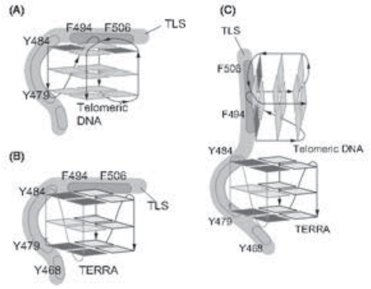

Fig. 2 Model of binary and ternary complex
(A) TLS in complex with telomeric DNA. (B) TLS in complex with TERRA. (C) TLS in complex with telomeric DNA and TERRA.

6. Toward the better utilization of woody biomass by wood degrading enzymes

Woody biomass is composed of cellulose, hemicellulose, and lignin. Cellulose has been turned into bioethanol. Although hemicellulose and lignin have potentials to be used to produce bioethanol and biomaterials, their chemical properties are not fully understood. This is mainly due to the complexity of their structure in woody tissue. We have started a study to investigate the structure-function relationships of the enzymes of white-rot fungus (highly selective lignin-degrading) that catalyze the degradation of cellulose, hemicellulose, and lignin. We are particularly focused on cellulases and manganese peroxidases (MnPs), the latter is known to degrade lignin. We have constructed the protein expression systems of several cellulases and MnPs with P. pastoris and E. coli, respectively. This year, we have obtained a high expression for one of the MnPs. This MnP was purified from inclusion body to a single protein after Ni-column chromatography, which was then followed by refolding procedure in the presence of iron-containing porphyrin, hemin. Formation of the MnP and hemin complex was confirmed by finding the maximum at 410 nm in UV spectrum. Moreover, we have found that this MnP possesses oxidase activity by using 2,6-dimethoxyphenol-based assay. Currently, we are optimizing the conditions to express, purify, and refold MnP in large scale. Preparation of cellulases is also underway. We are intending to solve the structure and elucidate the catalytic mechanism, by which we want to find the way to effectively enhance their activity.

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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

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Advanced Energy Utilization Division

Arivazhagan Rajendran, Program-Specific Lecturer

1. Introduction

DNA molecules are not merely associated with genetics and the carrying of information. They have been used as excellent building blocks in structural DNA nanotechnology due to their unique structural motifs, robust physicochemical properties, and self-assembling nature. In 1980's, Seeman proposed a theoretical model for the construction of nanomaterials using DNA, and subsequently DNA was used for the construction of increasingly complex shapes and patterns.[1] Using his method, various two-(2D) and three-dimensional (3D) structures have been prepared. However, the size of the nanostructures prepared in this method was relatively small which is not suitable for diverse applications. In the search for increasing the size of the DNA nanostructures, in 2006, Rothemund developed a versatile and simple method called "scaffolded DNA origami" for the preparation of larger nanostructures of almost any arbitrary shape with roughly 100 nm in diameter.[2] This method was successfully applied for the preparation of larger 2D (Fig. 1) and 3D structures of custom designed shapes. These nanostructures were also used for the nano patterning of various functional molecules, and single-molecule analysis of various chemical and biological reactions and functions.

One of the most salient features of DNA origami method is that each position on the structure has a precise address by means of sequence codes of the staple DNAs. The number of the staples define the number of such unique positions on the surface of the nanostructure, and the staple strands server as attachment point for different kinds of nanoobjects. This makes these structures as potential scaffolds for wide range of applications.

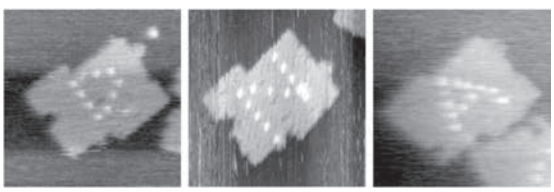

Fig. 1. Atomic force microscopy (AFM) images of the jigsaw-shaped DNA origami nanostructures prepared by "scaffolded DNA origami method" bearing the alphabets D, N, and A. Image size: 200 × 200 nm.

2. DNA origami preparation, self-assembly, and single-molecule analysis

I have been working on the preparation and self-assembly of DNA origami nanostructures to create micrometer scale structures that can be used for several applications such as fabrication of nanodevices (Fig. 1).[3-5] Further, I have been using these structures for the analysis of various biomolecular reactions and functions.[6-9] Now, I am using these DNA origami nanostructures for the assembly of enzyme cascades in predetermined patterns. Such an assembly is promising to mimic the biomolecular systems and can be successfully applied for the biomolecular energy conversion through controlled enzymatic reactions. Further, I aim to use these structures for the analysis of various proteins that play vital role in biomolecular energy conversion and utilization. Among the protein systems, human mitochondrial transcription factor A (TFAM) is one of the interesting proteins that is attractive to study using DNA origami method.

3. Human mitochondrial transcription factor A

Mitochondria are the small structures in cells that ranges from 0.5 to 1.0 μm in diameter. They generate energy for the cell to use and thus are often called "powerhouses" of the cell. They provide 30 molecules of adenosine triphosphate (ATP) per glucose, in contrast to two ATPs produced by glycolysis. They are essential for all higher organisms for sustaining life. Though most part of the human genome is located in the nucleus, mitochondria has its own DNA which is circular and double stranded, and its length is 16,569 base pairs. Mitochondrial DNA encodes two ribosomal RNAs (rRNAs), 22 transfer RNAs (tRNAs), and 13 of the about 80 subunits participating in oxidative phosphorylation. TFAM is a multifunctional protein which is essential for mitochondrial DNA packaging and maintenance. Further, it plays crucial role in transcription.[10]

The analysis of the structure and function of TFAM promises to offer the insights not only to the DNA packaging and maintenance, and its role in transcription, but also highly important for the biomolecular energy production and its utilization in higher organisms. Hence, I focus my studies on the analysis of DNA-TFAM interaction at molecular level using the DNA origami scaffold. The DNA folding nature of TFAM, the transcription initiation, and transcription machinery recruitment are investigated in detail. Further, the balance between the specific DNA sequence binding and non-specific binding, and their effect on the transcription and DNA packaging are studied in detail.

After successful investigations on the structure, function, and molecular interactions of TFAM with mitochondrial DNA, I aim to use this protein for the design of biomolecular switches for the development of biomolecular sensors.

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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) Binding of an RNA aptamer and a partial peptide of a prion protein: Crucial importance of water entropy in molecular recognition [1]

We have investigated the driving force for the binding of R12 (an RNA aptamer) and P16 (a partial peptide of a prion protein) during which P16 exhibits the global structural change. We calculate changes in thermodynamic quantities upon the R12-P16 binding using a statistical-mechanical approach combined with molecular models for water which is currently best suited to studies on hydration of biomolecules. The binding is driven by a water-entropy gain originating primarily from an increase in the total volume available to the translational displacement of water molecules in the system. The energy decrease due to the gain of R12-P16 attractive (van der Waals and electrostatic) interactions is almost cancelled out by the energy increase related to the loss of R12-water and P16-water attractive interactions. We can explain the general experimental result that stacking of flat moieties, hydrogen bonding, and molecular-shape and electrostatic complementarities are frequently observed in the complexes. The water-entropy gain is largely influenced by the geometric characteristics (overall shapes, sizes, and detailed polyatomic structures) of the biomolecules.

(A-2) Physical origins of the high structural stability of CLN025 with only ten residues [2]

CLN025 with only 10 residues folds into a specific β-hairpin structure (“native structure”). We have investigated its stabilization mechanism using our free-energy function F. F comprises two components, hydration entropy S and component related to the energetic dehydration effect Λ. S is calculated using the hybrid of the angle-dependent integral equation theory and our recently developed morphometric approach. A molecular model is employed for water. Λ is calculated in a simple but judicious manner accounting for physically the most important factors: the break of polypeptide-water hydrogen bonds and formation of polypeptide intramolecular hydrogen bonds upon structural change to a more compact one. We consider the native structure, compact nonnative structures newly generated, and a set of random coils mimicking the unfolded state. The loss of the conformational entropy upon folding is estimated using a simple but physically reasonable manner. We find that the key factor is the water-entropy gain upon folding originating primarily from an increase in the total volume available to the translational displacement of water molecules in the system, which is followed by the reduction of water crowding. The amino-acid sequence of CLN025 enables it not only to closely pack the backbone and side chains including those with large aromatic groups but also to assure the intramolecular hydrogen bonding upon burial of a donor and an acceptor when the backbone forms the native structure. The assurance leads to essentially no enthalpy increase upon folding. The close packing brings a water-entropy gain which is large enough to surpass the conformational-entropy loss.

(A-3) Statistical thermodynamics for functionally rotating mechanism of the multidrug efflux transporter AcrB [3]

AcrB, a homotrimer, is the pivotal part of a multidrug efflux pump. A "functionally rotating" picture was proposed for the drug transport by AcrB, but its mechanism remains unresolved. We have investigated energetics of the whole functional rotation cycle using our theoretical methods. We find that the packing efficiency of AcrB is ununiform and this ununiformity plays imperative roles primarily through the solvent-entropy effect. When a proton binds to or dissociates from a protomer, the packing properties of this protomer and its two interfaces are perturbed overall in the direction that the solvent translational entropy is lowered. The packing properties of the other two protomers are then reorganized with the recovery or maintenance of closely packed interfaces so that the solvent-entropy loss can be compensated. The functional structural change by an isolated protomer would cause a seriously large free-energy increase. By forming a trimer, any free-energy increase caused by a protomer is always cancelled out by the free-energy decrease brought by the other two protomers via the mechanism mentioned above. The functional structural rotation is thus accomplished using the free-energy decrease arising from the transfer of only a single proton per cycle. We also point out the similarities to F_1-ATPase.

(B-1) Study of bumpiness effect on fast ions generated by ICRF minority heating in Heliotron J [4]

The fast ion confinement and ion heating efficiency is studied using ICRF minority heating. The better confinement in the high bumpiness and the localization of fast ions in the high-field side heating in the medium bumpiness, have been found in the experiment and simulation.

Fast ion velocity distribution is investigated using fast protons generated by ICRF minority heating in Heliotron J, a low-shear helical-axis heliotron (R_0 = 1.2 m, a = 0.1-0.2 m, $B_0 \leq$ 1.5 T). Majority species is deuterium. The fast ions are measured by a charge-exchange neutral particle energy analyzer (CX-NPA) installed at the opposite position in the toroidal angle to the ICRF antennas. However, the detectable area is limited because of the diagnostic port arrangement for the CX-NPA. Therefore, the model calculation is important to understand fast ion distribution. We develop a Monte-Carlo calculation code for the fast ion confinement under the ICRF heating. This code is revised to estimate velocity distribution from bounded volume. The calculation is performed to estimate the toroidal dependence in each magnetic configuration.

In the low density condition of 0.4 × 10^{19} m^{-3} in line-averaged density, the on-axis proton cyclotron layer, the calculation was performed for three bumpiness configurations (high, medium and low). The plasma volume is divided into 16 areas in toroidal and poloidal directions. In the corner section of the plasma, the high-energy tail accelerated by ICRF heating is observed at about 60° and 120° in pitch angle for low bumpiness. The loss region in velocity space is located on both sides of 90° in vacuum Heliotron J magnetic field and the ICRF acceleration is basically perpendicular direction. From these effects, the high-energy tail is formed on the both sides of 90° in velocity space. The high-energy tail at 60° is very small in the high bumpiness and smallest in the medium bumpiness. In the straight section of the plasma, the high-energy tail at about 60° and 120° are clearly observed in the high bumpiness. The tail at 60° in the medium bumpiness is smallest in this position as well. In all cases, the tail at 120° is larger than that at 60°. The tail angle is slightly different each other. The tail near 120° is moved to smaller angle from the high bumpiness to the low bumpiness.

In the experiment, the acceleration of the fast ions injected by NBI heating is tried using ICRF heating in the high bumpiness configuration. The high-energy ion enhancement is considered to be useful to increase fusion reaction rate in the plasma core. Two units, BL-1 and BL-2 are used, of which power is 400 kW and 100 kW, respectively. ICRF injected power is about 250 kW in this case. The CX-NPA observes fast ions mainly injected by BL-2. The line-averaged density is 1.0 × 10^{19} m^{-3}, which value is larger than ordinary fast ion experiment because of the increase of absorption of injected NBI power. The ion temperature of the target plasma is from 100 eV to 200 eV. Near the injection pitch angle, the ions with the energy up to 38 keV are observed during ICRF pulse, where the injection energy (E_0) of BL-2 is 24 keV. Without ICRF pulse, the peak of $E_0/2$ and $E_0/3$ can be observed, however, the number of fast ions increases during pulse, then, the peak of $E_0/2$ disappears. Far from the injection pitch angle, the high-energy tail is observed up to 24 keV, however, this value is lower than that new injection angle.

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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，佐野史道，水内亨，長崎百伸，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、長崎百伸、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，長崎百伸、大島慎介、佐野史道、水内亨、岡田浩之、南貴司、小林進二、山本聡

核融合科学研究所, 先進ヘリカルによるプラズマ構造形成･不安定制御と閉じ込め磁場最適化の研究，佐野史道、水内亨、長崎百伸、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, ヘリオトロン J 装置における機械振動自己補正型干渉計の設計検討，水内亨、大島慎介、岡田浩之、佐野史道、門信一郎、長崎百伸、小林進二、南貴司

核融合科学研究所, トロイダル系閉じ込め装置における密度分布の動的挙動に係わる物理機構の解明と比較研究，佐野史道、水内亨、小林進二、南貴司、長崎百伸、岡田浩之

核融合科学研究所, ヘリオトロン J におけるビーム放射分光法による密度揺動の二次元分布計測, 水内亨、小林進二、大島慎介、岡田浩之、門信一郎

核融合科学研究所, 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，佐野史道、長崎百伸、水内亨、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，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, 佐野史道、水内亨、岡田浩之、長崎百伸、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, ヘリオトロン J における高エネルギー粒子の速度分布関数の解析，佐野史道、岡田浩之、水内亨、南貴司、小林進二、長崎百伸、山本聡

核融合科学研究所, ダイバーター熱流束分布モニタリングシステムの開発，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, ヘリオトロン J におけるコンパクトサイズペレット入射装置を用いたプラズマ高密度化研究, 佐野史道､門信一郎､長崎百伸、水内亨、岡田浩之

核融合科学研究所, ヘリオトロン J 装置における ICRF 加熱を用いた高速イオン閉じ込めの磁場最適化研究, 佐野史道、岡田浩之、水内亨、南貴司、小林進二、長崎百伸、山本聡、大島慎介

核融合科学研究所, 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, 佐野史道、岡田浩之、南貴司、長崎百伸、山本聡、大島慎介、水内亨

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核融合科学研究所，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, 佐野史道、岡田浩之、小林進二、山本聡、南貴司

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核融合科学研究所, 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, 佐野史道、山本聡、小林進二、大島慎介、岡田浩之、南貴司、長崎百伸、水内亨

核融合科学研究所, 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, 佐野史道、岡田浩之、水内亨、長崎百伸、山本聡、小林進二、南貴司

核融合科学研究所, ヘリオトロン J, CHS, LHD 装置における重水素プラズマの粒子輸送の研究, 佐野史道、山本聡、南貴司、水内亨、大島慎介、小林進二、長崎百伸、岡田浩之

核融合科学研究所，MHD 不安定性の閉じ込め性能に与える影響の研究，佐野史道、岡田浩之、長崎百伸、小林進二、山本聡、南貴司、水内亨

核融合科学研究所, ヘリオトロン J における偏光マルチパストムソン散乱システムの開発, 佐野史

道、南貴司、岡田浩之

Financial Support

Grant-in-Aid for Scientific Research
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S. Murakami, H. Oshima, T. Hayashi, M. Kinoshita, Theoretical Prediction of Thermal-Stability Changes upon Mutations of a Protein，Biophysical Society 59th Annual Meeting，Baltimore Convention Center, Maryland, USA，2015.2.7-11

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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 and the corresponding techniques, in areas of science and technology to private companies. The representative facilities, DuET & MUSTER, were historically dedicated for the research on energy science and technology, with the special emphasis on fusion reactor materials R&Ds. Due to this reason many of nuclear material relevant subjects are running in the beginning of the ADMIRE. The current project, however, is flexible to accept any new ideas from the industries 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 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 clear understandings of 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.

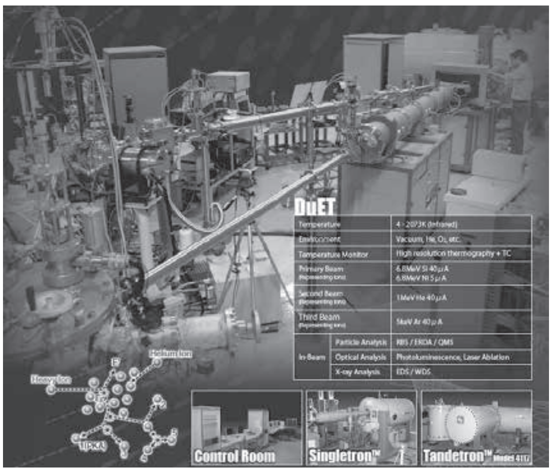

Fig. 1 Summary of the DuET facility set-up.

Testing by ion-irradiation is extremely useful to R&D of the nuclear materials because the flux "or damage rate" is very large (and it is easily controllable!) and conditions are accurate comparing to the testing in nuclear reactors. Thus, many advanced materials, such as silicon carbide and nuclear grade graphite, pro-vided by multiple commercial companies were tested within the ADMIRE framework. Although, we originally specialize in the irradiation study, some difficulties in testing the advanced materials, especially porous ceramic materials, were experienced. However, the developed methods (WO2014034829 A1) successfully revealed a unique irradiation effects observed in those materials, such as the anisotropic dimensional change of the graphite materials, which were presented at the internal and international con-francs.

On the other side of the DuET work is the creation of the functional materials, such as gradient materials, by implanting the specific ions which is originally absent in the matrix constituents. Unfortunately, most topics cannot be discussed 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.

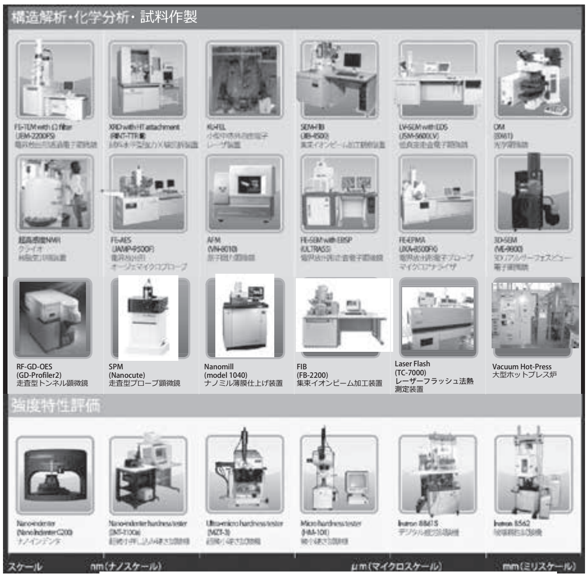

Fig. 2 Summary of the MUSTER equipment (selected).

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

Various analytical devices and mechanical testing machines are included in the MUSTER facility; each covers different 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 perticipated in the MUSTER in early 2013. Some upgrading and expanding of the MUSTER equipments, such as the installation of new 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 33 subjects are running, where the percentage of operating time for the ADMIRE related work is more than 50% (averaged, DEC 2013) 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 200kV 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 2015, faculty professors are excluded in the following list).

- Hideki Matsui, Ph. D., Specially Appointed Professor, Liaison officer.
- Reine Sakamoto, Secretary.
- Okinobu Hashitomi (IAE staff), Administrator of DuET accelerators.
- Takamasa Ohmura (IAE staff), Administrator of MUSTER facility and more.
- Yasunori Hayashi, Program-Specific Researcher.
- Aya Kitamura (WDB Eureka), Technical assistance and training staff.
- Yoosung Ha, Ph. D., Program-Specific Researcher.
- Siwei Chen, Ph. D., Program-Specific Researcher.
- Han Wentuo, Ph. D., Program-Specific Researcher.

Financial Support

MEXT Program on "Project for Creation of Research Platforms and Sharing of Advanced Research Infrastructure."

Publications

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近藤創介，SiC 材料の照射損傷研究への課題，原型炉開発にむけたブランケット工学開発の役割と強力中性子源の位置づけ，NIFS，2015.2.17

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3-3. AWARD

Top Prize of Poster Session Awarded at AESJ 2015 Spring Annual Meeting

Advanced atomic energy research section
Shutaro Takeda (D1)

Atomic Energy Society of Japan, founded in 1954, holds annual meetings twice a year, in spring and in autumn. At 2015 spring annual meeting, the author was awarded the top prize of poster session award.

The author presented his study, “LFC Simulation-Based Stability Analysis of Japanese Grid of 2040 under DEMO Fusion Plant Operation,” which was highly rated by the judges for its novelty and impact on the society. Current fusion plant design assumes a frequency target of 0.5 times per year for the plasma disruption; however, this target had not been evaluated quantitatively before. However, the Japanese power system in 2040 is expected to be much more unstable than that of today, because of larger renewables installation. Hence, a quantitative evaluation of the target was needed. In his study, the author carried out the first study of its kind, using a load frequency control simulator developed for this study. The results indicated that upon a sudden interruption of fusion output power, as represented by a plasma disruption, the frequency of the east power system of Japan ion 2040 would sustain a deviation of 0.4 Hz in 6.8 sec. Additionally, it was also indicated that the adverse effects of sudden interruption would ripple to the north and the middle-west system. Thus, the author suggested the necessity of development of an energy storage to mitigate these effects. An innovative energy storage, marine inverse dam, was also proposed in this study.

Best poster award – Second prize in 28th Symposium on Fusion Technology

Advanced Atomic Energy Research Section
Hyoseong Gwon (D3)

The symposium on fusion technology was founded in 1960. The symposium on fusion technology is the major event to exchange information on design, construction and operation of fusion experiments and on the technology for present fusion machines and future power plants. Symposium on fusion technology has been held once every two years in Europe.

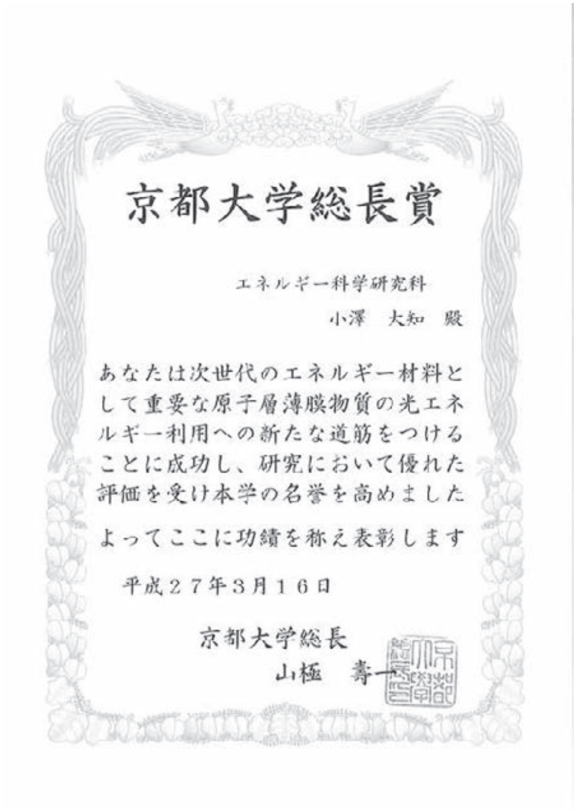
In the 28th symposium on fusion technology, I presented a work on thermal structural behavior of divertor under edge localized modes, ELMs. The heat flux to the target surface of the ITER divertor is assumed to be subject to average 10 MW/m^2 and 20 MW/m^2 in slow transient. However, recent researches recognize the possibility that ELMs would give a heat flux of several hundred MW/m^2 with short pulse width. ELMs-like pulse heat load would cause severe damages of plasma facing materials and affect the operation of the reactor. Thus thermal structural response should be considered. A YAG laser was introduced to simulate ELMs-like pulse heat load for the tungsten target in this study. The experimental results were compared with analytical results by finite element method, FEM. Based on the results the thermal structural behavior of tungsten target under ELMs was evaluated. When 0.25 MJ/m^2 of energy flux was applied to tungsten target, cracks and plastic deformation occurred at the target surface even though recrystallization was not confirmed. It implied that the tungsten target could be damaged by thermal stress even at below 0.5 MJ/m^2 which is the ITER divertor allowable heat load. In addition the compressive and the tensile stress along x axis were more dominant than the shear stress under ELMs.

Kyoto University president Award

Advanced Energy Materials Research Section
Daichi Kozawa (D3)

Kyoto University President Award annually recognizes students and student organizations that contributed to redounding the University's prestige through their achievements in academic, extracurricular, and public-service activities (http://www.kyoto-u.ac.jp/en/about/profile/honor/awards_b/president.html).

I won the award by the series of works on developing optoelectronic properties of two-dimensional crystals.



京都大学総長賞

エネルギー科学研究科
小澤　大知　殿

あなたは次世代のエネルギー材料として重要な原子層薄膜物質の光エネルギー利用への新たな道筋をつけることに成功し、研究において優れた評価を受け本学の名誉を高めました

よってここに功績を称え表彰します

平成２７年３月１６日

京都大学総長
山極　壽一

Poster Award

Advanced Energy Materials Research Section
Daichi Kozawa (D3)

Association for Condensed Matter Photophysics has been founded since 1990 to have a discussion on condensed matter photophysics with young researchers. Annual meetings have been held every year mainly in Kansai area.

In the 25th annual meeting, I presented a work on giant light absorption and photocarrier relaxation process in transition metal dichalcogenides.

Certificate of
Award for Encouragement of Research in
Condensed Matter Photophysics

Daichi Kozawa

Giant light absorption and photocarrier relaxation in atomic layers of transition metal dichalcogenides

石原　一
Hajime Ishihara
Chair of Organizing Committee
25th Symposium (December 12-13, 2014)
Association for Condensed Matter Photophysics, Japan

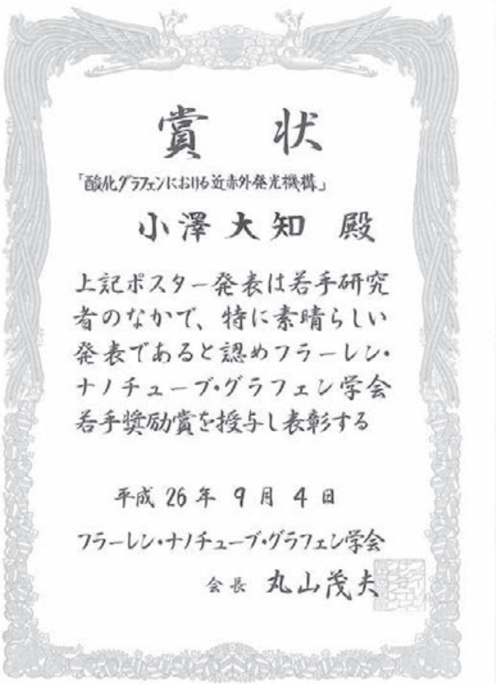
December 19, 2014
光物性研究会

Poster Award

Advanced Energy Materials Research Section
Daichi Kozawa (D3)

The Fullerenes, Nanotubes and Graphene Research Society has been established in 1991 to create an opportunity to provide information concerning basic science and applied technology relating to nano carbon based materials such as fullerenes, carbon nanotubes and graphene and to provide an opportunity for members to get together (http://fullerene-jp.org/en/main23_const.html). Bi-annual meetings are hold in every spring and autumn.

In the 46th Fullerenes-Nanotubes-Graphene General Symposium, I presented a work on Mechanisms of Near-Infrared Photoluminescence from Graphene Oxides.



賞　状

「酸化グラフェンにおける近赤外発光機構」

小澤大知　殿

上記ポスター発表は若手研究者のなかで、特に素晴らしい発表であると認めフラーレン・ナノチューブ・グラフェン学会若手奨励賞を授与し表彰する

平成26年9月4日

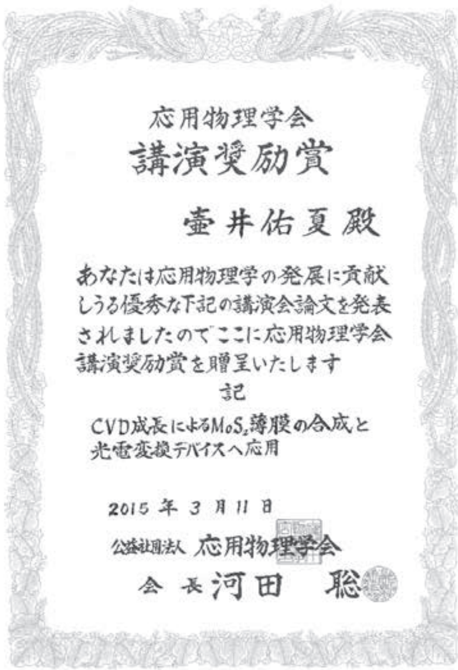
フラーレン・ナノチューブ・グラフェン学会

会長　丸山茂夫

Young scientist oral presentation award of the Japan Society of Applied Physics

Advanced Energy Materials Research Section
Yuka Tsuboi (M2)

The Japan Society of Applied Physics was founded in 1949 as a nonprofit, educational organization concerned with a broad range of applied physics. The meetings have been held two times every year.
In the spring autumn of 2014, I presented a work on CVD growth of MoS_2 thin film and its photovoltaic device applications.



応用物理学会

講演奨励賞

壷井佑夏殿

あなたは応用物理学の発展に貢献しうる優秀な下記の講演会論文を発表されましたのでここに応用物理学会講演奨励賞を贈呈いたします

記

CVD成長によるMoS_2薄膜の合成と光電変換デバイスへ応用

2015年3月11日

公益社団法人　応用物理学会

会長　河田　聡

Outstanding Poster Presentation Award in 14th International Symposium on Nucleic Acids Chemistry

Biofunctional Chemistry Research Section
Huyen Dinh (D1)

The International Symposium on Nucleic Acids Chemistry has started from 1973 as an annual domestic meeting of Nucleic Acids Chemists in Japan, and has become an international symposium in 2005 by inviting Nucleic Acids Chemists from all over the world. This symposium has been held every year in Japan.
In the 14th international symposium, I presented our research topic by following title, “Application of DNA binding proteins for assembling proteins RuBisCO and Carbonic Anhydrase on DNA nanoscaffold”. In living cells, many metabolic pathways are confined to specific compartments as solutions to facilitate efficient diffusion of intermediates from one enzyme to the others by substrate channeling and protein encapsulation. Despite of the generality of these strategies in nature, construction of rationally organized enzymes in vitro remains a major challenge for bioengineering. DNA nanostructures such as DNA origami are one of the ideal scaffolds for this purpose by taking advantage of the addressable nature. DNA origami has been used as a molecular switchboard to arrange cascade enzymes with nanometer scale precision. In this study, I have focused on carboxysome, which is a bacterial microcompartment that contains enzyme RuBisCO involved in carbon fixation and Carbonic Anhydrase (CA). In the carboxysome, CA helps to increase the local concentration of CO_2 in proximity to the carbon-fixing enzyme RuBisCO, consequently reducing its reaction with O_2, a competing substrate. DNA binding adaptors and DNA nanoscaffold has been used to construct an artificial assembly of RuBisCO and CA in order to study the effect of spatial factors and the ratio of two enzymes on the CO_2 fixation reaction. Adaptor-fused GCN4-RuBisCO and zif-SNAP-CA were constructed and their DNA-binding ability and enzymatic activity on DNA nanoscaffold were confirmed. Construction and characterization of the co-assembly of GCN4-RuBisCO and zif-SNAP-CA was discussed. The poster was well received, and even garnered a poster award.

Outstanding Oral Presentation Award in 2014. The 41st International Symposium on Nucleic Acids Chemistry

Biofunctional Chemistry Research Section
Annoni Chiara (Post-doc)

The International Symposium on Nucleic Acids Chemistry has been founded in 1973 and has become an international gathering in 2005 by inviting to Japan Nucleic Acids Chemists from all over the world. Nowadays, ISNAC is one of the biggest symposiums of bio-related chemistry which covers multiple aspects of genetic technology, molecular biology, nanobiotechnology, as well as therapeutic and diagnostic applications of this field.
In occasion of the 41st annual meeting, I participated giving an oral presentation about the progresses of our research topic of title “Assessment of both equilibrium and kinetic aspects of ATP-binding ribonucleopeptide (RNP) clusters arranged on DNA nanoscaffold”. Membrane receptors are often found to be arranged in the clustered state on the cell surface; receptor arrangements with specific density, distribution and clustering, may represent a key spatial feature, to gain a better knowledge of how many regulatory signal pathways work. DNA nanotechnologies, thanks to their fully addressable nature, provide a useful tool for the realization of *in vitro* systems to address this question. As we reported previously (*J. Am. Soc. Chem.*, 2006, **128**, 12932; *J. Am. Soc. Chem.*, 2013, **135**, 3465.), fluorescent ribonucleopeptide (RNP) sensors, obtained using as a framework the well-known complex between the Rev peptide and its RNA target, the HIV-1 Rev Responsive Element (RRE), provide a directly readable and highly sensitive detection system for specific ligands. Moreover the conversion to covalently linked sensors allowed handling at nanomolar order concentration proving to be a convenient detection tool also on DNA origami nanoscaffold. In this work, receptor clustering effect was investigated analyzing both the equilibrium and kinetic aspects of ATP-binding RNP sensors programmatically located at defined spatial orientations on DNA origami. The presentation received a satisfactory response from the audience and it was rewarded with an award.

Excellent presentation award in the 16th annual meeting of The RNA Society of Japan

Structural Energy Bioscience Research Section
Yudai Yamaoki (D3)

The RNA Society of Japan was founded in 1999 to provide the opportunity for presentation and exchange of information related to RNA study, which includes expression, function, and structure of RNA and RNA-binding protein, as well as RNA technology, and so on. The 16th annual meeting of this society was held in Aichi, Japan.

In the 16th annual meeting, I presented our latest work entitled "Creation of novel Tat-binding aptamer and ribozyme whose activities switch on in response to K^+ via quadruplex formation". 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. In other words, each of the newly designed molecules contain 5'-domain, R11, and 3'-domain (Figure 1). In the absence of K^+, they showed low activity because the 5'- and 3'-domains located far apart. On the other hand, 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 (Figure 1). We have also found that the induction of their activities is dependent on K^+ and not on Na^+. 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.

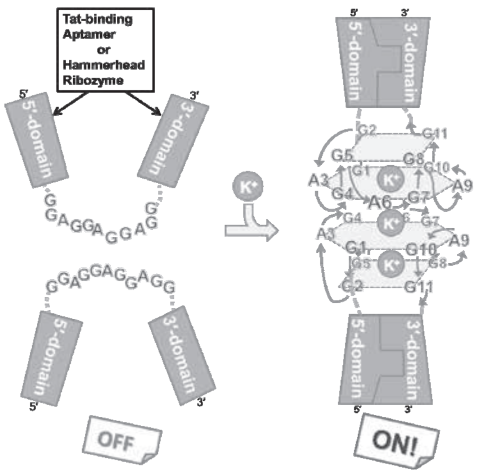


Figure 1. The scheme of the activation of newly designed Tat-binding aptamer and ribozyme.

4. JOINT USAGE/RESEARCH PROGRAM

Joint Usage/Research Program
"Zero-Emission Energy Research"

It is an urgent task to find out the best solutions against the energy and environmental problem for the sustainable development of human beings. 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.

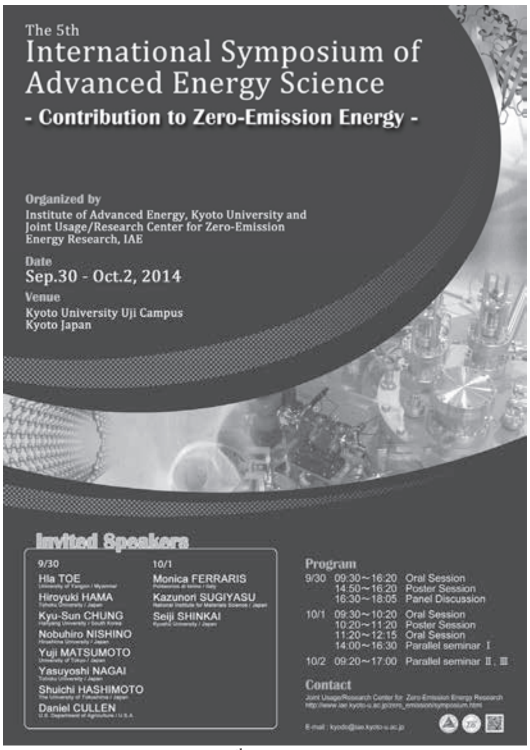


Fig. 1 Poster of the 5th International Symposium

Since FY 2011, we have operated a project, "Joint Usage/Research Program on Zero-Emission Energy", which is the program authorized by the MEXT. 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 new 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 photonics & energy nano-science research.

Many researchers have participated in this program. In FY 2014, Joint Usage/Research collaborations of total 82 subjects (including one workshop) on Zero-Emission Energy were performed with more than 390 visiting participants from 29 all-Japan Universities and Institutions including graduate/undergraduate students. The results of these collaborations are summarized in a report (in Japanese) "IAE Joint Usage/Research Program on Zero-Emission Energy 2014." Some of them were reported and discussed in a Research Summary Session of FY2014 held at Uji Campus on March 4, 2015. 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 5th International Symposium of Advanced Energy Science ~ Contribution to Zero-Emission Energy ~" on September 30 – October 2, 2014 at Uji Obaku Plaza, Kyoto University (Fig. 1). This symposium consists of plenary and poster sessions, panel discussions and parallel seminars. About 259 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/calendar2014.html)

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 2013

(Subject, Principal Researcher, IAE Key Person)

R&D of First-wall Component for Fusion Reactor Using Explosion Welding
K. Hokamoto, R. Kasada

Hydrogen isotope retention behavior for heavy ion implanted tungsten under higher temperature
Y. Oya, T. Hinoki

High value-added biomass originated from a bacterium often found in activated sludge
M. Takeda, M. Katahira

NMR analysis of the interaction between an artficial RNA and a transcription factor
T. Sakamoto, T. Nagata

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

NMR analysis of supramolecular structure of lignin in cell wall for advanced biomass utilization
K. Fukushima, M. Katahira

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

Multiple hydrogen trapping and thermal release at vacancies in high-fluence hydrogen plasma - tunsgten materials interaction
D. Kato, K. Morishita

Development of polymer hybrid nanofiber for the enzymatic transformation of carbon dioxide to alcohol
N. Tanaka, T. Morii

Mechanical properties of dissimilar bonding between low-activation ferritic steel and ODS steel
T. Nagasaka, A. Kimura

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

Phase stability in RAFM and ODS steels under ion irradiation
H. Abe, A. Kimura

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

Development of FP corrosion-resistrained cladding materials in fast reactor application,
K. Fukumoto, A. Kimura

Study on Mechanisms of Radiation Resistance of Advanced Tungsten Alloy
A. Hasegawa, A. Kimura

Effects of Damage and Helium Generation Rates on Bubbles/Voids Formation in Fusion Reactor Structural Materials
T. Yamamoto, A. Kimura

Stuctural analysis of lignin by ultra-high sensitivity NMR for biorefinery
T. Watanabe, M. Katahira

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

Study on Discharge chracteristics of D-T Burning in Discharge Fusion Neutron Source
H. Osawa, K. Masuda

Optimization of a high particle and high temperature loading experiment system using the ion beam test stand, and experiment of a fusion diverter system II
Y. Yamamoto, S. Konishi

Experimental study on chemical behavior of lithium oxide in lithium lead alloy
M. Kondo, S. Konishi

Energy enhancement of KU-FEL using laser photocathode rf gun and its applications
R. Kuroda, H. Ohgaki

Damage Formation Mechanism of Tungsten Under Repetitive and Pulsed High-Heat Load Conditions (Part 3)
K. Ezato, A. Kimura

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

Corrosion properties of Advanced Joints of Reduced Activation Ferritic/Martensitic Steel
T. Hirose, A. Kimura

Study of electron bunch length by measuring

coherent synchrotron radiation with narrow-band detectors
N. Sei, H. Ohgaki

Creation of hierarchical self-assembling architectures in a microfluidic device
M. Numata, E. Nakata

Structural study of the mechanism of signal transduction in eukaryotic translation initiation factor complex
E. Oobayashi, T. Nagata

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

Measurement of active radicals produced by atmospheric pressure plasma jet in the gas-liquid interface
H. Matuura, S. Kado

Development of novel guanine-tethered antisense probes
M. Hagihara, T. Morii

Investigation of methodology for Deliberative Polling based on science education to better reflect public opinion for nuclear power and other energy sources
H. Iwakiri, K. Morishita

A fluorescent probe for imaging of energy metabolism in cells
S. Sato, T. Morii

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

Development of the zero-emission energy oriented boron neutron capture-type antitumor agents.
Y. Uto, E. Nakata

Transport analysis for high energy particles using numerical simulation codes in three-dimensional plasmas
Y. Nakashima, S. Kobayashi

Development and Microstructure Control of Composite Materials for High Thermal Conductivity
G. Sasaki, T. Hinoki

Diagnostics of Plasma Turbulence by Using Micro-Wave
S. Inagaki, K. Nagasaki

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

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

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

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

Study on Fatigue Life Evaluation Method of SiC/SiC Composite
S. Nogami, T. Hinoki

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

High temperature properties of advanced SiC-based materials under multiple environments
K. Shimoda, T. Hinoki

Beat wave ion heating/current drive by EC range waves
H. Shidara, K. Nagasaki

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

Study of atomically thin materials toward novel energy conversion
S. Konabe, K. Matsuda

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

Modeling and simulation of irradiation field dependence on microstructural change in material
Y. Watanabe, K. Morishita

Effects of ion irradiation temperature on dimensional stability and microstructure of advanced SiC/SiC composites
K. Ozawa, T. Hinoki

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

Comparative study of negative triangularity tokamak and helical
M. Kikuchi, K. Nagasaki

Development of Pulsed Radiation Detection Method Emitted from IEC Device
T. Misawa, K. Masuda

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

Control of metallic nanostructure on glass substrates by ion irradiation induced dewetting
T. Shibayama, T. Hinoki

Analysis on molten tungsten motion during the laser material processing and the ion beam irradiation for the robustness evaluation of nuclear fusion reactor walls
K. Ibano, S. Konishi

Study of nonlinear dynamics and structure formation of turbulence in helical plasmas
A. Ishizawa, Y. Kishimoto

Experiment and theory/simulation of the interaction between ultra-short CEP-controlled laser pulses and cluster medium
Y. Fukuda, K. Matsuda

Development of electric double layer capacitors with an extremely high capacity based on surface-induced phase transition in nanoporous electrodes
K. Fukami, M. Kinoshita

Unraveling the optical properties of atomic layers by microscopic spectroscopy
Y. Miyata, K. Matsuda

Assembly of the rare metal binding protein on the DNA nano-structure (DNA origami) towards the development of a rare metal recovery system with high efficiency
Y. Mori, T. Morii

Design of artificial proteins targeting modified nucleic acids
M. Imanishi, T. Morii

Construction of microdevice for multifunctional protein enzymes
Y. Aizawa, T. Morii

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

Radiation effects of ion irradiated 3C-SiC
J. Kai, T. Hinoki

Feasibility Study of Micro Power Plant with 6 Phase Generator for Rural Electrification in Sarawak
H. Ping, H. Ohgaki

Hydrogen isotope behavior under complex fusion irradiation environment
Y. Ueda, A. Kimura

Effect of SFE on irradiation microstructure in Fe-Cr-Ni alloys
K. Yabuuchi, A. Kimura

Microstructure evolution of ion irradiated Ni-based precipitation/dispersion strengthened alloys (for advanced nuclear materials)
S. Ukai, A. Kimura

Microstructure evolution of ion-irradiated oxide/nitride ceramics ～ Role of electronic excitation and selective displacement damage～
K. Yasuda, A. Kimura

Effect of temperature and micro structure on mechanical property in low-activation steel
H. Kinoshita, A. Kimura

Development of attosecond laser pulse generator for measuring ultrafast optical response on solid surfaces
G. Miyaji, K. Matsuda

Study on photocatalytic film synthesis and biological CO2 fixing using infrared free electron laser
T. Sakae, H. Ohgaki

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

Mode-selective phonone excitation in wide-bandgap semiconductor by mid-infrared free-electron-laser
K. Hachiya, H. Ohgaki

Corrosion behavior of advanced structural materials in supercritical pressrized water
Ge-Ping Yu, A. Kimura

Development of a radiative transfer code in Heliotoron J

H. Kawazome, T. Mizuuchi

Study on Photo- and Electronic- Properties of Atomic Layer Materials using Photoluminescence Spectroelectrochemistry
N. Nakashima, K. Matsuda

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

Development of the site-directed RNA mutagenesis for regulating an energy production in the cell
M. Fukuda, 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 in 1996 simultaneously with the institute as an attached facility for research on advanced processes of energy production, conversion and application. On the other hand, resource and energy problems as well as global warming problems become very serious in recent years. We must concentrate all our knowledge and wisdom to find solutions to these problems. From such a viewpoint, the laboratory has been recognized again since FY2006 so that 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. 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 system 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 and MUSTER 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 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 field by utilizing the existing devices such as System for Creation and Functional Analysis of Catalytic Materials, SEMs, SPM, Solar Simulator, TW fs laser, MIR-FEL, 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 project

Summary of the standard cooperative research subjects carried out in the year of 2014.

A public collection of cooperative research application was carried out, in this year, for a program which consists of three groups of “Kiban”, “Syorei” and “Kikaku-chosa” cooperative research. The “Kiban” cooperative research means a program to promote leading research themes of the institute projects. The “Syorei” cooperative research means a program to promote general research themes with respect to the institute projects. The “Kikaku-chosa” cooperative research means a program to promote the cooperative research through a seminar or symposium.

As a result, the research themes of 23 were applied and applications of 23 were accepted after the approval by a steering committee of the laboratory. 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 23

		category A			B	total
		A1	A2	A3		
Kibann	inside	1	1	1	0	3
	outside	0	0	0	0	0
Syorei/Kikaku-chosa	inside	4	11	5	0	20
	outside	0	0	0	0	0

"inside" or "outside" : Numbers applied by the inside or outside of the Institute

The individual research subjects are as follows.

A1

"International Collaborative Research on Advanced Biorefinery"

(1) B. Jin. Lee
(2) K. Gardner
(3) J-H. Lee
(4) S.L. Lam
(5) A. Shekhtman
(6) M. Katahira , T. Morii, M. Kinoshita, T. Kotaki, E. Nakata, T. Nagata, S. Nakano T. Mashima, K. Kondo

(1) College of Pharmacy, Seoul Natl. Univ.
(2) Univ. Texas Southwestern Medical Center
(3) Dept. Chem. Gyeongsang Natl. Univ.
(4) Dept. Chem. The Chinese Univ. Hong Kong
(5) State Univ. New York
(6) Institute of Advanced Energy, Kyoto University

A2,

"Promotion of Advanced Plasma and Quantum Energy Studies"

(1) T. Mizuuchi, F. Sano, A. Kimura, S. Konishi, K. Nagasaki, K. Morishita, K. Masuda, H. Okada, T. Minami, R. Kasada, S. Kado, U. Takeuchi, S. Kobayashi, S. Yamamoto, S. Ohshima, K. Hata, K. Jimbo, S. Kondo, Z. Linge, S. Konoshima
(2) Y. Nakamura
(3) Y. Nakajima
(4) M. Ohnishi, Y. Yamamoto
(5) T. Fukuda
(6) S. Kitajima
(7) T. Akiyama, K. Tanaka,

(1) Institute of Advanced Energy, Kyoto University
(2) Graduate School of Energy Science, Kyoto University
(3) University Tsukuba
(4) Kansai University
(5) Kobe University
(6) Tohoku University
(7) National Institute for Fusion Science

A3

"Research on establishment of Photo-Energy Nano Science"

(1) K. Matsuda, Member of Photo-Energy Nano-Science

(1) Institute of Advanced Energy, Kyoto University

A1

"International Collaboration Research on Plasma Production Using Microwaves"

(1) M. Preynas, N. Marushchenko, H. Laqua
(2) E. Ascasibar, A. Cappa
(3) F. Volpe
(4) Y. Yoshimura
(5) Y. Nakamura
(6) K. Nagasaki, S. Yamamoto, K. Masuda, S. Ohshima, K. Sakamoto, F. Sano, T. Mizuuchi, T. Minami, H. Okada, S. Kado, S. Kobayashi, S. Konoshima,

(1) Max Plank Institute, Germany
(2) CIEMAT, Spain
(3) Columbia University USA
(4) National Institute for Fusion Science
(5) Graduate School of Energy Science, Kyoto University
(6) Institute of Advanced Energy, Kyoto University

"Visualization and Extension of System Code for Fusion Reactor Design"

(1) R. Kasada, S. Konishi
(2) R. Hiwatari
(3) H. Takeda
(4) A. Kobori

(1) Institute of Advanced Energy, Kyoto University
(2) Central Research Institute of Electric Power Industry
(3) Graduate School of Advance Leadership Studies, Kyoto University
(4) Graduate School of Energy Science, Kyoto University

"Standardization and Verification of Lifetime Evaluation Method of W-Divertor Structural Component"

(1) A. Kimura, H. Wentuo, O. Hashitomi, T, Ohmura

(1) Institute of Advanced Energy, Kyoto University

"Development of a Highly Efficient Bioethanol Production Yeast by Genetic Engineering"

(1) T. Kodaki, T. Nagata
(2) S. Sawayama

(1) Institute of Advanced Energy, Kyoto University

(2) Graduate School of Agriculture, Kyoto University

A2

"Conductive Sub-Layer of Turbulent Heat Transfer for Heating of Water in a Circular Tube"
(1) K. Hata
(2) K. Fukuda
(1) Institute of Advanced Energy, Kyoto University
(2) Graduate School of Maritime Science, Kobe University

"Observation of Divertor Plasma Behavior with High-Speed Video Cameras"
(1) T. Mizuuchi, Z. Linge, S. Kobayashi, H. Okada,
(2) D. Oda
(1) Institute of Advanced Energy, Kyoto University
(2) Graduate School of Energy Science, Kyoto University

"Preliminary Study of Innovative Cu Alloys Towards Breakthrough of Divertor Concept"
(1) R. Kasada, S. Konishi,
(2) K. Aoki, H. Gwon
(1) Institute of Advanced Energy, Kyoto University
(2) Graduate School of Energy Science, Kyoto University

"Multiscale modeling of materials behavior Under Fission and Fusion Environments and its Application to Research for Establishment of Advanced Nuclear Safety"
(1) K. Morishita
(2) T. Nakasuji
(3) Y. Yamamoto
(4) Y. Kaneta
(5) Y. Watanabe
(6) D. Kato
(7) X. Qui
(8) M. Miyamoto
(9) H. Iwakiri
(1) Institute of Advanced Energy, Kyoto University
(2) Graduate School of Energy Science, Kyoto University
(3) Institute of Nuclear Safety System
(4) Akita National College of Technology
(5) Japan Atomic Energy Agency
(6) National Institute for Fusion Science
(7) Kyoto University Research Reactor Institute
(8) Interdisciplinary Faculty of Science and Engineering, Shimane University
(9) Dep. Education, University of Ryukyu

"Study of Mechanism of Ion Cyclotron Range of Frequency Heating of Plasma In a Non-Axisymmetric Magnetic field"
(1) H. Okada, S. Kobayashi, S. Yamamoto, T. Minami, S. Ohshima, T. Mizuuchi, K. Nagasaki, F. Sano, S. Kado
(2) Y. Nakamura
(3) T. Mutoh
(4) Y. Nakashima
(5) N. Nishino
(1) Institute of Advanced Energy, Kyoto University
(2) Graduate School of Energy Science, Kyoto University
(3) National Institute for Fusion Science
(4) Tsukuba University
(5) Graduate School of Engineering, Hiroshima University

"Development of Fluctuation Analysis Technique using Analytic Function"
(1) S. Ohshima, S. Yamamoto, S. Kobayashi, K. Nagasaki, F. Sano, T Mizuuchi, H. Okada, L. Zang, S. Konoshima,
(1) Institute of Advanced Energy, Kyoto University

"Investigation and Evaluation of Zero-Emission Energy System and Scenario with Fusion, Biomass and Microgrid"
(1) S. Konishi, R. Kasada
(2) K. Namba
(3) S. Takeda
(1) Institute of Advanced Energy, Kyoto University
(2) Graduate School of Energy Science, Kyoto University
(3) Graduate School of Advance Leadership Studies, Kyoto University

"Investigation of Isotope Effect on Improved Confinement Mode for Advanced Helical Plasma"
(1) T. Minami, F. Sano, T. Mizuuchi, S. Kado, H. Okada, S. Kobayashi, S. Yamamoto, S. Ohshima, S. Konoshima
(2) K. Tanaka
(1) Institute of Advanced Energy, Kyoto University
(2) National Institute for Fusion Science

"Analysis for Spatial Structure of Density Fluctuation in Core Plasmas Based on Development of Beam Emission Imaging"
(1) S. Kobayashi, T. Mizuuchi, F. Sano, K. Nagasaki, H. Okada, T. Minami, S. Yamamoto, S. Kado, S. Konoshima,
(2) Y. Nakamura, M. Kirimoto, T. Harada
(3) Y. Suzuki, K. Nagaoka, Y. Takeiri, S. Okamura K. Mukai, T. Ohishi
(4) S. Murakami,
(5) T. Estrada
(6) Lee Hyunyong
(1) Institute of Advanced Energy, Kyoto University
(2) Graduate School of Energy Science, Kyoto University
(3) National Institute for Fusion Science
(4) Graduate School of Engineering, Kyoto University

(5) CIEMAT, Spain
(6) Korea Advanced Institute of Science and Technology

"Studies on MHD Equilibrium and Stability of High Density Plasmas Utilized by Soft X-Ray Computer Tomography in Heliotron J"

(1) S. Yamamoto, H. Okada, F. Sano, T. Minami, T. Mizuuchi, S. Kobayashi, K. Nagasaki, S. Kado, S. Ohshima, S. Konoshima, L. Zang
(2) Y. Nakamura
(3) S. Ohdachi
(4) H. Lee
(1) Institute of Advanced Energy, Kyoto University
(2) Graduate School of Energy Science, Kyoto University
(3) National Institute for Fusion Science
(4) Korea Advanced Institute of Science and Technology

"Measurement of the Impurity Line Spectra in Heliotron J for the Plasma Diagnostics"

(1) S. Kado, S. Yamamoto, H. Okada, F. Sano, T. Minami, T. Mizuuchi, S. Kobayashi, K. Nagasaki, S. Ohshima, S. Konoshima
(2) Y. Nakamura
(1) Institute of Advanced Energy, Kyoto University
(2) Graduate School of Energy Science, Kyoto University

A3

"Time-Resolved Spectroscopy of a Thin Polymer Film Using KU-FEL"

(1) T. Nakajima, H. Zen, T. Kii, H. Ohgaki, E. Ageev
(2) K. Mizobata
(1) Institute of Advanced Energy, Kyoto University
(2) Graduate School of Energy Science, Kyoto University

"Analysis of Structure-function Relationships on Wood Degrading Enzymes for Better Utilization of Woody Biomass"

(1) T. Nagata, M. Katahira, T. Morii, T. Kodaki, E. Nakata
(1) Institute of Advanced Energy, Kyoto University

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

(1) E. Nakata, T. Morii, T. Kodaki, S. Nakano
(1) Institute of Advanced Energy, Kyoto University

"Development of Compact THz-FEL System"

(1) H. Ohgaki, K. Masuda, T. Kii, H. Zen
(2) S. Suphakul, Y. Tsugamura
(3) K. Damminsek
(1) Institute of Advanced Energy, Kyoto University
(2) Graduate School of Energy Science, Kyoto University
(3) Chaingmai University

"Upgrade of Kyoto University Mid-Infrared Free Electron Laser by Photocathode Operation"

(1) H. Zen, T. Kii, H. Ohgaki, K. Masuda, T. Nakajima
(1) Institute of Advanced Energy, Kyoto University

SYMPOSIUM IN THE LABORATORY

Symposium

The Symposium has been arranged in order to introduce the research activities in sections and to enhance the mutual cooperation among different fields. In2014, three regular meetings and the annual meeting for the cooperative research results were held with following theme.

1. The regular meeting

(1) **May 15, 2014**

F. Sano "Overview of Recent Heliotron J Experiment"
Institute of Advanced Energy, Kyoto University

(2) July 18, 2014

Brahim Lounis, "Optical Detection and Spectroscopy of Individual Nano-Objects"
Univ. Bordeaux, Institut d'Optique & CNRSLP2N, France

(3) September 18, 2014

Y. Kishimoto, "Plasma and Fusion Research Based on the Idea of Zero-Emission Energy - Formation of Structure and Creation of Function Using Infinitesimally Small Energy -",
Institute of Advanced Energy, Kyoto University

(4) February 3, 2015

G. Eda, "Charge Carriers and Excitons 2D Crystals of Transition Metal Dichalcogenides"
National University of Singapore

The Annual Meeting for the Cooperative Research Results, April 3, 2015

(1) T. Mizuuchi, "Promotion of Advanced Plasma and Quantum Energy Studies"
Institute of Advanced Energy, Kyoto University

(2) T. Minami, **"**First results of Electron Internal Transport Barrier Formation Experiment in Advanced Helical Plasma**"**
Institute of Advanced Energy, Kyoto University

(3) H. Okada, **"**Study of Fast Ions by Using ICRF Heating in Heliotron J**"**
Institute of Advanced Energy, Kyoto University

(4) K. Matsuda, **"**Research on Establishment of Photo-Energy Nano Science**",**
Institute of Advanced Energy, Kyoto University

(5) E. Nakata, **"**Development of the Methodology to Construct the High-Efficient Material Conversion System on DNA Nanostructure**"**
Institute of Advanced Energy, Kyoto University

(6) H. Zen, "Upgrade of Kyoto University Mid-Infrared Free Electron Laser by Photocathode Operation"
Institute of Advanced Energy, Kyoto University

(7) M. Katahira, **"**International Collaborative Research on Advanced Biorefinery**"**
Institute of Advanced Energy, Kyoto University

(8) T. Kodaki, **"**Development of a Highly Efficient Bioethanol Production Yeast by Genetic Engineering**"**
Institute of Advanced Energy, Kyoto University

(9) K. Nagasaki, **"**International Collaboration Research in Helical System Community**"**
Institute of Advanced Energy, Kyoto University

(10) R. Kasada "Visualization and Extension of System Code for Fusion Reactor Design"
Institute of Advanced Energy, Kyoto University

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

Professor Kazunari Matsuda's group aimed to develop a novel strategy for light energy utilization by nano-carbon materials in his research entitled "Optical Properties of Novel Nano-materials for Light Energy Applications." In addition to the nano-carbon material, novel nanomaterials have attracted a great deal of interest from viewpoint of fundamental physics, chemistry and potential applications for the light energy. Since the discovery of graphene, the studies of atomically thin-layered materials, such as transition-metal dichalcogenides called as “beyond graphene,” have drastically been emerged. The atomically thin-layered transition-metal dichalcogenides (MX_2, M=Mo, W, X=Se, S) shows the strong light absorption (5-10%) even in atomically thin materials. Potential application of light energy utilization using atomically thin-layered transition-metal dichalcogenides has been discussed.

Professors Tetsuo Sakka and Kazuhiro Fukami studied metal modified semiconductor electrodes to overcome the problem of semiconductor electrodes, which often show low catalytic activity for photoelectrochemical reactions in his research "Semiconductor electrodes modified with metal nanoparticles for the application to photoelectrochemical reactions." For the utilization of silicon as a photoelectrode, platinum modification has been studied for more than a decade. To elicit the highest performance, the size of metal nanoparticles as well as the interparticle distance should be precisely controlled. The research focuses on the utilization of porous silicon electrodes whose pore size and thickness of pore wall is ~3 nm. Electrodeposition of metals into porous silicon is normally difficult because metal ions are preferentially reduced at the pore opening. He reported new methods to control the electrodeposition in porous silicon. In the first example, platinum is chosen as metal for deposition because silicon modified with fine-particles of platinum is often used as an electrode for photoelectrochemical cell. Copper modified porous silicon was also characterized by measuring EXAFS spectra. It has been clarified that copper oxide is preferentially formed when the size of particles are small. Formation of copper oxide has been suggested to limit the efficiency for photoelectrochemical reduction of CO_2.

Prof. Takashi Sagawa's group developed nanostructured ZnO by his research entitled "Hierarchical Construction of ZnO Nanorods on Nanofibers for Hybrid Solar Cells." Zinc oxide (ZnO) is known for its high electron mobility, acceptable refractive index, and the ease in process when tuning its size and shape. Continuous electron pathways in ZnO are essential for the transport of the generated charge upon exciton separation at the ZnO/polymer interface to the electrode. Recently, his research group that the surface area of ZnO nanofibers (NFs) substrates was further increased by the deposition of nanorods (NRs) to form hierarchical-structured ZnO substrates. In fact, Photovoltaic performance of hybrid ZnO NFs/poly(3-hexylthiophene) (P3HT) solar cell is enhanced through the deposition of ZnO NRs. The improvement of VOC can largely be attributed to the higher JSC due to the higher surface areas and the suppression of reverse current saturation density (J0) due to better electrode coverage. These increases led to ten times improvement in power conversion efficiency. The hierarchical structure based on NFs anchored on thin-films of ZnO nanoparticles (NPs) with NR deposition can solve the trade-off of surface area and the direct electron pathway of the NRs and NPs morphology.

Professor Hideaki Ohgaki's group carried out a research on “Accelerator based Infrared Light Sources" at Institute of Advanced Energy, Kyoto University. A mid-infrared free electron laser (MIR-FEL) based on compact linear accelerator is routinely operated for various user experiments. A broadband millimeter-wave radiation can also been provided from same accelerator. A THz-FEL device is now under construction, which will be useful in the characterization of materials developed for the zero-emission energy system.

Production of solar fuels

Professor Takashi Morii's group pursued a research entitled "Artificial metabolic channeling on the molecular switchboard." Construction of an artificial photosynthesis system requires ordered assembly of functional components, such as the dyes to absorb sunlight and the enzymes to drive each step in the multiple chemical transformations. The Morii group focused on development of an assembly of enzymes that efficiently drives the multistep chemical transformation. Molecular switchboards use the DNA-origami nanostructure as an addressable template to arrange enzymes with nanometer-scale precision. Construction of molecular switchboard that converts xylose into xylitol, then to xylulose was currently underway.

Professor Hiroshi Sakaguchi's group succeeded in the synthesis of graphene nanoribbon (GNR), which was predicted to behave as semiconductor in the research of "Bottom-Up Produced Graphene Nanoribbons by Surface Polymerization." His group has demonstrated Radical-polymerized Chemical Vapor Deposition (RPCVD) and Electrochemical Epitaxial Polymerization as bottom-up massive growth techniques of GNRs under normal condition. For RPCVD, poly(perianthracene) can be produced under extremely low vacuum condition (ca. 1 Torr) from 10,10'-dibromo-9,9'-bianthryl. This new reaction technique was demonstrated to be useful for other organic monomers such as 3,9-, and 3,10-dibromoperylenes to produce narrowest GNR poly(perinaphthalene). The group has also succeeded in for the first time the synthesis of multilayered GNR, transfer onto insulator substrate and FET fabrication of bottom-up synthesized GNR. Also demonstrated for the first time is an electrochemical method to produce GNR under room temperature in metal-solution interface. These new techniques open the door to the device fabrication and unknown features of bottom-up fabricated GNRs.

Efficient conversion of biomasses to useful chemicals

Wood biomasses are produced by solar energy. Therefore, development of new bio-refinery methods also contributes on exploring novel principles for highly efficient utilization of solar energy. Although NMR is recognized as one of the most powerful tool to achieve this and is widely used in many fields, variation in a molecular size of components distorts quantitation due to size-dependent decay of magnetization. Professor Masato Katahira's group developed a new method to correctly quantify the amounts of each component was developed by combined use of HSQC and TROSY in the research entitled "Development of New NMR Methods for Correct Quantitation of Biomass Components." The new method was applied to a solution that contains biomass-related components whose molecular sizes largely differ, and the validity of the method was proved. This method is also tolerant to other factors that distort quantitation such as either variation in $^{1}J_{CH}$ or imperfectness of pulses. Thus, the method developed in Professor Katahira's group is applicable to a variety of situation to correctly quantify the amounts of components in solution.

Bidirectional Collaborative Research Program

Since 2004, the Heliotron J group at Kyoto University has joined the bidirectional collaborative research program of National Institute for Fusion Science (NIFS). The purpose of this program is to extend the activities of nuclear fusion research at universities in Japan after the Committee of the Science Subdivision under the Council for Science and Technology has decided to set up its master plan for Japanese fusion research and development by promoting collaborative research activities. This plan was summarized in the report "Policy for executing Japanese nuclear fusion research", where it was pointed out that continuous scientific research activities for comprehensive understanding of toroidal plasma physics are needed under the parameters which can be extrapolated to the fusion reactor.

The main objective of the research is to improve the confinement and stability performance for advanced helical magnetic configurations such as the helical-axis heliotron, Heliotron J. Six topics for the collaboration research for this FY are selected; (1) confinement improvement by controlling magnetic configuration and related plasma self-organization, (2) ECH/EBW heating physics, (3) NBI plasma formation with assistance of micro wave and high beta plasma (4) boundary plasma control, (5) instability suppression by controlling magnetic configuration, and (6) toroidal current control and so on. The results of several subjects are described below.

Study of parallel flow dynamics in NBI heating plasmas [1]: It is an important subject to understand the driving and damping mechanisms of plasma flow in magnetically confined plasmas, because the parallel plasma flow plays an important role in suppression of MHD activity and control of turbulence. It is affected by parallel viscosity. The parallel flow velocity has been investigated from the viewpoint of the magnetic ripple strength γ, since the neoclassical (NC) toroidal viscosity in the plateau regime is proportional to γ^2. The effect of γ on the parallel flow was investigated in NBI plasmas of Heliotron J. In the plateau regime, the parallel flow velocity at the core region in the high γ configuration was measured to be 2-3 times smaller than that in the standard γ case. The experimental observation of the flow velocity was generally consistent with that predicted by the NC transport analysis. The flow velocity outside the core region was not sensitive to the ripple strength and the NBI direction.

A toroidally symmetrical electric field fluctuation with radially elongated structure [2]: The fluctuation has dominant frequency components less than 4 kHz and shows electrostatic characteristics without density perturbations. These characteristics are quite similar to those of zonal flows, however, its radial wavelength is, unlike those in other devices, comparatively large. The electric field fluctuation generates the velocity shear synchronized with the fluctuation around LCFS since the fluctuation exists in the low frequency range. Cross-correlation analysis indicates that turbulence structure drastically changes at the boundary of LCFS, which results in the steep increase of Reynolds stress inside LCFS. Consequently, radial shape of the Reynolds stress is similar to that of the symmetric fluctuation amplitude. This observation implies that the generation of the symmetric fluctuation is coupled with the Reynolds stress.

External Control of Energetic-ion-driven MHD Instabilities by ECH/ECCD [3]: Energetic-ion-driven magnetohydro dynamic (MHD) instabilities such as energetic particle modes (EPMs) have been studied in NBI-heated Heliotron J plasmas with low magnetic shear. We clarified the characteristics of the observed EPMs. The observed EPMs have low-m/n (m and n are the poloidal and toroidal mode numbers) such as m/n=2/1 or 4/2 with a single helicity, and localize at plasma edge region of ~ 0.8 in normalized minor radius where frequency of passing particle in toroidal direction intersects with shear Alfven continua of m/n=2/1 or 4/2. We scanned plasma current by the parallel refractive index $N_{//}$ in order to vary the magnetic shear which is a key parameter for continuum damping rate of EPM. We demonstrated that EPMs could be controlled by means of both positive and negative magnetic shear induced by electron cyclotron (EC) driven plasma current.

References

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[2] S. Ohshima, et al., "Observation of a Totoidally Symmetrical Electric Field Fluctuation with Radially Elongated Structure in Heliotron J", ibid., EX/P4-26.
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Application of DuET and MUSTER for Industrial Research and Engineering (The ADMIRE Project)

1. Introduction

The ADMIRE Project at the Institute of Advanced Energy (IAE), Kyoto University is one of the MEXT (Ministry of Education, Culture, Sports, Science and Technology of Japan) -supported programs "*Project for Creation of Research Platforms and Sharing of Advanced Research Infrastructure*" to provide private companies 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. In the “Trial use mode” the users can use these facilities free of charge for a limited time period.

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 private industries 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.

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

a) Trial use mode

In this mode, users are allowed to utilize the ADMIRE facilities free of charge for six months for the MUSTER facilities or twelve months for the DuET facilities. The term may be repeated once if requested and approved. The only obligation of the user is to submit a short report at the end of the term. If the user requests to postpone the immediate dissemination of the outcome in order to secure its IPR, a moratorium up to two years may be given.

b) 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.

DuET, the dual-ion beam irradiation facility

c) 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.

d) 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.

3. 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:
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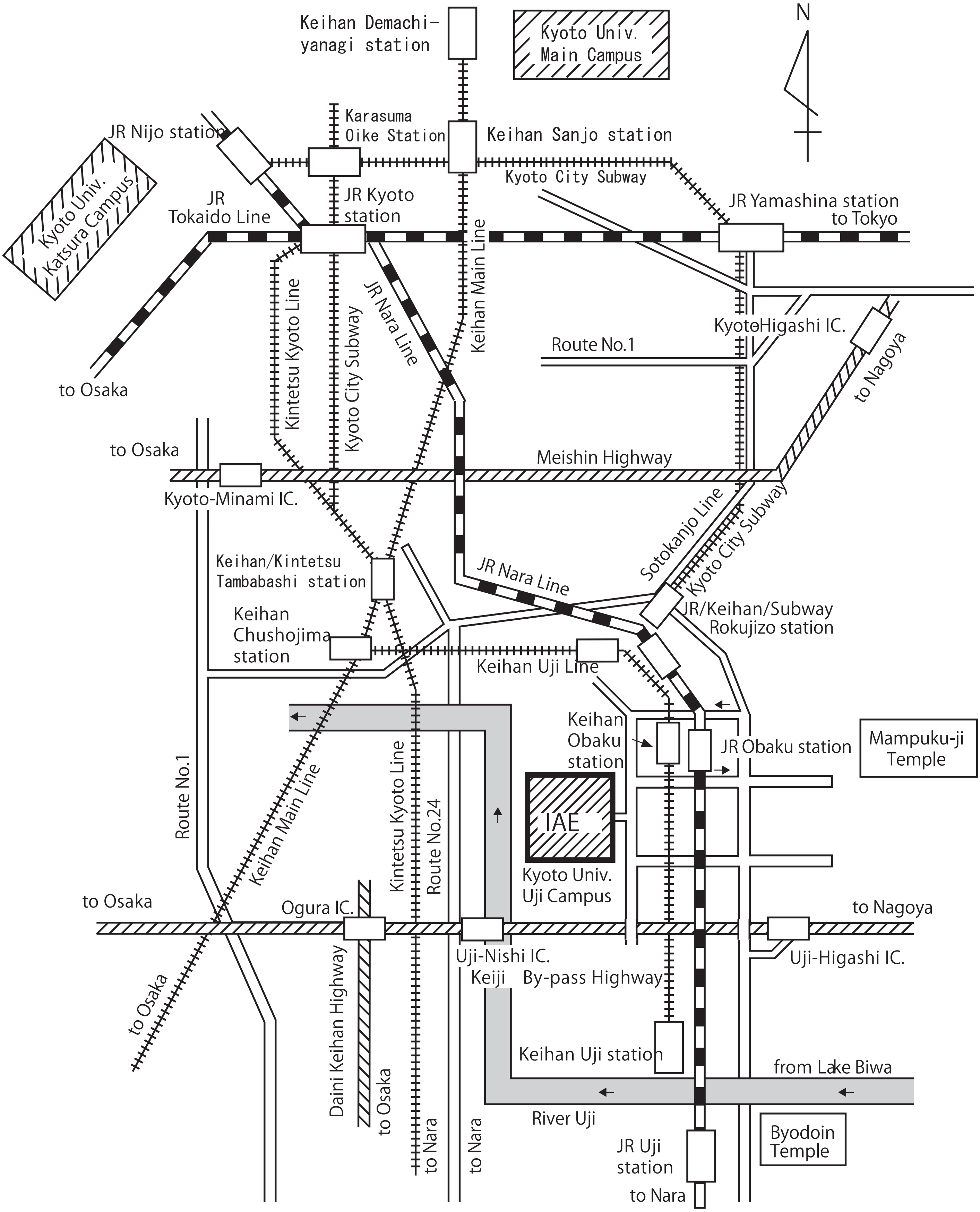
7. HOW TO GET TO THE IAE



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

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

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