

ISSN 1342-3177

IAE-AR-2013

Institute of Advanced Energy
Kyoto University

ANNUAL REPORT

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

ANNUAL REPORT

2012

**Institute of Advanced Energy
Kyoto University**

Gokasho, Uji, Kyoto 611-0011
Japan

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FOREWORD



The year of 2012 was again a tough year domestically and internationally in the political situation as well as the economical condition. Progress of the recovery from the March 11 disaster seems still sluggish. Universities also cannot be independent of the situation. The basic budget of universities has been reduced. Kyoto University has started to think of strategies to cope with the difficult situation: downsizing of personnel and expenditure without reducing the activities. Under these circumstances, we have carried forward important projects.

FY2012 was the third year in the second period of the 6-years operation plan (FY2010-FY2015). In this second period, the competency of the research institute is strictly assessed since the government urges national universities to accelerate their full-scale reform action. From this point of view, we have to further strengthen our capabilities of research and education based on the accomplishment of our academic activities, and to exhibit our prospective future. Self-check and external-review for our activities are scheduled in next fiscal year. The “Joint Usage/Research Program on Zero-Emission Energy”, which is a program authorized by the MEXT (FY2011-FY2015), is going well. The past 2-year activities will be evaluated next fiscal year. The result will be reflected in the budget in coming years, and also in the adoption of the successive program after FY2016 if any. The Global COE program “Energy Science in the Global Warming Era” (2008–2012), which we have acted as a core institution, fulfills successfully. So does the international collaboration program, Asian Core, with China and Korea.

We are working hard toward further progress in research and education, and conducting a lot of collaborative researches in the fields of advanced energy science and technology; we especially lay stress on “Advanced Plasma and Quantum Energy” and “Photo- and Energy Nano-Science”. We aim at the realization of Zero-Emission Energy Society through the research. We start a new project sponsored by the MEXT: Development of solar energy utilization with revolutionary high-efficiency. This project will be a great support and encouragement for our activities.

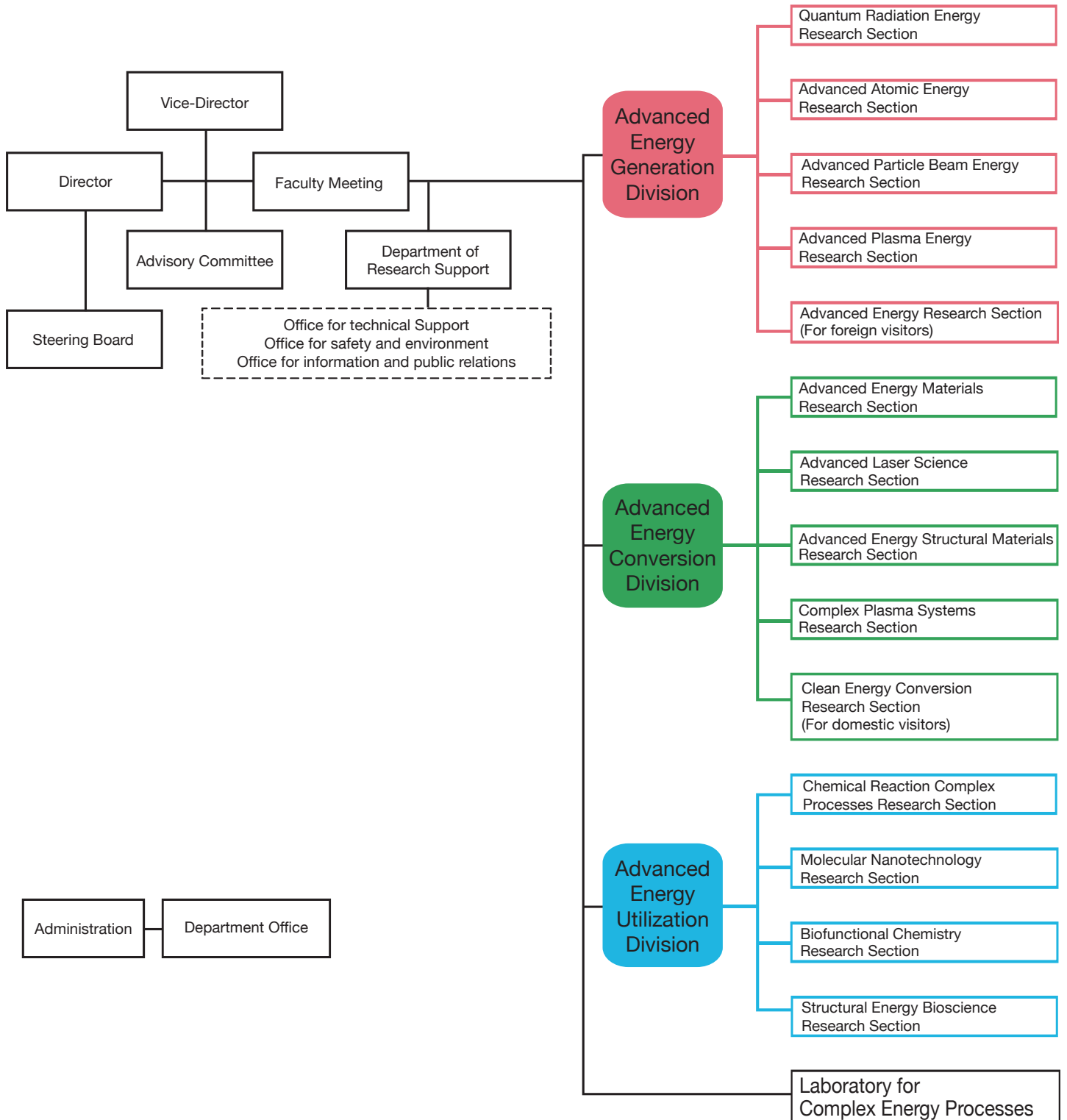
The worldwide concern regarding energy supplies and global warming drives our efforts, and energy issues are urgent priority subjects especially after the Fukushima accident. We shall renovate our efforts toward a new period, through research and education on advanced energy science and technology, to cope with these critical issues and contribute to the benefit of future generations. It is our great pleasure to issue this Annual Report. We hope that it provides you with good understanding of the activities of the Institute of Advanced Energy, Kyoto University.

A handwritten signature in black ink, appearing to read 'Y. Ogata'.

March 2013

Yukio H. OGATA
Director
Institute of Advanced Energy
Kyoto University

2. ORGANIZATION CHART



3. RESEARCH ACTIVITIES

3-1. TOPICS

Integration of Liquid-State Theory and Electrochemistry: Molecular-Scale Picture of Electrochemical Reactions within Nanoporous Electrodes

K. Fukami, Assistant Professor (Chemical Reaction Complex Process Research Section)

M. Kinoshita, Professor (Laboratory for Complex Energy Process Section)

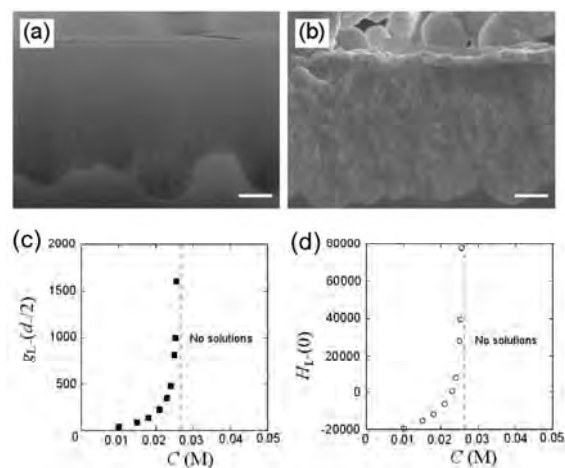
Porous electrodes have become important materials in the field of sensing, (photo)catalysis and batteries. Although the specific surface area becomes larger with an increase in the porosity, it is difficult in chemical or electrochemical reactions to elicit suitably high performance originating from the large specific surface area. This is because the reaction efficiency within nanoporous media is lowered by the difficulty in supply of reactants from the bulk and in ejection of products to the bulk. By applying the diffusion equation to the description of supply and ejection, we know that they are strongly disturbed by the porous structure and this disturbance is more serious whose pores are deeper and smaller in diameter. As a consequence, reactions occur primarily on the top surface of porous structure which is advantageous in terms of supply of reactants from the bulk. The control of such reactions within nanoporous media is much more difficult than one simply imagines.

In order to understand molecular-scale mechanisms of chemical or electrochemical reactions within nanoporous electrodes, we have started an original collaboration aiming at the integrating of liquid-state theory and electrochemistry. We carried out detailed experiments on the effects due to the concentration of platinum complex ions in the bulk aqueous electrolyte solution and the affinity of the pore wall surface with water. A surprising finding was as follows. When the ion concentration in the bulk was gradually increased, at a threshold concentration the deposition behavior exhibited a sudden change, leading to drastic acceleration of the electrochemical deposition. This result is strongly suggestive of the occurrence of a transition phenomenon. When the affinity of the surface with water was gradually reduced (i.e., the hydrophobicity of the surface was gradually strengthened) with fixing the ion concentration, qualitatively the same phenomenon was observed. With the aid of our statistical-mechanical theory for confined molecular liquids, we attribute the finding to a surface-induced phase transition upon which the confined nanospace is abruptly filled with the second phase: The ion concentration is orders of magnitude higher in the second phase than in the bulk. The transition occurs even when the bulk is thermodynamically stable as a single phase.

Occurrence of the surface-induced phase transition is not limited to this particular system. It can occur for many chemical reactions as long as the surface-induced

hydration structure is carefully controlled. For the precise control of surface-induced structure, analyses based on statistical mechanics using a molecular model for the solvent as well as experimental investigations are crucially important. The finding that the surface-induced phase transition occurs at a lower ionic concentration for $[\text{PtBr}_4]^{2-}$ than for $[\text{PtCl}_4]^{2-}$ was first predicted by the theory and then verified by experiments.

Our collaboration has presented stimulating results overcoming the problem described in the first paragraph and opens a novel field of science. The surface-induced phase transition in nanoporous materials will shed new light on design and control of highly efficient chemical systems in a nanospace in the near future.



(a,b) Cross-sectional SEM images of the porous silicon electrodes after electrochemical deposition of platinum. Concentrations of platinum ions were (a) 0.009 M and (b) 0.010 M for $[\text{PtCl}_4]^{2-}$. The platinum electrodeposition was abruptly and drastically accelerated above the threshold concentration. White bars in the figures (a, b) indicate 0.5 μm . (c,d) Relation between $g_L(d/2)$ (the normalized number density of platinum complex ions) or $H_L(0)$ (the Fourier transform of the total correlation function at zero wave vector) and C (the concentration of anions, platinum complex ions) near an extended hydrophobic surface. Both $g_L(d/2)$ and $H_L(0)$ diverge at $C^* \sim 0.0255$ M, suggesting the occurrence of a phase-transition phenomenon.

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3-2. RESEARCH ACTIVITIES IN 2012

Quantum Radiation Energy Research Section

H. Ohgaki, Professor
 T. Kii, Associate Professor
 H. Zen, Assistant Professor
 (T. Hori, Research Professor)

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, such as high-efficiency solar cells, energy conversion in bio materials. Figure 1 shows a schematic drawing of the KU-FEL system. The KU-FEL consists of a 4.5-cell thermionic RF gun, a 3-m travelling wave accelerator tube, a beam transport system, and a 1.8-m undulator and an optical resonator.

In last year, the 1.6-m undulator was replaced with 1.8-m one to have higher laser gain. At the same time, the optical resonator mirrors have also been replaced with new ones for smaller optical loss and higher gain. After those modifications, FEL lasing and power saturation at 7.5 μm has already been achieved. After fine tuning, we have already achieved the FEL lasing from 5

to 15 μm . Now the KU-FEL facility is open for internal and external users of our institute under the Joint Usage/Research Program on Zero-Emission Energy Research, Institute of Advanced Energy, Kyoto University.

Another topic of KU-FEL development is introduction of photo-cathode RF gun, which enables us to generate MIR-FEL with higher peak power and wider tunable range. A Multi-bunch UV-laser system for illuminating photo-cathode has been developed under the collaboration with Dr. R. Kuroda, Researcher of AIST. The laser system consists of a mode-locked Nd:YVO₄ oscillator, two two-pass Nd:YAG amplifier, a 2nd harmonic generation crystal and a 4th harmonic generation crystal.

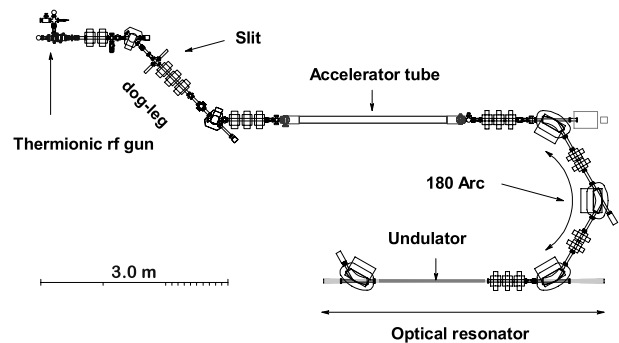


Fig. 1 Schematic drawing of the KU-FEL

2.2 MIR-FEL Application in the Energy Science

It is well known that an infrared region light has a good resonance with molecular vibration and lattice vibration in some liquid or solid compound. In particular, wide-gap semiconducting materials such as ZnO, SiC, and TiO₂ show unique electrical and optical properties, resulting in photochemical phenomena with microwave irradiation. For deep understanding the electronic structure of the ZnO treated by microwave (MW-ZnO), the precious photoluminescence of the MW-ZnO was measured. As the results, we found the MW-ZnO has specific electronic structure coupling with phonon. Therefore, it is considered that the irradiation of MIR-FEL on such semiconducting materials possibly excites the phonon selectively, and then gives rise to the

changes in electronic structures. For the verification of selective phonon excitation and for the observation of electronic structure change induced by MIR-FEL irradiation, the low temperature Raman scattering and photoluminescence (PL) measurement system with MIR-FEL irradiation has been developed (Fig. 2). By using these spectrometers, we suggested that a method for verification of the selective phonon excitation by anti-stokes scattering, and the preparation of the experiment has been developing. This study aims at development of new evaluation technique of electron-phonon interaction in such wide-gap semiconducting materials by MIR-FEL.

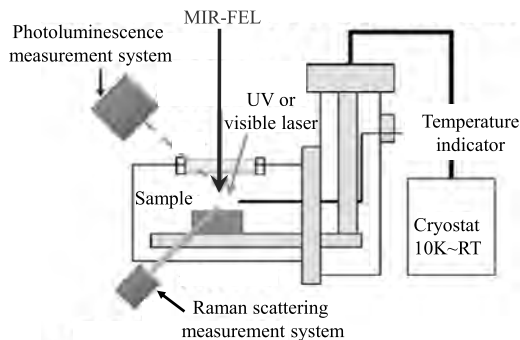


Fig. 2 Conceptual drawing of PL and Raman scattering measurement system combined with MIR-FEL.

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 strong periodic field. The Bulk HTSC SAU consists of stacked bulk high-Tc superconductors (HTSs) and a solenoid magnet as shown in Fig. 3.

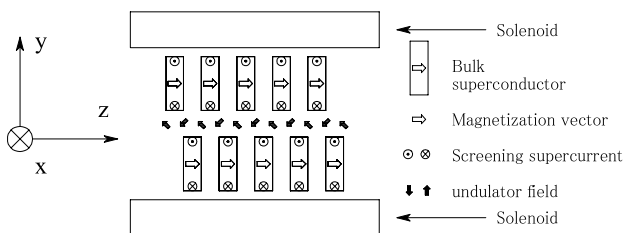


Fig. 3 Conceptual drawing of the bulk HTSC SAU and generation principle of the periodic undulator field using an induced current.

We performed low temperature operation of the undulator, and strong periodic magnetic field was successfully generated. Measured undulator field strength B_0 was 0.85 T for period length of 10 mm and gap width of 4 mm. This value exceeds the theoretical limit can be

achieved by using permanent magnet.

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 homeland security such as a nondestructive measurement of containers at airports or harbors, detection or identification of special nuclear materials (SNM). The required performances of the detector used in the NRF facility are high energy resolution, high full energy efficiency, and high counting rate. $\text{LaBr}_3(\text{Ce})$ scintillator is a strong candidate to meet these requirements because of its superior energy resolution and high counting rates. We have constructed a 8 $\text{LaBr}_3(\text{Ce})$ detector array (Fig.4) consisted of 1.5 inches in diameter and 3 inches in length. The performance of the array detector has been examined in the GACKO at New Subaru, Ni-shi-Harima, and HI γ S facility in Duke University, North Carolina.



Fig. 4 $\text{LaBr}_3(\text{Ce})$ scintillator array detector tested at HI γ S facility.

Acknowledgment

These works were partially supported by the Grant-in-Aid for Scientific Research B, the Grant-in-Aid for challenging Exploratory Research by the Ministry of Education, Culture, Sports, Science and Technology of Japan, Strategic Funds for the Promotion of Science and Technology, Kyoto University Global COE program, the Collaboration Program of the WAKASA WAN Energy Research Center, and The Collaboration Program of the Laboratory for Complex Energy Processes, Institute of Advanced Energy, Kyoto University.

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Advanced Atomic Energy Research Section

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

1. Introduction

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, conversion and utilization systems. The attractiveness of the total energy system considered by the socio-economic analysis of future society and markets in the global scale and the scope covering 21st century and beyond is reflected. Typically, we propose a Zero-emission energy scenario based on fusion energy for biomass-based recycling system.

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

- (1) Design of small and realistic biomass-fusion hybrid energy system
- (2) Development of advanced fusion blanket and divertor with liquid LiPb and SiC composite for high temperature heat
- (3) Conversion of waste biomass by endo-thermic reaction to generate hydrogen and liquid fuel
- (4) Design and analysis of DC micro-grid 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.
- (7) Materials R&D for the above-mentioned issues

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

The surface of the target of the divertor suffers high heat flux localized onto the 5-10 cm surface area. This study examines the feasibility of the divertor concepts to distribute the heat load on the target surface to coolant by the heat pipe mechanism, utilizing the latent heat in phase change. A comparative evaluation was performed about the heat transport capability of Na and H₂O as working fluid to be used for our diverter concept. Existing heat pipe data base provides some of the basic parameters required for the design of the structure of the dual phase heat sink.

The result in Fig. 1 clearly shows that evaporation of both H₂O and Na provides sufficient cooling capability to distribute heat load on the anticipated divertor surface. And, considering the operating temperature for efficient use of heat, Na system is suitable for the application to the divertor. The heat-transport capacity of heat flux in the Na system with inner diameter 40mm is expected to exceed 100MW/m² in the operating temperature 727-1027 degree under no MHD effect on the movement of a conductive liquid that requires further evaluation. The result is expected to relax the stringent requirements on the divertor design for the reactor.

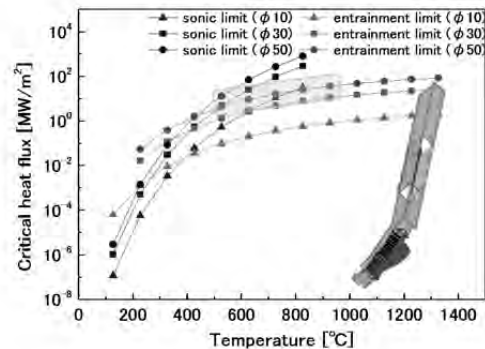


Fig. 1 The relation between limit heat-transport capacity of heat flux and operation temperature in the Na system.

3. R&D of neutron beam source using cylindrical discharge type fusion device for medical applications

As shown in Fig. 2, we propose an application of a cylindrical discharge tube type fusion neutron beam source for medical purpose. In this study, practicality and possibility of the medical irradiation plan were evaluated from the standpoint of engineering and medicine. Cancer treatment by BNCT (Boron Neutron Capture Therapy) was selected as an effective application to take advantage of this neutron source. Neutron transport in a phantom was calculated with the MCNP5 (Monte Carlo Neutron Particle calculation code version5), and the distribution of dose on the affected part medicated with a boron agent sug-

gested satisfactory focusing. Since this neutron source is small size, it is designed to irradiate the affected part from many directions by crossfire irradiation. Flexibility of attitude and operation modes permits irradiation in a supine position from arbitrary directions. Because of low neutron flux, irradiation therapy is planned for multi-fractionation in a manner similar to CHART (Continuous Hyperfractionated Accelerated Radio Therapy). Crossfire irradiation and CHART will allow us to achieve new cancer therapy with a relatively lower dose rate than conventional BNCT. It causes apoptosis selectively to a cancer cell, reducing side effects and a patient's recuperation burden. This result suggests the possibility of advanced cancer treatment which improves QOL (Quality of Life) of the patients.

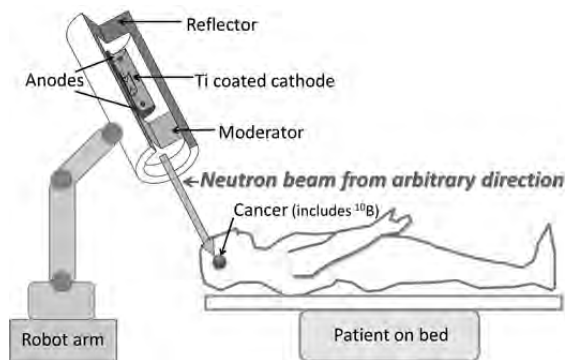


Fig. 2. Schematic view of the new cancer therapy method using a cylindrical discharge type fusion neutron beam source

4. An innovative method for tritium extraction from liquid Pb-17Li

In our previous studies, the authors confirmed that deuterium release from falling liquid Pb-17Li droplets in vacuum was approximately three hundred times faster than release from a static diffusion condition. Using these results, a prototype design study for a tritium extraction device was performed. The tritium extraction ratio was first analyzed for an optimum inventory condition; then, the dimensions of the device were studied. A case study of the extraction device for a fusion powered ITER class reactor with a Pb-17Li blanket was performed. The optimum extraction ratio was 35%. For the design study, the extraction chamber had an inside diameter of ϕ 2.5[m] with a height of 0.25[m], and the 1-stage structure had the required capabilities for the optimum inventory condition. The overall size of the device was approximately ϕ 3[m] with a height of 1[m], as shown in Fig. 3. This result is expected to be applicable for the Pb-17Li based tritium blanket system.

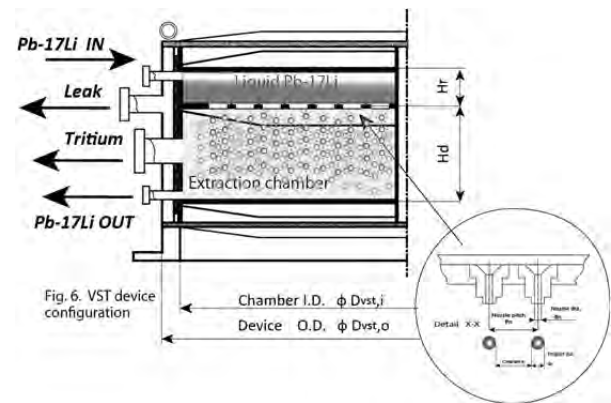


Fig. 3. Schematic view of the newly-designed vacuum sieve tray device for tritium extraction from Li-Pb.

5. Nano and meso scale mechanics of ion-irradiated fusion reactor materials

Irradiation hardening/embrittlement is one of the essential degradation issues of fusion reactor materials. Heavy ion irradiation techniques using MeV accelerators such as DuET have many advantages to investigate the irradiation effects on the fusion reactor materials. In order to evaluate irradiation hardening in the ion-irradiated materials, an instrumented indentation test, which is generally called as “nanoindentation test”, has been used because the irradiation damage is limited in the surface up to a few micron meters. However, the nanoindentation hardness of metals generally exhibits an “indentation size effect (ISE)”. Moreover the ion-irradiations generate a displacement damage gradient into the materials so as to cause an additional hardness gradient. These complex nano- and meso scale mechanics should be understood for an evaluation of “universal” bulk-equivalent hardness of ion-irradiated materials. In the present study, therefore, we propose a new composite hardness model in order to explain the bulk-equivalent hardness depth profile of ion-irradiated Fe-based model ferritic alloys as shown in Fig. 4. Validity of this method will be judged through the application to other materials irradiated at different ion-species and energies and doses.

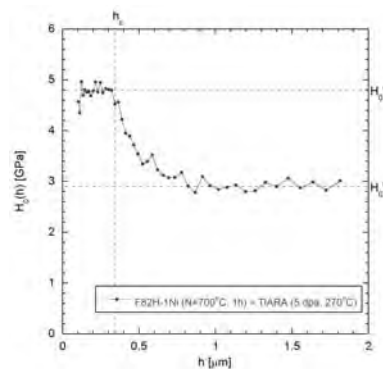


Fig. 4. Depth dependence of bulk-equivalent hardness of F82H-1Ni steel irradiated at TI-ARA.

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Advanced Particle Beam Energy Research Section

K. Nagasaki, Professor
 K. Masuda, Associate Professor
 S. Ohshima, Assistant Professor
 K. Tanaka, Part-time Lecturer

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. Main research subjects are now focused on the following; 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 plasmas and production/diagnostics of highly brilliant relativistic electron beams for advanced light sources such as free electron lasers.

2. Simultaneous X-ray and neutron radiography by use of IECF

Inertial Electrostatic Confinement (IEC) is a compact and highly controllable nuclear fusion device. A glow discharge driven D-D IEC fusion device is one of the candidates as a neutron source especially for the neutron radiography since conventional neutron sources cannot simultaneously satisfy all the requirements, i.e. compactness, portability and controllability of the system. The glow discharge driven IEC fusion device has been developed technically and can be applicable to practical use. In particular, the IEC fusion device can work as a source of not only neutrons but also X-rays, therefore, identification of materials by the simultaneous neutron and the X-ray radiography, i.e. two beam radiography is feasible in principle by evaluating R values which are the ratio of attenuation rate of X-ray and neutron in the materials. The R value corresponds to μ_n/μ_X (μ_n and μ_X are mass attenuation coefficient of X-rays and neutrons), and is inherent value of the material. It can be evaluated independently on the shape, thickness or density of the samples.

As an initial experiment, we irradiated samples with X-rays and neutrons simultaneously for 120 minutes using our IEC system with the neutron yield of 2.7×10^7 n/sec. Numerical simulation showed that thermal neutron flux density and the fluence were 2.2×10^2 n/cm²/sec and 1.6×10^6 n/cm²

at the sample position. This is enough to obtain a neutron image on the neutron imaging plate (IP) because the minimum fluence larger than 10^4 n/cm² is required for the IP measurement. .

A simple calculation predicts the plastic material containing the hydrogen such as Acrylic or Polyethylene has larger R value. Actually, we experimentally discriminated the plastic materials of Polyethylene and Acrylic from the other metals to evaluate R values, as shown in Figure 1.

These results demonstrate the two beam radiography using the glow discharge driven D-D IEC fusion device is applicable to the practical usage in near future although the improvement of the neutron output in the IEC system is necessary.

3. Design of a Coaxial RF Cavity for Thermionic Triode RF Gun

Low gain free electron lasers require electron beams with high brightness, high peak current, and long macro-pulse duration. In the Kyoto University Free Electron Laser (KU-FEL) facility, a 4.5 cell thermionic RF gun is being studied intensively to meet these requirements in an extremely compact and low-cost system. A thermionic triode type RF gun is being developed to mitigate the adverse effect of electron back-bombardment onto the cathode. Therefore an additional small coaxial RF cavity with a thermionic cathode on the inner rod shall be installed into currently used 4.5 cell thermionic RF gun.

Figure 2 shows schematic structure of conventional and triode type thermionic RF gun. The prototype coaxial cavity was designed and fabricated for resonance frequency of 2856 MHz corresponding to

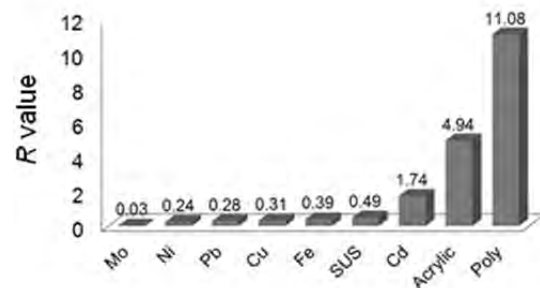


Fig. 1 R value for the various materials. Specific value by materials is shown by R value.

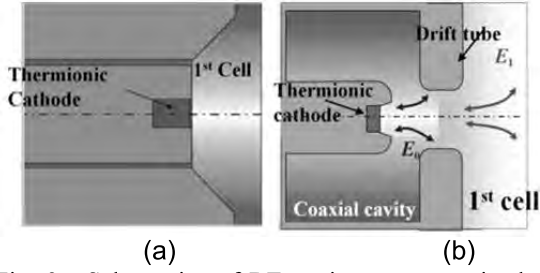


Fig. 2 Schematics of RF cavity structures in the vicinity of the thermionic cathode in (a) a conventional type, and (b) the triode-type RF gun.

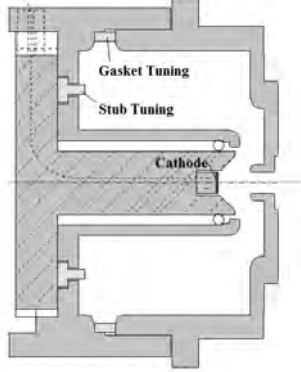


Fig. 3 Cross section of the new designed coaxial cavity for thermionic triode type RF gun. The Drawing includes the stub and gasket tuning systems.

the operational frequency of KU-FEL thermionic RF gun. However, the measured value has deviation of 429 MHz. Furthermore the low power test of prototype coaxial cavity revealed the resonance frequency dependence on the cavity temperature. As the consequence for operational conditions of cathode at ~ 1500 K the resonance is shifted for -10MHz.

Design refinement has been done based on these prototype test results in order to meet the resonance frequency requirement. A new cavity equipped with stub tuning and gasket tuning mechanism for frequency adjustment was fabricated and tested. The cross-sectional schema of the new designed cavity is shown in Figure 3.

The resonance frequency for the new coaxial cavity is measured to be 2862 MHz with 1 mm long tuning stub and 2 mm thick gasket. This value meets the requirements under consideration of thermal resonance shift at operational conditions and the frequency tolerance of ± 5 MHz.

This cavity is suitable for application to the KU-FEL thermionic RF gun, which will be done near future.

4. Development of AM reflectometer for fluctuation measurement in high temperature plasmas

Transport property of high temperature, fusion plasmas is believed to be influenced by various fluctua-

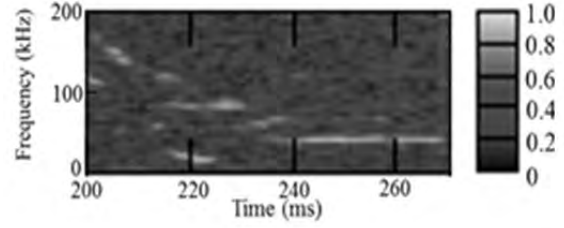


Fig. 4 Coherence between phase signal of AM reflectometer and signal of magnetic probe.

tations caused from a variety of instabilities. In this study, we have developed an Amplitude Modulation (AM) reflectometer for measurement of electron density fluctuation in a helical-axis heliotron device, Heliotron J. Previously in Heliotron J, we had developed a Frequency Modulation (FM) reflectometer using up-converter for the same purpose. However, the FM reflectometer system had large system noise and low measurement resolution. Therefore, we started to develop a new reflectometer system. In this AM reflectometer system, we use a voltage controlled oscillator (VCO) which can sweep the output carrier frequency. The microwaves are injected at O-mode with the carrier frequency ranging from 24.75 to 42 GHz, corresponding to the O-mode cut-off plasma density of $0.76\text{--}2.2 \times 10^{19} \text{ m}^{-3}$. The injected microwave is modulated in the frequency of 100 MHz using a PIN switch, and the phase shift originated from the density fluctuation at a cut off layer is detected using I/Q detector in the intermediate frequency.

Density fluctuations were measured with the newly developed AM reflectometer in a neutral beam injection (NBI) plasma with additional fueling of supersonic molecular beam injection (SMBI) in Heliotron J. In this experiment, the carrier frequency was fixed at 25.4 GHz of which cut off density is $n_e^c = 0.82 \times 10^{19} \text{ m}^{-3}$. Plasma density was in the measurable range of this reflectometer system since the maximum line average density was $n_e = 1.1 \times 10^{19} \text{ m}^{-3}$ and the cut off layer exists inside the plasma. Figure 4 shows the coherence between a phase signal of the AM reflectometer and a magnetic probe signal. Clearly, correlation between these two signals exists in a specific frequency range, which means fluctuation of an energetic ion driven MHD mode was successfully measured in this reflectometer system. Compared to the experimental results obtained by the previous FM reflectometer system, the signal to noise ratio was obviously improved in the new AM reflectometer system, resulting in clearer information about electron density fluctuations.

Collaboration Works

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、長崎百伸

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/ダイバーター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、花谷清

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

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、長崎百伸、大島慎介、水内亨、佐野史道

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ANU（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、長崎百伸、佐野史道

Stuttgart Univ.（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

V.G. Khlopin Radium Inst.（ロシア）、Low-background Spectroscopic Position-Sensitive Neutron Detector for Detection of Nuclear Materials in Cargo Containers、増田開

自然科学研究機構連携、磁場閉じ込めプラズマ中の乱流、磁気島及び磁力線の研究のための国際共同研究拠点ネットワーク活動の推進（分担）先進閉じ込め配位、長崎百伸、佐野史道、水内亨、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、Heliotron J 装置における電極バイアスによる径方向電場制御、佐野史道、水内亨、長崎百伸、岡田浩之、小林進二、山本聡

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、水内亨、長崎百伸、岡田浩之、南貴司、小林進二、山本聡

核融合科学研究所、ダイバータープラズマにおける熱流束に関する実験的研究（ヘリオトロン J における周辺プラズマの揺動と熱輸送の計測）、佐野史道、水内亨、岡田浩之、小林進二、大島慎介

核融合科学研究所、トリムコイルを用いたヘリオトロン J の磁場配位最適化、佐野史道、水内亨、長崎百伸、岡田浩之、南貴司、小林進二、山本聡

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、長崎百伸、岡田浩之、南貴司、小林進二

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、水内亨、長崎百伸、岡田浩之、南貴司、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 におけるビーム放射分光法による密度揺動の空間分布計測、水内亨、岡田浩之、小林進二、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 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、水内亨、長崎百伸、岡田浩之、南貴司、小林進二、山本聡、大島慎介

核融合科学研究所、極低磁場での電子バーンシュタイン波加熱のヘリオトロン J プラズマの閉じ込めと MHD 特性への影響、佐野史道、水内亨、長崎百伸、岡田浩之、南貴司、小林進二、山本聡、大島慎介

核融合科学研究所、高速カメラを主体とした周辺乱流計測と乱流物理の解明-Helical Heliotron 磁場装置 Heliotron J での乱流計測-、佐野史道、水内亨、長崎百伸、岡田浩之、南貴司、小林進二、山本聡、大島慎介

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、小林進二、山本聡、大島慎介

核融合科学研究所、多様な磁場配位を有するヘリカル系プラズマにおけるプラズマフローと磁気島の理解、佐野史道、水内亨、長崎百伸、岡田浩之、南貴司、小林進二、山本聡、大島慎介

核融合科学研究所、低磁気シアプラズマにおける高速イオンと高速イオン励起 MHD 不安定性の相互作用に関する研究、佐野史道、水内亨、長崎百伸、岡田浩之、南貴司、小林進二、山本聡

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

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核融合科学研究所, 電子サイクロトロン電流駆動の物理と回転変換制御, 長崎百伸

核融合科学研究所, 方向性プローブを用いた揺動による粒子異常輸送の研究, 佐野史道, 水内亨, 長崎百伸, 岡田浩之, 南貴司, 小林進二, 山本聡, 大島慎介

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Financial Support

Grant-in-Aid for Scientific Research

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K. Nagasaki, Nuclear Fusion Technology and Plasma

Advanced Plasma Energy Research Section

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

1. Introduction

The current subjects of this research section are to study the properties of high temperature plasmas in order to control and improve the plasma energy confinement from the physical viewpoint of nuclear fusion research. The experimental and theoretical investigations for the optimization of the helical-axis heliotron configuration are in progress under the collaboration with other groups of the institute and also groups of other universities/institutes under the auspices of the Collaboration Program of the Lab. Complex Energy Processes, IAE, the Collaborative Research Program of NIFS (National Institute for Fusion Science), etc.

In this report, some remarkable results obtained in the Heliotron J experimental study in FY2012 are reported focusing on (1) the effect of parallel magnetic ripple on plasma flow and (2) the characteristics of low-frequency density fluctuation in ECCD plasmas.

2. Effect of Parallel Magnetic Ripple on Plasma Flow*

Plasma flow plays an important role in stabilization of magnetohydro-dynamic (MHD) instabilities and improvement of the confinement in tokamaks. Since the parallel magnetic ripple of the confinement field causes the damping of parallel flow (v_{\parallel}) due to the neoclassical (NC) parallel viscosity, it is important subject to investigate the effect of magnetic field ripple on parallel plasma flow and to clarify experimentally its damping mechanisms in Heliotron devices, which have higher ripple than tokamaks.

To study the effect of the magnetic ripple strength, three different configurations are selected; high, standard and reversed mirror configurations. These configurations have different ripple configurations along the field line and the magnetic ripple strengths (γ) are 0.073, 0.031 and 0.027 m^{-1} at the plasma core, respectively. Radial profile of parallel flow velocity is measured using Charge eXchange Recombination Spectroscopy (CXRS) in Heliotron J. This system measures a CVI emission line (529.05 nm) through CXR process. Figure 1 shows the measured parallel flow velocity (v_{\parallel}) and ion temperature (T_i) profiles during the quasi-steady

state phase. Here the data in $\rho > 0.8$ are omitted due to the low signal-to-noise ratio. The ion temperature near the plasma center ($\rho = 0.07$) in the high mirror configuration is approximately 20 (40) eV higher than that in the standard (reversed) mirror configuration. In the plasma core ($\rho < 0.5$), v_{\parallel} in the standard and reversed mirror configurations are 2-3 times larger than v_{\parallel} in the high mirror configuration.

The external momentum input ($F_{\parallel\text{ext}}$) by NBI is changed by the balance of Co- and Counter-NBI power. Figure 2 show v_{\parallel} at $\rho = 0.07$ as a function of $F_{\parallel\text{ext}}$, which is evaluated using a Fokker-Planck code. A positive value of $F_{\parallel\text{ext}}$ denotes the co-direction. The line-averaged electron density in these discharges was almost $1.0 \times 10^{19} \text{ m}^{-3}$ within approximately 20% of variance, and this density variance gives 5-6 % uncertainties of $F_{\parallel\text{ext}}$ at $\rho = 0.07$. The parallel flow velocities increase as a function of $F_{\parallel\text{ext}}$ in the three configurations. The variation of parallel flow velocity with the external momentum input ($dv_{\parallel}/dF_{\parallel\text{ext}}$) in the high mirror configuration is clearly small compared to those in the other configurations. This result suggests that the damping force of v_{\parallel} in the high mirror configuration is much larger than those values in the standard and

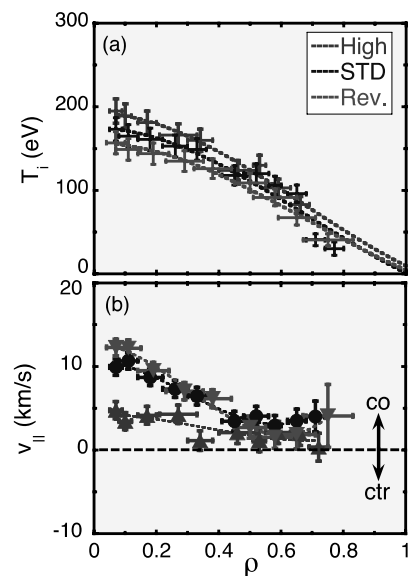


Fig. 1. Measured radial profiles of (a) ion temperature and (b) parallel flow velocity.

*H. Lee, S. Kobayashi, *et al.*, Plasma Phys. Control. Fusion **55** (2013) 035012.

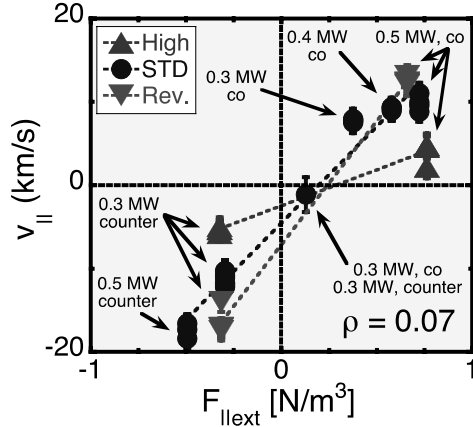


Fig. 2. Measured parallel flow velocities at $\rho = 0.07$ as a function of the external momentum input in the three mirror configurations.

reversed mirror configurations. In addition, counter-directed non-zero parallel flow is expected even in the condition of $F_{||\text{ext}} = 0 \text{ N/m}^3$ in every mirror configuration.

Further studies are necessary to quantitatively evaluate the offset parallel flow and to understand the flow driving mechanism in Heliotron J.

3. Control of Low-frequency Density Fluctuations by ECCD

It is an important subject to control the MHD activities related with the existence of the rational surface. Mitigation of MHD activities by using the electron-cyclotron-current-drive (ECCD) has been demonstrated. Density fluctuation measurement by using a beam emission spectroscopy (BES) reveals effects of ECH/ECCD on the characteristics of low-frequency density fluctuations in Heliotron J.

The toroidal current was controlled from +0.5kA (Co) to -1.5kA (Ctr) by changing the parallel refractive index $N_{||}$ of ECH waves from 0 to 0.3 (see Fig. 3). Here, the positive sign of the toroidal current means the current increases the rotational transform. Figure 4(a) shows the power spectrum of the density fluctuation measured with BES in the case of $N_{||} = 0.3$. The density fluctuations in the low frequency range ($f = 0.3\text{-}5 \text{ kHz}$) are observed in the peripheral region ($r/a > 0.7$). The coherence of the BES fluctuation signals at different radial positions to that at $r/a = 0.72$ was higher than 0.6. The phase difference is around zero. These indicate that this low-frequency density oscillation occurs only in the peripheral region. Since the coherence of the BES intensity to the Mirnov signal is around 0.3, an excitation of MHD activity is expected in the peripheral region. From the equilibrium calculation using VMEC code, the appearance of the $m/n = 8/4$ rational surface is predicted at $r/a \sim 0.6$ when the equivalent toroidal current around -1.5 kA is assumed. Here m and n are the poloidal and toroidal

mode numbers, respectively. As shown in Fig. 4(b), the position of the excited fluctuation shifts inwardly when $N_{||}$ changed from 0.3 to 0.2. In the case of $N_{||} = 0.15$ and 0.05, where no rational surface is expected from the equilibrium calculation, the fluctuation intensity stays in the noise level. These observations suggest that the observed low- f fluctuation is connected to the existence of a rational surface.

Although the further analysis is required to identify the fluctuation, the result obtained in the experiment has a capability to control the excitation of low- f fluctuation by ECCD in Heliotron J.

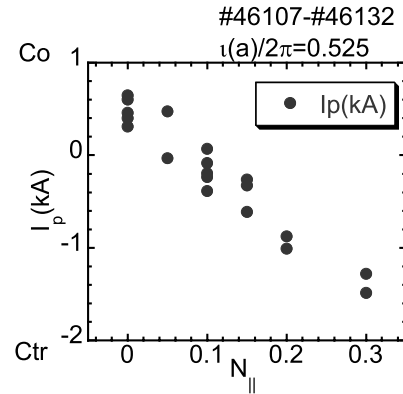


Fig. 3. Toroidal current (I_p) as a function of parallel refractive index $N_{||}$.

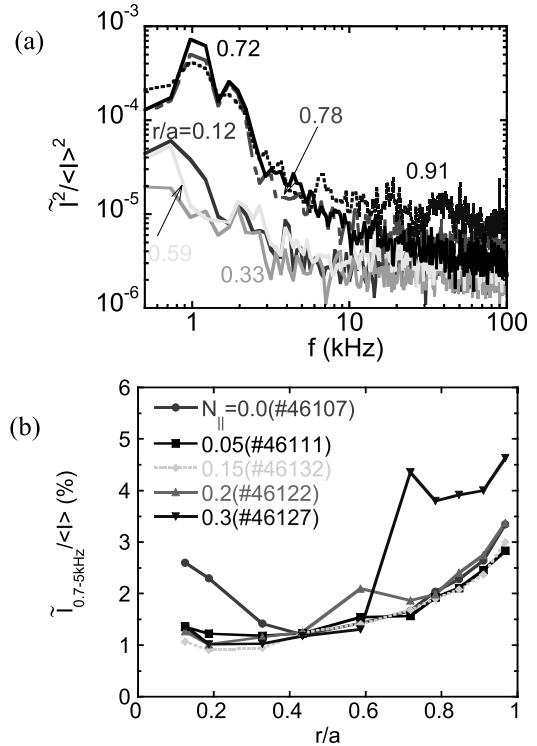


Fig. 4. (a) power spectrum of density fluctuation in case of $N_{||} = 0.3$ and (b) radial profile of density fluctuation in low- f range.

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/ダイバーター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, 花谷清

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Advanced Energy Research Section

Chonghong Zhang, Foreign Visiting Associate Professor
(Institute of Modern Physics, Chinese Academy of Science, China)

1. Summary

The effects of helium implantation and high-energy Ne-ion irradiation on the Ti-added Al-free ODS ferritic steel and a RAMS, which are candidate materials to fusion reactor blankets, have been investigated, and it is shown that the ODS steel is much more resistance to helium embrittlement than the RAMS.

2. Introduction

Oxide-dispersion-strengthened (ODS) ferritic steels were developed to remedy the high temperature creep strength of reduced activation martensitic/ferritic steels (RAMS), which are candidate structure materials for fusion reactor blankets. The recently developed 16Cr Ti-added ODS ferritic steel was proven to have good high-temperature mechanical properties meanwhile show high resistance to the corrosion from super-critical water (SCW) coolant (Kimura et al, J.Nucl.Mater. 417(2011)176). Our more recent investigation of the microstructures with TEM shows that there are fine oxides of Y-Ti-O, with an average diameter of 3.9 nm, in a high-density about $7 \times 10^{16} \text{ cm}^{-3}$ in the grains of the 16Cr Ti-added and Al-free ODS ferritic steel. Because the first wall and blankets have to endure intensive irradiation from 14 MeV neutrons in prototype fusion reactors, effects of production of crystal defects and the nuclear transmutation products including helium are crucial concerns for the application of the materials in fusion reactors.

In the present paper, results of our recent study of helium implantation and heavy ion-irradiation on the ODS ferritic steel are presented.

3. Effects of helium-ion implantation

Well polished $\phi 3$ mm disks of a 16Cr Ti-added Al-free ODS ferritic steel and a commercial ferritic/martensitic steel (T92B) were implanted simultaneously at ambient temperature with helium ions at the ECR 320 kV high-voltage platform in the Institute of Modern Physics (IMP), CAS in Lanzhou. The energy of helium ions was degraded successively from 540 keV to 10 keV to produced a box-shape distribution of helium atoms from the near-surface to a depth about 1.2 μm . Three

concentration levels (3000, 6000, 12000 appm He) were reached. The specimens were subsequently thermal annealed at 800°C in vacuum. Plan-view TEM samples were prepared subsequently from the specimens with dimple polishing and ion-milling. Thin areas of the samples were investigated in a transmission electron microscope (JEOL 2100F).

Bubbles were observed in both the specimens. Typical morphologies were shown in Fig.1. Obviously bubbles in the ODS ferritic steel have a smaller average diameter than in T92B. Anymore, there is less difference in size between bubbles at the grainboundaries and those within the grains in the ODS ferritic steel. It is indicated that the growth of bubbles especially at grainboundaries was significantly suppressed in the ODS steel, probably due to trapping of helium atoms and recombination of point defects at the oxide/matrix interfaces, showing a high potential of resistance to helium accumulation.

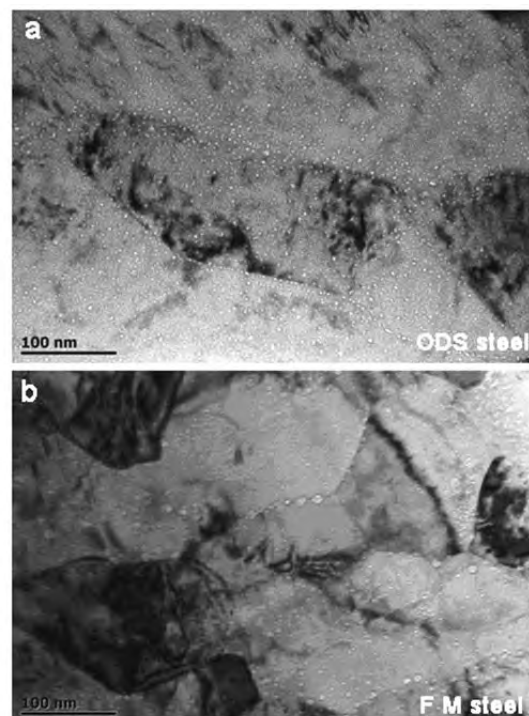


Figure 1 Typical morphologies of microstructures of helium-implanted (to 6000 appm) and subsequently annealed at 800°C, (a) Ferritic ODS steel and (b) Commercial ferritic/ martensitic (F/M) steel.

4. Effects of 122 MeV Ne-ion irradiation

In order to understand the response of the mechanical properties of the 16Cr ODS ferritic steel to intense irradiation, further irradiation experiment of the ODS ferritic steel was performed at the terminal of the sector focused cyclotron (SFC) in IMP, Lanzhou, with ^{20}Ne ions with a kinetic energy of 122 MeV. The recently developed chamber at the terminal of SFC includes an energy degrader which enables a uniform distribution of atomic displacement damage and injected ions within the projective range in specimens, a cooling (liquid nitrogen) stage, a hot (up to 600°C) stage of specimens. An overview of the chamber is shown in Fig.2.

According to previous work (Marokov, Goodhew, J.Nucl.Mater. 158 (1988) 81; Zhang et al, J.Nucl.Mater. 375(2008)185), Ne ions can be effectively used to simulate helium implantation and meanwhile produce a higher rate of atomic displacement damage (in dpa) in metals. In the present experiment, a uniform distribution of Ne concentration and atomic displacement damage (in dpa) was produced from the near surface to a depth about 31 micro-meters in the specimens, as shown by the SRIM estimate in Fig.2. Two dose levels of 690, 1600 appm of Ne concentration, corresponding to 0.56, 1.3 dpa were approached.

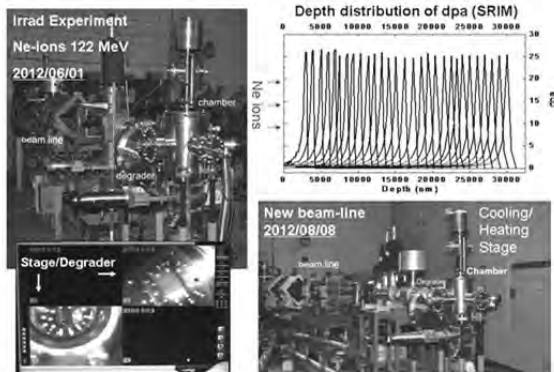


Figure 2 Irradiation chamber at the SFC, with an inset showing a SRIM estimate of depth distribution of atomic displacement damage (in dpa).

Tests of the mechanical properties were carried out using a special equipment of Small-ball Punch Test in Paul Scherrer Institut (PSI). Disks with 3 mm in diameter of the ODS steel were tested with Small Punch test at 500°C. The obtained load-displacement curves of the steel in different conditions (un-irradiated or irradiated to different doses) are shown in Fig.3. Hardening and embrittlement were hardly observed in the ODS ferritic steel. The ODS ferritic steel do not exhibit observable loss of ductility even to the highest dose level (1600 appm

Ne, corresponding to 1.3 dpa), indicating that the ODS ferritic has good resistance to helium embrittlement, probably due to the trapping of helium atoms at the oxide/substrate interfaces and thus the reduction of transport of helium atoms to grain-boundaries. Results of the present work show the advantage of ODS ferritic steels which are proposed to be used in harsh environments with strong irradiation at high temperatures. Further investigations of the fractured area with scanning electron microscopy (SEM) and with transmission electron microscopy (TEM) is being carried out to know in detail the fracture mode, behavior of the defect accumulation and evolution in the ODS steel to build up a correlation of mechanical properties with microstructures.

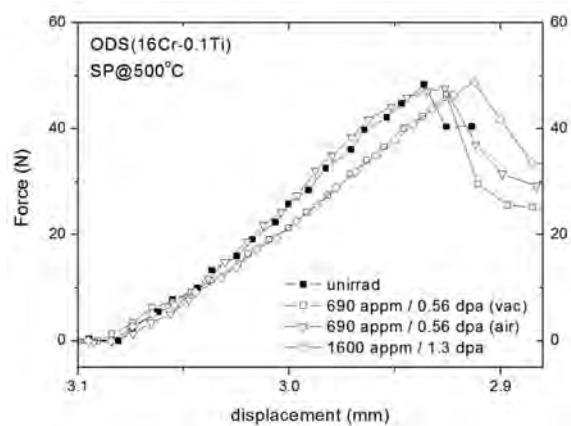


Figure 3 Effects of Ne-ion implantation on load – displacement curve in small-punch test of the ODS ferritic steel at 500°C.

5. Resistance to helium embrittlement

Transmutation helium atoms generated in the structural materials under operation of fusion reactor will cause a severe damage of blanket component where neutron irradiation embrittlement is enhanced by helium-induced embrittlement. The neutron irradiation embrittlement is due to the formation radiation defects such as vacancy clusters and interstitial clusters as well as irradiation induced precipitation of secondary phases, which are accompanied by hardening to cause embrittlement. Helium-induced embrittlement is due to formation of helium bubbles at grain boundaries, which reduces grain boundary strength and results in grain boundary cracking.

Nano-scaled oxide particles are well known to play a role to trap defects and helium atoms at the interface of the particles and matrix. This study clearly indicates that the helium bubble growth is suppressed in the ODS steel, resulting that the ODS steel is much more radiation tolerant than the RAMS.

Advanced Energy Research Section

Jan Valenta, Foreign Visiting Associate Professor
 (Associated Professor, Department of Chemical Physics & Optics,
 Faculty of Mathematics & Physics, Charles University, Prague, Czech Republic, EU)

Silicon nanocrystals for the third generation photovoltaics

The principles of the 3rd generation photovoltaics (PV) are presented on the background of the current status of PV research and development (R&D). The possible contribution of silicon (or other group-IV-A nanomaterials) is discussed with some examples of the author's research results.

1. Factors limiting PV-cell efficiency

There are three types of *intrinsic losses* in an ideal single p-n junction PV-cell as described by Shockley and Queisser [1] (S-Q) and setting the power efficiency (PE) limit to about 33 %:

- non-absorbed energy of below-band-gap photons
- energy of hot-carriers converted to heat (entropy)
- energy lost by radiative recombination

2. Development of photovoltaics

The following three generations of PV devices are commonly distinguished [2] (Fig. 1):

1st generation – based on bulk material p-n junction is represented by the bulk Si PV-cells made of mono- or poly-crystalline wafers.

2nd generation – based on the thin film technology and possibly using various materials (a-Si, CdS, CdTe, CIGS-copper indium/gallium diselenide etc.).

3rd generation – high-efficiency PV cells that overcome the S-Q limit by reducing losses due to non-absorbed photons and thermalized hot carriers. It is using advanced concepts employing several energy levels to harvest the solar spectrum more efficiently. The main concepts include: tandem cells, light-frequency converters (up- and down-conversion), multiple-exciton generation or carrier multiplication, hot-carrier exploitation through selective contacts, intermediate band cells etc.

The 1st generation PV-cells still represent the major part of the PV production as the Chinese producers of bulk Si PV-cells continue to push price per power beyond limits (currently the panel cost dropped to ~0.5 USD/Wp) that were anticipated when the 2nd generation was developed for production. This effect has considerably limited the share of market by thin-film PV cells (it persists between 10-20% already for about two decades). Therefore the plot in Fig. 1 evolved from the original

publication by M.A. Green in 2001 – i.e. the 1st generation merged with the 2nd generation. One can suppose that different “generations” and concepts will coexist and possibly find different (niche) application fields under the severe economical conditions.

There are three basic routes to be followed in

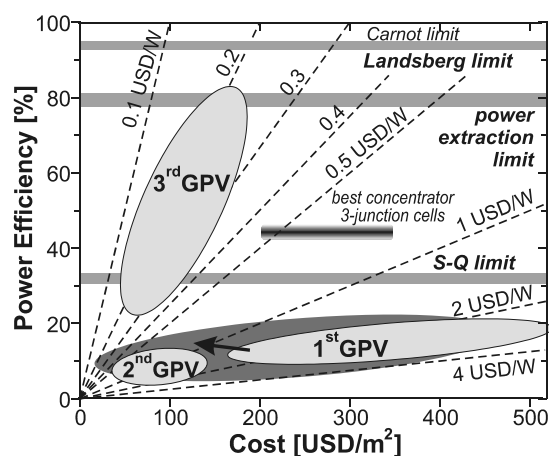


Figure 1. The three PV generations plotted in coordinates of price per m² and energy efficiency as proposed by M.A. Green [2]. The tilted dashed lines indicate price per power (taking solar power of 1 kW/m²). Different theoretical limits are indicated. Light gray ellipsoids show position of PV generations according to Green. Dark gray area shows recent evolution of the 1st generation toward low price and improved efficiency (15-20 %).

order to improve solar-spectrum harvesting by the 3rd generation PV-cells:

(a) Increasing number of energy bands which can absorb separately different parts of the spectrum.

(b) Create more low-potential electron-hole pairs from one absorbed photon of high-energy or inversely, create one high-potential electron-hole pair from several low-energy photons.

(c) Capture highly-excited (hot) photo-carriers before their thermalization (relaxation) to the band minima.

3. Silicon nanostructures for 3rd PV generation

Semiconductor nanostructures are extensively studied for about three decades. Their possible role in solar cells includes mainly the *better exploitation of the solar spectrum* and/or *increase of light trapping*. Many different materials could be used for such purpose but for large-scale application only

cheap and abundant materials with well mastered and scalable technology can be suitable. Therefore, large part of the research focuses on the materials containing elements from the group-IV (more exactly IV-A, or group 14) of the periodic table – mostly Si and C.

The only 3rd generation PV principle which is already used in commercial production is **tandem cell** (GaInP/GaInAs/Ge triple-cells are currently the most efficient PV-cells with $\eta = 43.5\%$ under concentration of 480 Suns [3] and even 44% at ~950 Suns). Similar type of **stacked tandem cells** (upper cell absorbs high-energy photons, transmitting low energy part of the spectrum for the lower cell; cells are connected in series by a tunnel diode between them) can be, in principle, built out of semiconductor nanostructures taking advantage of the *quantum confinement effects* which blue-shifts the band-gap energy with decreasing size of the structure. Silicon nanocrystals (Si-NCs) seems to be very promising material for such tandem cells and they are being developed e.g. by Conibeer's group in Sydney [4,5] or within our European project NASCEnt [6]. The main effort is now concentrated on the optimization of transport properties, reduction of defects, efficient doping of Si-NCs etc.

Another possible application of Si-NCs is the **photoluminescence down-shifter**. Si-NCs deposited on a conventional PV cell efficiently absorb high energy photons and emit low-energy photons [7]. The advantage of this conversion consists in deeper penetration of low-energy photons into the bulk PV-cell, where the charge collection is more efficient. The improvement of PV-cell internal quantum efficiency (QE) of 14% has been reported using thick layer of Si-NCs in oxide [8]. However, for effective increase of power efficiency, the luminescence down-shifters must be combined with appropriate light management design.

Obviously, the above described down-shifting of photon energy cannot reduce energy loss of short-wavelength photons. This can be achieved by **down-conversion** (production of more than one low-energy photon from one high-energy photon) or **carrier multiplication** (CM) (also called multiple-exciton generation), where one hot carrier generated by one photon is converted to more than one “cold” carrier. The effect of CM can be understood as an analog of the impact ionization in bulk material. CM was reported in Si-NCs by Beard et al. using ultrafast transmittance spectroscopy [9] and by collaboration of the author with Gregorkiewicz' group [10]. The later observation is based on measurement of photoluminescence quantum yield (PL QY) as function of excitation wavelength. This technique reveals step-like enhancement of the PL QY with increasing energy of excitation photons in densely spaced ensembles of Si-NCs (see Fig. 2) but

not in sparsely organized Si-NCs. The model called *Space-Separated Quantum-Cutting* (SSQC) was proposed considering interaction of neighbour NCs.

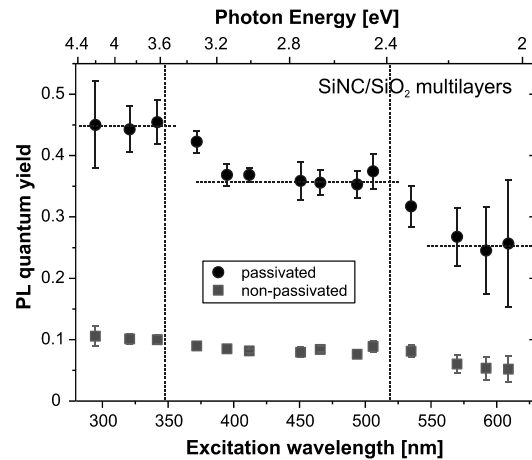


Figure 2. PL QY excitation spectra for a pair of SiNC/SiO₂ multilayer samples: Non-passivated (gray rectangles) and passivated by annealing in H (black circles). [11]

CM can be exploited either in tandem solar-cells with Si-NCs or in PL down-converters.

The PL QY technique proved to be very convenient for studies of CM under conditions similar to the solar radiation, in contrast to the ultrafast-laser spectroscopy. However, the technique must be perfectly mastered in order to avoid large errors. Therefore, we recently developed (theoretically and experimentally) correct methodology for precise determination of PL QY with use of an integrating sphere [11]. Currently, we are testing an extension of this methodology allowing for low-temperature measurement of PL QY.

In conclusion, Si nanostructures can be produced by techniques compatible with the major trends in semiconductor microelectronics at competitive prices. Also the knowledge of excitation and relaxation processes in such nanostructures is quite deep. Therefore, these materials are considered as one of the best options for development of the 3rd generation PV-cells as was illustrated by a few examples in this report.

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Advanced Energy Research Section

Francesco Volpe, Foreign Visiting Researcher
 (Assistant Professor in the Department of
 Applied Physics and Applied Mathematics,
 Columbia University, New York, USA)

1. Summary

The author spent the summer of 2012 as a visiting assistant professor at the Uji campus of Kyoto University, hosted by the Heliotron J group.

Here the author reports about a radiometer he developed for future Electron Bernstein Wave (EBW) emission measurements at Heliotron J, and discussions he had on ray tracing calculations aimed at interpreting such measurements.

2. Introduction

Electron Bernstein Waves (EBWs) are electrostatic waves propagating in hot magnetized plasmas at densities not accessible to Electron Cyclotron (EC) waves polarized in the Ordinary (O) or extraordinary (X) mode. This aspect, along with the high localization of their emission and absorption, makes EBWs highly attractive for heating, current drive and emission measurements in hot dense fusion plasmas.

Being electrostatic waves, EBWs can only exist in a medium (in this case, the plasma). However, they can be coupled to an external transmitter or receiver by means of mode conversions. Of various schemes proposed, the O-X-B mode conversion and the reverse, B-X-O process, are particularly attractive because they can be geometrically optimized by adopting a special line of sight. This is in contrast with other methods relying on the thinness of evanescent layers in the plasma edge.

Clear demonstrations of OXB-enabled EBW heating/current drive and of a BXO-enabled EBW emission measurements were obtained in the W7-AS stellarator device [1][2]. Also, overdense plasmas were effectively heated both at the second and third harmonic resonance condition in the Heliotron DR helical device.

Diagnostic uses of EBW emission (EBE) were explored in tokamaks, spherical tori and helical systems. The main application of EBE is as electron temperature profile diagnostic [2] but, more recently it has also been proposed to measure the angular dependence of the BXO mode conversion to diagnose the magnetic pitch angle profile [3].

The complicated three-dimensional field of helical systems has to be taken into account in the calculation for evaluating how waves propagate, mode-convert and are absorbed, or emitted. This can

be done by means of a ray tracing code adopting the geometrical optics approximation.

3. Ray tracing code for EBE

The B-X-O process is a reversal process of O-X-B process. Using this physical principle, we are able to estimate the EBE position in plasmas when antenna position is determined. Let us consider an overdense plasma in which the O-mode cut-off determined by the plasma frequency. In toroidal geometries, an incident O-mode launched from the low field side can be converted into a slow X-mode at the O-mode cut-off layer if the O-mode is injected at the optimal angle oblique to the magnetic field. The optimal angle at the O-mode cut-off is given by

$$\cos \theta^{opt} = \sqrt{\frac{Y}{1+Y}} \quad (1)$$

where θ is the angle that the magnetic field makes with the wave vector, $Y = \omega_{ce}/\omega$, ω_{ce} is the electron cyclotron frequency and ω is the wave frequency. After conversion, the X-mode propagates toward high-density region until it turns back and propagates toward the upper hybrid resonance (UHR) layer satisfying the relation, $\omega_{pe}^2 + \omega_{ce}^2 = \omega^2$. When the X-mode approaches the UHR layer, the perpendicular component of the refractive index rapidly increases, resulting that the phase velocity of the wave slows down. In this process, the electric field of the X-mode begins to lie parallel to the wave vector, that is, the wave turns to have an electrostatic nature. As the wave approaches the UHR, its phase velocity approaches the electron thermal velocity, making kinetic effects significant and causing the X-mode to be converted into the EBW. This propagates backward into the high-density region (towards the plasma center) and the wave energy is transferred to electrons at the position where the Doppler shifted cyclotron resonance condition,

$$\omega \left(1 - \frac{N_{\parallel} v_{\parallel}}{c}\right) = \frac{\omega_{ce}}{\gamma} \quad (2)$$

is satisfied. Here γ is the relativistic factor, and v_{\parallel} and N_{\parallel} is the parallel components of the thermal velocity and refractive index, respectively.

A ray tracing code is being developed to calculate the ray trajectory and the EBE profile for Heliotron J. The code solves the radiative transfer

equations under the geometrical optics approximation. Assuming that the non-uniformity of the plasma parameters is weak on the distance of a wavelength, the wave trajectory can be calculated from the following set of differential equations:

$$\frac{d\mathbf{r}}{d\sigma} = \frac{\partial D}{\partial \mathbf{k}}, \quad \frac{d\mathbf{k}}{d\sigma} = -\frac{\partial D}{\partial \mathbf{r}}, \quad \frac{dt}{d\sigma} = -\frac{\partial D}{\partial \omega}, \quad (3)$$

where $D(\omega, \mathbf{k}, \mathbf{r})=0$ is the local dispersion relation of the wave, and $\mathbf{r}(\sigma)$, $\mathbf{k}(\sigma)$ and $t(\sigma)$ denote the position, wave vector and time along the wave trajectory respectively, which are related to each other through the parameter, σ . The dispersion relation for the electromagnetic waves is given by a cold plasma approximation. The dispersion relation for electrostatic waves is given by a hot plasma approximation,

$$D = \frac{\mu^2 N^2}{X^2} + 1 + z \sum_m \exp(-\lambda) I_m(\lambda) Z(z - m\alpha) = 0 \quad (4)$$

where

$\mu = v_{th} / c$, $z = 1 / \sqrt{2} \mu N_{||}$, $X^2 = \omega_{pe}^2 / \omega^2$, $Y = \omega_{ce} / \omega$, $\alpha = Yz$, $\lambda = \mu^2 N_{\perp}^2 / Y^2$, v_{th} is the electron thermal velocity, I_m is the modified Bessel function, and $Z(z)$ is Fried-Conte function. The ray initially starts from the vacuum region where the refractive index is unity and the ray propagates straight until it enters the plasma. Once it enters the plasma, the differential equations are numerically solved using the dispersion relation for cold plasma. When the ray reaches the O-mode cut-off layer with optimal angle, it is converted into the X-mode propagating inside the cut-off layer. When the X-mode reaches the UHR layer, the dispersion relation is changed into the eqn. (4) to trace the EBW ray. The calculation is continued until 99.9% of power is absorbed. The imaginary part of the wave vector is given by solving the non-relativistic dispersion relation, eqn. (4). The inclusion of relativistic corrections, which absorption might be sensitive to, is being evaluated.

The three-dimensional magnetic field structure of Heliotron J will be taken into account, and present single-ray calculations will be upgraded to multiple rays in order to more accurately estimate the power absorption profile.

4. Radiometer system for EBE diagnostic

An EBE radiometer system was assembled and tested in the laboratory, and is awaiting installation on the Heliotron J device, where it is expected to measure the T_e profile under overdense conditions not accessible to Electron Cyclotron Emission (ECE). Furthermore, as the radiometer will be connected to the transmission line and steerable antenna normally used for 70 GHz second harmonic X-mode heating, it will be possible to perform angular scans of conversion efficiency that could provide guidance to

EBW heating.

The radiometer consists of a 28GHz Gunn oscillator, a balanced mixer, a step attenuator, low-noise amplifiers, a power divider, band-pass filters, Schottky-barrier diodes and video-amplifiers. Manual replacement of the filters allows tuning the 4 channels of the radiometers to frequencies in the 30-46GHz range. Accessing EBE at these frequencies by means of BXO conversion requires the plasma densities of $1.2-2.7 \times 10^{19} \text{m}^{-3}$ which, indeed, are routinely obtained at Heliotron J.

A waveguide switch will be installed in the transmission line to switch between ECH/ECCD and EBE. A Gaussian-optics antenna is used to attain high gain, and can simultaneously measure two cross-polarizations. These will be matched to the elliptical polarizations of the oblique O-mode and X-mode by means of a universal polarizer, possibly consisting of a $\lambda/4$ plate and waveguide rotary joint. Note that, although the desired signal is polarized in the O-mode, simultaneous X-mode measurements would contain information on stray radiation and less-than-optimal conversion efficiency, as due for example to density fluctuations.

Preliminary tests showed that the radiometer can detect 35 GHz microwaves of nW level intensity. The radiometer system is planned to operate in the forthcoming experimental campaign.

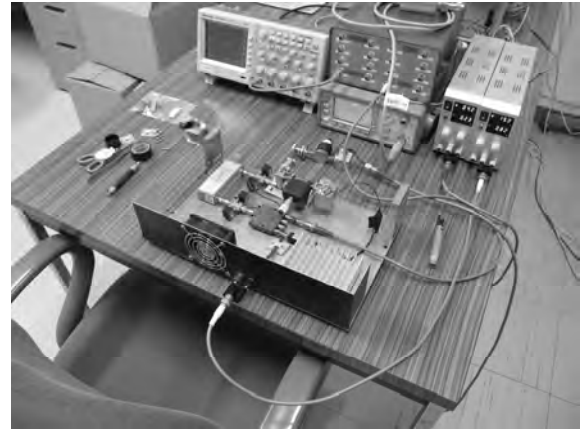


Fig. 1: Radiometer system for Heliotron J

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Advanced Energy Materials Research Section

K. Matsuda, Professor
 T. Hinoki, 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 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 2012.

1. Observation of Negative and Positive Trions in the Electrochemically Carrier-Doped Single-Walled Carbon Nanotubes

The electronic and optical properties of single-walled carbon nanotubes (SWNTs) have been the subjects of intense investigation because of their importance in nanoscience and for various promising applications. The optically generated electron-hole pair in a 1-nm cylinder structure forms exciton as the strongly bound state, such as the hydrogen atom (H), due to the attractive Coulomb interaction. Because of the strong Coulomb interaction, the formation of a charged exciton, called a trion, has been expected in carrier doped SWNTs. The trion is the three-particle bound state of a doped carrier (electron or hole) and an optically generated electron-hole pair, such as H^- or H^{2+} . Since the trion has an extra charge and nonzero spin, the trion physics has been of strong interest especially in the field of spin manipulation, and has been studied in various semiconducting materials. Very recently, the positive trion (bound state of two holes and one electron) was detected in the hole-doped SWNTs by chemical doping at room temperature. The negative trion (bound state of two electrons and a hole) has also been expected to be stable in the electron-doped SWNTs according to the theoretical prediction. However, the negative trion in the SWNTs has not yet been observed by means of chemical doping using a dopant molecule.

We reported the detection of both the positive trion (positively charged exciton) and negative trion (negatively charged exciton) as a three-particle bound state in the SWNTs at room temperature by an in situ photoluminescence (PL) spectroelectrochem-

istry method for an isolated SWNT film cast on an ITO electrode (upper panels of Fig. 1). The electrochemical hole and electron dopings enable us to detect such trions on the SWNTs. The large energy difference between the singlet bright exciton and the negative and positive trions showing a tube diameter dependence is determined by both the exchange splitting energy and the trion binding energy. In contrast to conventional compound semiconductors, on the SWNTs, the negative trion has almost the same binding energy to the positive trion, which is attributed to nearly identical effective masses of the holes and electrons (lower panel of Fig. 1).

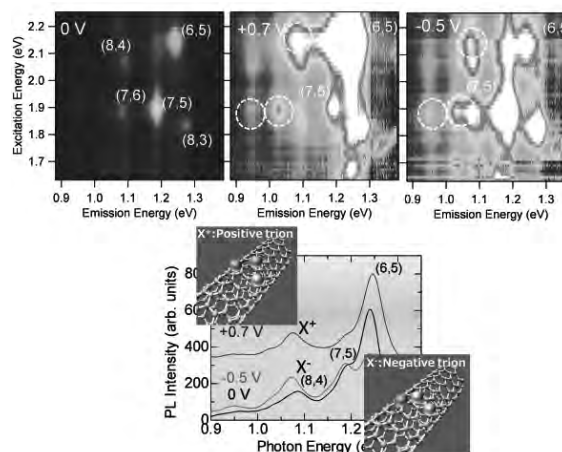


Fig. 1 Upper panel; PL maps of SWNTs by electrochemically doping method. Lower panel; PL spectra of electrochemically doped SWNTs.

2. Implications of Trion Localization Studied by Temperature Dependence of Photoluminescence Spectra in Hole-doped Single-Walled Carbon Nanotubes

Charge carrier doping is an effective method for modifying the optical properties of low-dimensional materials. The interplay between the excitons and doped charge carriers due to strong Coulomb interactions in SWNTs causes intriguing excitonic properties such as exciton dephasing by unusual exciton-hole interactions, the blueshift of the exciton energy, and the formation of trions (charged exciton), which is a bound state of two holes and an electron (or two electrons and a hole). Despite their importance, the

dimensionality of the trions, i.e., whether they are itinerant (1D) or localized (0D-like) in 1D SWNTs, is still under discussion. From the previously obtained experiment, we infer the localization of trions. However, no clear evidence of trion localization has been observed. Temperature-dependent PL spectroscopy is a powerful method to probe the dimensionality of quasiparticles such as excitons and trions because the PL intensity is associated with the effective radiative decay rate determined as a function of temperature T , which depends on the effective dimensionality of the excitonic states. Thus, the PL spectral change under different temperatures is expected to provide important information for understanding the dimensionality of the excitons and trions in SWNTs.

We investigated the temperature dependence of the PL spectra of hole-doped SWNTs from 5 to 300K to clarify the dimensionality of the excitons and trions. We observed considerably different behavior of the PL from the trions and excitons; the PL intensity of the trions was nearly independent of temperature, whereas that of the 1D excitons changes according to $T^{-1/2}$ dependence. These behaviors are attributed to the difference of the dimensionality of excitonic states; the $T^{-1/2}$ dependence of the PL reflects the 1D radiative decay rate of the excitons and the nearly temperature-independent trion PL indicates the 0D radiative decay rate suggesting spatial localization of the trions.

3. Development of Pseudo Ductile Porous Silicon Carbide Ceramics

Silicon carbide (SiC) ceramics are very attractive engineering ceramics in particular for high temperature use and nuclear application due to high temperature strength, oxygen resistance, chemical stability, low activation, radiation resistance and so on. However the application of SiC ceramics is limited due to brittle feature. Novel porous SiC composites were developed at Kyoto University. The objective of this work is to develop pseudo ductile porous SiC ceramics by SiC fiber reinforcement.

The composites consisted with just SiC fiber and crystalline porous SiC matrix without fiber/matrix interphase like carbon (C). The SiC matrix was formed with C powder by liquid phase sintering or reaction sintering method. The porous SiC matrix was formed following decarburization process. The composites showed pseudo-ductile behavior and complicated fracture behavior due to frictional stress at debonded fiber/matrix interface. Three point flexural strength was approximately 300 MPa in case of the material with 30 % porosity.

Compared to current porous SiC ceramics, strength is more than three times with pseudo-ductile feature by fiber reinforcement. High temperature use is expected above metal applied temperature. Silicon carbide composites require fiber/matrix interface

layer like C for pseudo-ductile fracture behavior. The control of thickness and quality for the interface layer is very difficult, although it is the key to determine mechanical properties of the composites. The novel material has pseudo-ductile behavior and reliability and applicable as structural material. The novel material doesn't require fiber/matrix interphase like C. It decrease material cost significantly. Productivity is also excellent compared to current SiC composites. The material just consists with SiC. Excellent resistance to high temperature oxygen and chemical corrosion is expected.

4. Simulation of Neutron Damage on Nuclear Ceramics by Ion Irradiation

Due to the lack of operating research reactors and fusion reactors, research on nuclear materials relies on simulation experiments such as ion-irradiation. A Material Irradiation Research Facility (DuET), composed of two accelerators for heavy ions and He^+ , respectively, can be a useful tool to simulate the neutron bombardments. The highly controllable irradiation conditions would help to understand the underlying mechanisms of the irradiation effects. Our research group has focused on the irradiation performance of SiC composites and nuclear grade graphite. The exceptionally high irradiation tolerances, such as the retaining of the initial strength after irradiation in a wide T_{irr} range (280-1400°C), have been demonstrated for SiC composites. Recently, the unique irradiation and analysis method combined with MUSTER facility demonstrated the irradiation-induced contraction of the graphite and clarified that the dimensional stability is largely depends on the graphite grade.

5. Horizontal Laser Cooling of Magnesium Ion Beam by Synchro-Betatron Resonance at S-LSR

As collaboration research with Advanced Research Center for Beam Science, Institute for Chemical Research, Jimbo engages in a laser cooling experiment of magnesium ion beam at Small Laser-equipped Storage Ring (S-LSR). Prolongation of sideband amplitudes in the right side of the revolution frequency of $h=99$ and in the left side of the revolution frequency of $h=101$ were observed adjacent to the 2.5MHz RF frequency ($h=100$) in analysis of frequency spectrum of bunched ion beam. We would like to achieve an energy transfer between the longitudinal and the horizontal directions of the ion beam to realize the horizontal cooling. Now optical method is the only way to diagnose a bunched ion beam. As less ions are in the beam, however, it is more difficult to observe such a beam optically. We hope that observed asymmetries of frequency spectrum are utilized as another diagnosis method.

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

Oak Ridge National Laboratory (米国), TAITAN (Tritium, Irradiation and Thermofluid for America and Nippon) Task2-2 接合・被覆システムの健全性, 檜木達也

Oak Ridge National Laboratory (米国), TAITAN (Tritium, Irradiation and Thermofluid for America and Nippon) Task2-3 動的変形挙動, 檜木達也

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核融合科学研究所, 液体ブランケット二重冷却システム用炭化珪素材料の開発, 檜木達也

Financial Support

1. Grant-in-Aid for Scientific Research

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毛利真一郎, 若手(B), 局在光電場中の単一カーボンナノチューブ電子状態の解明とその制御

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Advanced Laser Science Research Section

K. Miyazaki, Professor
 T. Nakajima, Associate Professor
 K. Hata, Assistant Professor
 G. Miyaji, Assistant Professor

1. Introduction

Our research interest is focused on the development of advanced laser science for the purposes of pioneering new fields of photon energy technology. The laser development is aiming at the generation of high-intensity, few-cycle laser pulses with stabilized carrier envelope phase (CEP). The intense laser pulses allow us to approach sub-fs ($< 10^{-15}$ s) to attosecond (10^{-18} s) time regions in the experimental study of ultrafast strong-field interaction with atoms, molecules and solid surfaces. The goal is to demonstrate potential abilities of high-intensity coherent radiation in new regimes and to contribute to the progress of future science and technology.

2. High-intensity ultrashort pulse lasers

Three Ti:sapphire laser systems using the chirped-pulse amplification (CPA) technique are working in the laboratory, which emit high-intensity fs laser pulses at the center wavelength of ~ 800 nm. One of them produces a peak power of 1 TW (40 mJ in 40 fs), which has been used for the study of ultrafast strong-field interactions with atoms and molecules. The other CPA laser system, producing 10 mJ in 100 fs pulses with a well-defined intensity distribution in the beam, has been applied to the study of nano-processing of materials.

An advanced fs Ti:sapphire CPA laser system (Fig. 1) is operating for the study of attosecond science. This system consists of a mode-locked oscillator producing 5 fs pulses at 80 MHz, a pulse stretcher, a pulse selector, a multi-pass amplifier, and a grating compressor. The CEP of output pulses can be



Fig. 1. CEP stabilized Ti:sapphire CPA laser system (5 fs, 0.1 TW, 1 kHz).

locked and precisely controlled. The average output power is 1.6 W with CEP-locked 25 fs pulses at a repetition rate of 1 kHz. The output pulses can be compressed to less than 5 fs in duration with a pulse compressor consisting of a gas-filled hollow fiber and chirped mirrors for dispersion compensation.

3. High-order harmonic generation with few-cycle fs laser pulses

The intense few-cycle laser pulses are used to produce attosecond EUV pulses through the high-order harmonic generation (HHG) in a gaseous medium. The experimental apparatus for the HHG (Fig. 2) consists of a pulsed gas jet operated at 100 Hz, vacuum chambers for differential pumping, a flat-field grating EUV spectrometer with a CCD detector.

Atomic and molecular gases, Ne, Ar, N₂, and CO₂, were used as the nonlinear media for HHG. The HHG spectra, especially in the cutoff region, were observed to shift, strongly depending on the CEP shift ϕ_{CEP} . The largest wavelength shift was observed for Ne having the highest ionization potential of the nonlinear media used in the experiment. We have found that the wavelength shift periodically changes with the change in ϕ_{CEP} .

When ϕ_{CEP} is not fixed in the HHG, the harmonic spectrum tends to be continuum in the cutoff region. This phenomenon is certainly associated with the wavelength shift induced by the random change in ϕ_{CEP} of the output pulses at the repetitive operation. The wavelength shift of harmonic peaks can be larger than the separation of adjacent harmonic peaks, especially in Ne atoms interacting at high in-



Fig. 2. Experimental apparatus for the HHG.

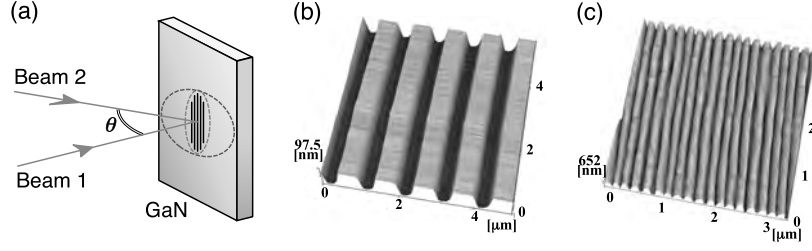


Fig. 3. (a) Optical configuration in the experiment, (b) scanning probe microscope (SPM) image of the interference pattern on the GaN surface ablated with a single fs pulse from two beams, and (c) SPM image of the nanograting.

tensities. This was confirmed with a theoretical simulation of the HHG depending on ϕ_{CEP} . The results obtained suggest that a single attosecond EUV pulse can be produced by stabilizing the CEP of the few-cycle fs laser pulses.

4. Patterning of nanogratings with fs laser pulses

We have demonstrated that intense 100-fs laser pulses can directly imprint a homogeneous nanograting on solid surfaces in air by controlling the excitation of surface plasmon polaritons (SPPs).

A simple two-step process of fs laser ablation was designed to fabricate a nanograting with a period less than 200 nm. In the first step, the fs laser output was split into two beams and focused onto the target, as in Fig. 3(a), so that the two beams ablate the surface to create an interference fringe pattern with the period Λ . The scanning probe microscope image (SPM) of ablated surface with $\Lambda = 937$ nm is shown in Fig. 3(b). In the second step, the fringe period Λ was reduced by irradiating superimposed multiple shots of low-fluence fs laser pulses from beam 1. Figure 3(c) shows the nanograting formed on GaN.

Figure 4 shows the SEM image and its period distribution in the surface structure after irradiation with superimposed multiple shots of fs laser pulses $N = 10$ and 40 from beam 1. We note that the nanograting period d formed is equal to $\sim \Lambda/5$, and the downsizing process develops at $d \sim \Lambda/q$ with the integer q . The nanograting period d was observed to discretely change with a higher fluence.

The cross-sectional surface shape of the nanograting was observed with a scanning transmission electron microscope. We found that the bottom of valleys was deeply ablated at a uniform period on a smooth horizontal level, whereas the height of protrusions was $h = 530 - 730$ nm. The result demonstrates that intense near-fields having a uniform peak of fluence were generated with the excitation of SPPs to periodically ablate the valley bottom.

These results obtained represent exactly the nature when a spatial standing SPP wave mode is formed in the period Λ . To see the origin of the nanograting period d in the second step, we calculated the SPP wavelength λ_{spp} , based on a model surface structure

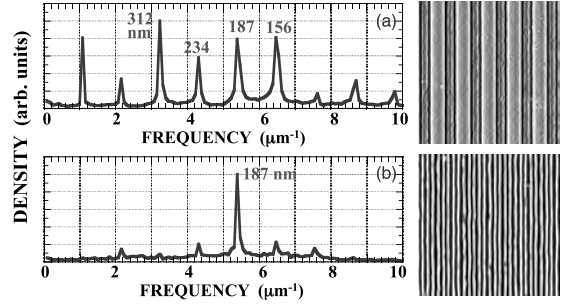


Fig. 4. SEM image and the period distribution in structure on the GaN surface after irradiation with superimposed fs laser pulses $N = 10$ (a) and $N = 40$ (b) from beam 1. The laser polarization direction is horizontal.

consisting of the excited thin layer on the GaN substrate. The results have shown that the nanograting period $\lambda_{\text{spp}}/2$ should be 150 - 300 nm, being in good agreement with the observations. This period restricts the SPP wave mode.

5. Theoretical study of ultrafast laser-matter interactions

We have studied how the electromagnetic waves pass through the interface between two lossy media, and found that the physical interpretation of the meaning of negative refraction have to be reinterpreted. In addition we have proposed an efficient scheme to produce ps VUV pulses utilizing high atomic coherence. Collaborating with the FEL group, we have experimentally demonstrated the single-shot measurement of mid-infrared FEL spectra using an up-conversion technique, and also developed a new technique to estimate the wavelength stability.

6. Twisted-tape-induced swirl flow heat transfer in a circular tube

The thickness of conductive sub-layer δ_{CSL} and the non-dimensional thickness of conductive sub-layer y^+_{CSL} for the turbulent heat transfer on the circular tube with the twisted-tape insert are clarified, based on the numerical solutions. The correlations of δ_{CSL} and y^+_{CSL} for twisted-tape-induced swirl flow heat transfer in a vertical circular tube are derived.

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Univ. of Brawijaya (インドネシア), 超短パルス高強度レーザーによる分子配向と高次高調波発生, 宮崎健創

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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Advanced Energy Structural Materials Research Section

A. Kimura, Professor
 K. Morishita, Associate Professor
 H. Kurishita, Part-time Lecturer
 (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. Development of advanced ferritic steels for fusion systems

The objective of this research is to evaluate the susceptibility to stress corrosion cracking (SCC) of nano-scaled ODS ferritic steels in supercritical pressurized water (500°C, 25MPa) by means of steady strain rate tests at strain rates between 1×10^{-4} /sec to 1×10^{-6} /sec. Fractured surface and specimen side surface were observed by FE-SEM and the chemical compositions of the surface oxide layers were analyzed by FE-EPMA.

The SCC susceptibility of different steels was evaluated by the fracture mode determination, which indicated that SUS316L showed more significant TGSCC than ODS steel. The specimen side surface of the ODS steel is shown in Fig.1 with the results of chemical analysis of ODS steel, SUS316L and F82H.

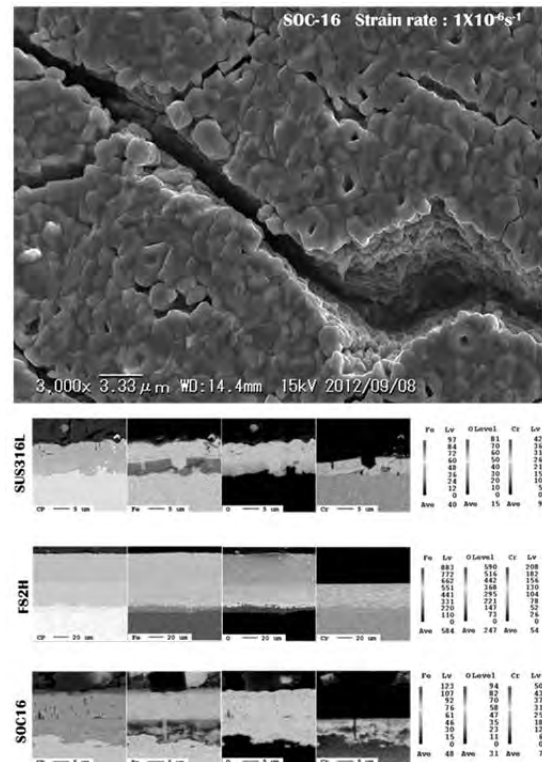


Fig. 1 Oxide products on the specimen side of steel (Fe-15Cr- 4Al-2W-0.1Ti-0.35Y₂O₃) and chemical analysis results of SUS316L, F82H and ODS steel

FSW was performed for an ODS steel with high Cr concentration at a rotating speed of 800 rpm with a line-scanning speed of 50 mm/min. The FSW treatment resulted in a growth of the grains, and consequently, a remarkable reduction of the strength at RT. However, the reduction of strength at elevated temperatures was so small that the FSW is adequate for the application of ODS steels to practical blanket fabrication.

SSDB was carried out at 1200°C at 25MPa for 1 hr with and without insert material. Since the melting temperature of the insert material was lower than 1200°C, the insert material is melted and the method is often called as transient liquid phase bonding (TLPB). Tensile strength of both the SSDB and TLPB was not degraded by the bonding treatment. The elongation of TLPB was reduced to about a half of the material. However, the elongation of SSDB was not reduced at all, indicating the SSDB joining method is very suitable for ODS steels.

3. Theoretical evaluation of oxidation rate of Zr

In nuclear light water reactors, zirconium (Zr) alloys are used as fuel cladding material due to their small thermal neutron cross-section and good corrosion resistance. One of the main issues to be solved for improvement of fuel cladding material is Zr-water oxidation reaction, which may cause embrittlement of Zr alloy, a reduction in thermal conductivity, and so on. Also, at the accident at the Fukushima Daiichi nuclear power plant, hydrogen explosion occurred where hydrogen gas was produced by the Zr-water oxidation reaction. Thus, the oxidation of fuel cladding is significant and should be suppressed as low as possible, not only during normal operation but also in an accident. However, the precise mechanism of oxidation process is not yet understood well.

The oxidation process is caused by atomistic scale oxygen diffusion process in a Zr oxide film. The diffusion process is considered to be a key to the oxidation rate, where the film may act as a barrier against the diffusion. It has been reported by experiments that the early stage of oxidation proceeds in proportion to the cubic root of time, which cannot be explained by the so-called diffusion-controlled process. It may indicate that there may be some factors that reduce the diffusion rate of oxygen in the film. In this study, we investigated diffusion process as a function of the applied stress, which is caused at the oxide/metal interface due to the difference of equilibrium volumes between the oxide and the metal.

Since an oxygen atom is supposed to diffuse in Zr oxide film by the vacancy mechanism, the formation and migration energies were calculated by first principle calculations using the SIESTA code as a function of applied stress. It was found from our calculations that both the vacancy formation and migration energies increase in direct proportion to the compressive

stress as shown in Fig. 1. The calculated increase is as small as 0.05eV even at a maximum compressive stress of 1 GPa, but such a small difference in energy will cause a large difference in diffusion coefficients by several factors.

With the energies thus obtained the oxidation rate of Zr was evaluated by solving diffusion equations. When the stress effect is considered, the oxidation rate decreases with increasing oxide thickness, and finally, oxide thickness increases in approximately proportion to the *cubic* root of time. It is consistent with experiments. We concluded that the stress effect is a key to explain the experimental observations.

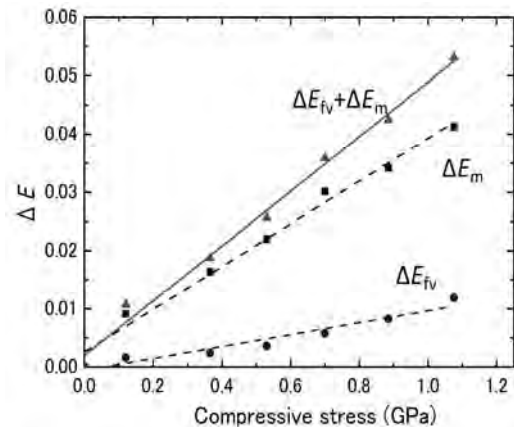


Fig. 2 Variation in calculated defect energies due to compressive stress

4. W-ODS steel joints for fusion divertor

In this study, we show a relaxation technique of thermal expansion coefficient mismatch by application of vanadium (V) alloys as an intermediate insert to bonding of tungsten (W) and oxide dispersion strengthened steel (ODSS). In view of the diffusion bonding (DB) interface between a V alloy and ODSS, precipitation of a sigma phase in the Fe-V system is a critical issue. The DB part of ODSS/V alloy hence needs to be investigated. DB was carried out at 1250C, which is high enough to avert sigma phase formation. However, the anticipated temperature in the reactor blanket is 700~800C, and embrittlement caused by sigma phase formation will be a serious concern for a long time operation. Therefore, we introduced a barrier layer between the V alloy and ODSS and examined the applicability of a barrier layer for fusion reactor components by three-point bending tests for the joint with and without a diffusion barrier layer. It was shown that the joint strength without a barrier layer decreased by 25% after aging at 700C for 100 hr, but that with a barrier layer showed no decrease after the aging treatment. The result indicates that the introduction of a barrier layer leads to the prevention of the sigma phase during aging.

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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 inherent safety features, waste which will not be a burden for future generations, no greenhouse gases and 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 (MHD). 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 confinement in Heliotron J. A topic of Heliotron J experiments in FY2012 is described as follows:

Novel approaches of high-density ($n_e > 10^{20} \text{ m}^{-3}$) plasma operation of Heliotron J have been advanced, in which the plasma start-up for neutral beam injection (NBI) heating was performed with a short pulse ($t < 50 \text{ ms}$) of 2nd-harmonic 70 GHz ECH ($P < 250 \text{ kW}$) or of 2.45 GHz non-resonant microwaves ($P < 5 \text{ kW}$) at magnetic field strength $B=1.3 \text{ T}$ in the unexplored magnetic configuration where the lower toroidicity (ϵ_r) of the magnetic Fourier components in the Boozer coordinates features prominently as compared with that of the standard configuration. This configuration has an elongation higher than that of the standard configuration so that the beneficial effects of recycling on particle confinement might be manifested through the plasma-wall interaction. Another key to this high-density operation was the novel

gas-puff fuelling scenario using high-intensity gas-puff fuelling (HIGP) technique or supersonic molecular beam injection (SMBI) technique. Especially, HIGP, a strong gas-puff fuelling whose intensity was several times larger than that of the standard continuous fuelling with a short-pulse (10-20 ms), was eminently successful in this configuration to produce for the first time high-density NBI-only plasmas ($n_e > 10^{20} \text{ m}^{-3}$) at simultaneous core electron and ion temperatures of 200-300 eV. Two types of high-density operation depending on the different plasma start-up schemes were found to show appreciably different density profiles during the ramp-up phase of plasma stored energy: a very peaking profile in the case of 70 GHz ECH start-up and a very fat profile in the case of 2.45 GHz non-resonant microwaves start-up. Understanding of the effects of different plasma start-up schemes remains as a future work, but these observations are found to contribute to the studies of fusion performance designs of a helical-axis heliotron line where the physics of configuration optimization should be combined with the physics of gas-puff fuelling in the initial target plasmas to tailor the density profile to achieve an efficient neutral beam absorption for the required confinement evolution. Upcoming experiments are planned to continue developing this high-density performance as a candidate operation for advanced confinement modes of Heliotron J.

2. Energetic-ion-driven MHD instabilities in a low shear helical plasmas

Energetic alpha particles in a fusion reactor such as ITER would resonantly couple with MHD modes related to the Alfvén and/or sound wave in the slowing down process of alpha particles, and excite these MHD modes. The MHD modes could enhance the transport and/or induce the loss of alpha particles before their thermalization. This leads to reduction of net gain of fusion burn and significant damage of first wall of a reactor. The existence and stability of energetic-ion-driven MHD instabilities such as Alfvén eigenmodes (AEs) are characterized by the magnetic configuration. Our purpose is to clarify the energetic-ion-driven MHD instabilities in advanced helical plasmas configuration having low

magnetic shear and low toroidal field period, we have experimentally and numerically investigated the energetic-ion-driven MHD instabilities in both helical-axis heliotron Heliotron J and flexible heliac TJ-II plasmas. Both have three-dimensional magnetic configuration, low magnetic shear and low field period $N_p = 4$. In addition, both share similar parameters such as plasma major and minor radii, and energy and power of tangential NBI. The rotational transform (iota), which is the main difference between both devices and a key parameter to characterize the shear Alfvén spectra, can be varied in the range $0.45 \sim 0.65$ and $0.9 \sim 2.0$ in the Heliotron J and TJ-II, respectively. The studies utilizing the similarities and differences among two devices with low magnetic shear or high magnetic shear and high N_p device are an effective method to clarify the energetic-ion-driven MHD instabilities in helical plasmas. We will show that effect of iota on shear Alfvén spectra through the experimental and simulation results of Heliotron J and TJ-II.

Figures 1 (a) and (b) respectively show the global AE (GAE) frequency as a function of iota at plasma core in Heliotron J, obtained from numerical simulations and experiments, respectively. We have selected the condition of electron density as $\langle n_e \rangle \sim 1.5 \times 10^{19} \text{ m}^{-3}$ where the GAEs have been seen clearly in almost all magnetic configurations. Experimental results show two trends that the GAE frequencies respectively decrease and increase with an increase of iota as shown in Fig. 1 (b). This is the same tendency found in the numerical simulations in Fig. 1 (a). In numerical simulations, we found a few GAEs consisting of single and same Fourier components. Helicity-induced AEs (HAEs) should exist in high frequency region above 500 kHz in our experimental condition of Heliotron J. We concluded that GAE is the main AE in low iota case.

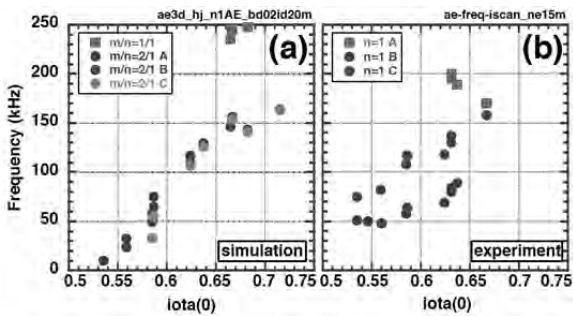


Fig. 1. Dependence of AE frequency on iota obtained from (a) simulation and (b) experiment in Heliotron J with low iota.

Figures 2 (a) and (b) show the dependence of AE on iota obtained from experiment and numerical simulation in TJ-II. We plotted all observed mode frequencies without the classification of mode number in Fig. 2 (a) because we cannot correctly identify mode numbers in our study. We found many AEs in-

cluding TAE, GAE and HAE in the frequency gap without the intersection of shear Alfvén spectra, as shown in Fig. 2 (b). It is clearly seen that GAE frequency corresponding to close ($N_f = 1$) and open ($N_f = 2$) circle symbols in Fig. 2 (b) has dependence on iota. However, the dependence of HAE frequency (square symbol) on iota is not clear because the HAE gap structure is gradually changed when we change the magnetic configuration. We concluded that observed modes are both GAEs and HAEs in high iota configuration although we could not explain all experimental results by using numerical simulations.

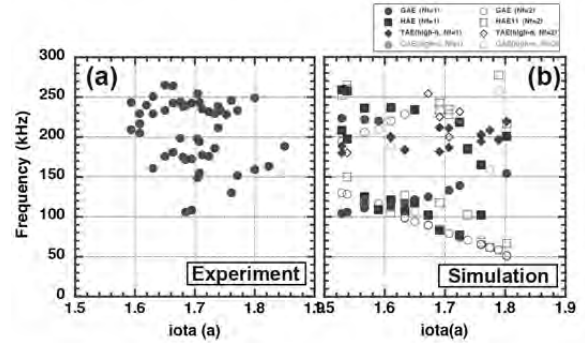


Fig.2. Dependence of AE frequency on iota obtained from (a) experiment and (b) numerical simulation in TJ-II with high iota.

3. Development of lost ion probe for Heliotron J

In order to clarify the mechanism of loss of the energetic ions caused by MHD instabilities discussed in section 2, we have designed lost ion probe (LIP) that can directly measure the lost ions just outside of last close flux surface (LCFS). We have chosen the Faraday cup type detector, which can absolutely measure the ion flux corresponding to lost ion flux. LIP consists of double apertures and detector region. Double apertures restrict the incoming of energetic ions. Detector consists of some thin metal foils where the lost ion flux will convert to current signal. LIP can give us the information of pitch angle and energy of lost ions. Figure 3 shows the detector map consisted of pitch angle and energy for Heliotron J. LIP can detect the lost ions having the energy of 7~40 keV and pitch angle of $100 \sim 160$ deg. in our design corresponding to co.-going energetic ions which can destabilize MHD instabilities.

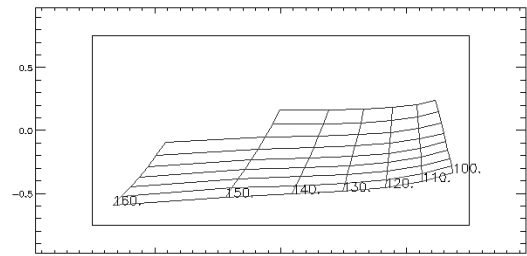


Fig. 3. Detector design of LIP for Heliotron J.

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, 花谷清

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Clean Energy Conversion Research Section

Shinzaburo Matsuda, Visiting Professor
(Tokyo Institute of Technology)

1. Introduction

The most important role of the fusion DEMO reactor is the demonstration of electricity in a plant level. It requires advanced plasma performance and technologies, and therefore realistic DEMO concepts could be found in a narrow design window. The critical issues for the components have been discussed in each special field, but on the basis of some performance expectations or assumptions. Therefore, sometimes efforts are concentrated in a maze of very little solution. It is a role of the overall system study to guide the basic structure of these research works. Present study intends to review issues and to balance the design from a view point of a fusion power plant system.

Amongst several important issues, the present paper deals with the removal of heat from the in-vessel components as most critical.

2. Steady state heat load

Even with a large size of a reactor comparable to ITER, due to a narrow heat deposition profile, the power handling capability in the divertor plate is limited to a level of 50MW. However, in DEMO at about 3GW burning operation with $Q \sim 30$, a heat generated by the produced α particles (600MW) and the injected heating power $P_{heat}(= P_{fusion}/Q)$ (~ 100 MW) will generates about 700MW continuous heat inside the main plasma boundary. Therefore, a difference between the generated heat and the power absorbed by the divertor has to be dissipated by the main plasma radiation etc. (~ 100 MW) and mostly by the SOL

(scrape off layer) plasma radiation (500-600MW) in the divertor region[1]. Namely, a total of

$$\left(\frac{1}{5} + \frac{1}{Q}\right) \times P_{fusion} - P_{target} \sim 650\text{MW}$$

has to be absorbed in the wall of the machine.

Assuming such radiation be realized, then it is necessary to follow where these radiated power will be ultimately absorbed and the design should incorporate such a power.

As an example of the Slim CS design, the total surface area of the first wall and the divertor room are 670m^2 and 210m^2 , respectively. The radiated power will be absorbed by these surfaces, with an average power density of $\sim 0.7\text{MW}/\text{m}^2$. If we incorporate non-uniformity of a factor 3, a power level of $\sim 2\text{MW}/\text{m}^2$ has to be absorbed by the first wall in addition to the neutron wall loading.

Instead, if all the wall of the divertor room is covered by the same divertor plates (heat removal capability of $\sim 10\text{MW}/\text{m}^2$) and the configuration of the divertor room is made in a way that radiated power may not enter into the plasma main chamber, the estimated average power density is about $3\text{MW}/\text{m}^2$. With an assumption of a factor 3 non-uniformity, the peak power density in about $9\text{MW}/\text{m}^2$ in addition to the normal heat flux.

Thus in any case of the design concepts, finding of distributions of heat within technically achievable flux density is a critical job. More detailed design simulation analysis and experimental verification are necessary. If not, the DEMO performance target of 3GW with a size of ITER should be relaxed.

3. Transient heat load

In the case of the transient heat load, evolution of the surface temperature and the heat conduction into the depth of the materials are important. In a thin plate analytical model, the critical heat flux exceeding the temperature rise ΔT due to a constant pulsed heat load is calculated to be:

$$q_0 \Delta t = \rho c \delta_0 \Delta T$$

,where the notations are, q_0 : 1D heat flux, Δt : pulsed heat load time, ρ : mass density, c : specific heat, δ_0 : thickness of the plate, and ΔT : the temperature rise, respectively.

In an actual geometry for the plasma disruption or ELM heat load, the heat can be conducted into the material during the pulse, and the analytical model gives a solution of:

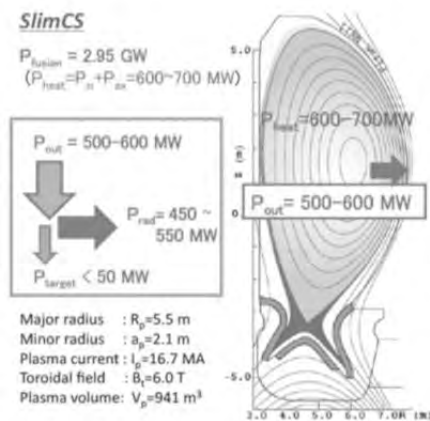


Fig.1 Power flow of a DEMO power plant

$$q_0\sqrt{\Delta t} \geq \frac{\Delta T}{2} \sqrt{\pi c \rho \lambda}$$

It is also clarified that the most of the energy is accumulated in a depth of $\delta \sim \sqrt{\alpha \Delta t}$ from the surface of the plate. For example, in the case of tungsten, most of the heat stays within a depth of 0.12mm for a pulse duration of 0.4ms.

4. ELM heat load

In addition to the steady state heat load, high energy confinement modes in toroidal plasmas are characterized by the repetitious transient heat load named ELM(edge localized mode). The peak heat flux in present Tokamaks extends as high as several tens of MW/m², so that study has to be made from a view point of melting or erosion of the divertor plate surface.

T. Eich et al. [2] analyzed the energy decay length λ_g of the SOL plasma in the median plane of the machine by the regression analysis of the ASDEX U, and JET attached plasmas and deduced a scaling with an very steep estimate of ~ 1 mm in the case of ITER. However, the heat deposition profiles have been studied extensively including many other machines and M.A. Makowski et al. [3] have revealed that the deposition profiles at the divertor plates are not determined by λ_g with a simple multiplication by the expansion of the poloidal flux to the divertor plate but mainly by the diffusion and convection of the SOL plasma between the X-point and the divertor plate. They proposed an integral scaling of the profile characterized by $\lambda_{int} \cong \lambda_q + 1.64w_{pvt}$, where w_{pvt} spreads in a range of 0.5~2.0. Taking the value of ASDEXU, 1.5, where the cross section of the plasma is similar to that of ITER, $\lambda_{int} \sim 3.5$ is obtained. This value, if multiplied by the flux expansion factor (~ 6 in ITER and ~ 3 in SlimCS), will give expanded profiles at the divertor surface. In the case of de-touched or semi-de-touched plasma, the heat distribution becomes a more broader one.

In the case of ELM heat load, the author proposes a ratio of heat deposition during one peak pulse to the total heat deposition during one ELM cycle as a measure of significance. Not all the ELM peak load causes surface melting even the peak load is significant. For instance, the peak load in Fig.2(a) of the Ref. [2] showed a peak heat load as high as 80MW/m², but the duration was 0.4msec and a constant power of ~ 10 MW/m² is absorbed in the rest of the time for 40msec. Since an estimated energy deposition by the peak ELM is $q_0\sqrt{\Delta t} = 80MW \times \sqrt{4 \times 10^{-4}} \sim 1.6 MJm^{-2}s^{-1/2}$, the consequent surface temperature rise by one peak pulse is only 110 degrees. Since the divertor plate can cope with a constant load of 10-15MW/m², and the operating surface temperature will be less than ~ 1000 degrees, the effect by the peak ELM pulse is negligible. Since a typical heat conduction time scales as $x \sim \sqrt{\alpha \Delta t}$, the heat deposited by one peak pulse can be

transported to a sufficiently deep position before the next ELM visit. Therefore, there is no accumulation of heat.

On the contrary, as shown in Fig.2(b) of Ref. [4], the transient ELM pulse covers most of the cycle. In such a case, the influence of the ELM pulse becomes significant. Therefore, it is important to know the heat deposited by one ELM and the repetition period accurately.

There are a lot of data on the divertor by the surface temperature measurement, and the heat flux is calculated from this measurement. However, attention should be made on this translation, because the equation includes time dependency as seen before.

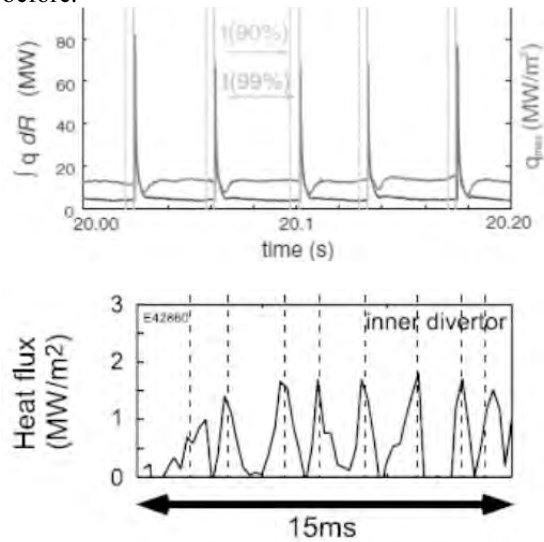


Fig.2 (a) type 1 ELM from Ref. [2] and Grassy ELM from Ref. [4]

5. Summary

Research works by many plasma scientists are focused how to achieve such a high radiative plasma, and some promising computer simulation results [1] have been obtained, yet a level of requirements by extrapolation to DEMO engineering requires more careful investigation and analysis. On the other hand, more attention have to be paid whether the experiments in the component R&D really simulate the heat transfer problem from the plasma to the solid plates.

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Clean Energy Conversion Research Section

Takahisa Ikegami, Visiting Associate Professor
(Institute of Protein Research, Osaka University)

1. Introduction

I am applying nuclear magnetic resonance (NMR) to studying biomolecules including proteins, nucleic acids, glycopeptides, and lipids. NMR is a powerful tool for the analyses of protein structures and dynamics at an atomic resolution. NMR targets solution states of samples, which are closer to natural conditions compared to crystal states. Therefore, NMR allows for the analyses of proteins containing flexible regions, for which crystallization is often difficult. I mainly determine the three-dimensional structures of proteins using NMR as described in the following, as well as study dynamics of proteins and develop methodology of related NMR techniques.

2. Determination of protein structures

It has recently been more and more important to describe biological functions in terms of the three-dimensional structures of associated proteins. At least three methods are currently known to determine structures with the atomic coordinates: X-ray crystallography, electron-microscopy, and NMR. NMR is characteristic in that it can analyze the structures of biomolecules in solution states, providing data that reflect more natural conditions. Although it is considered that the procedures of determining the structures of small proteins (M.W. < 30 k) by NMR have mostly become protocols, a

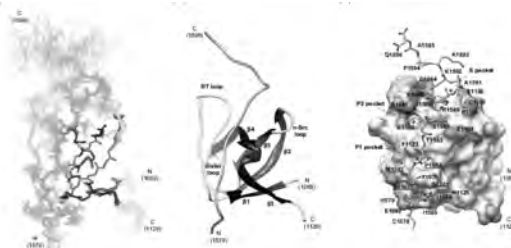


Fig.1: The structure of the complex between the SH3 domain of DDEF1 and a SAMP1 peptide of APC was determined by NMR. The affinity between the two components was significantly strong from the biological point of view, but not enough to provide a large amount of distance information between them. To overcome this problem, I determined the complex structure by fusing the two components by a flexible linker. The connected protein exhibited many NOE peaks, which determined the complex structure precisely and accurately [1].

lot of problems have to be practically solved when flexible and large proteins (M.W. > 40 k) are targeted, such as ones containing multi-domains inside (Fig. 1) [1, 2, 3].

3. Analyses of protein dynamics

NMR is also suitable for detection of flexibility, providing information as to which parts of proteins fluctuate in solutions. The fact that NMR exhibits dynamic structures distinguishes NMR from X-ray crystallography, which normally provides only static structures. A lot of biological functions are related to protein-motions. In particular, slow dynamics occurring in a time range of microsecond to millisecond are very important for biological functions. Since much faster motions alone ranging from picosecond to nanosecond have so far been analyzed by NMR, new parameters representing slower dynamics will elucidate real characters of proteins as well as mechanisms of protein folding/unfolding and protein-protein associations [4]. The above-mentioned dynamics are generally probed by investigating nuclear magnetic relaxation rates of associated nuclei (T_1 , T_2 , and NOE relaxation parameters for amide ^{15}N nuclei in most cases). Much slower motions in a time range of microsecond to hour can be detected by the hydrogen/deuterium (H/D) exchange rates of labile amide protons. I am studying the dynamics of a relatively large protein related to photosynthesis by combining the analyses of its nuclear magnetic relaxation rates and H/D exchange rates, and beginning to demonstrate that the dynamics in and around the substrate binding region regulate the turnover of the substrate, and hence, the activity of the protein in photosynthesis.

4. Analyses of protein-ligand interactions

NMR can detect which part of a protein interacts with the related ligands such as nucleic acids, other proteins, peptides, and in/organic chemicals. The simplest and most frequently used method is the chemical shift perturbation experiments where the interacting nuclei are determined as the corresponding resonances undergoing shifts or broadening by some effects from the ligands. Chemical shift perturbation experiments combined with the titration of ligands allow us to calculate the dissociation constants of the interactions (Fig. 2).

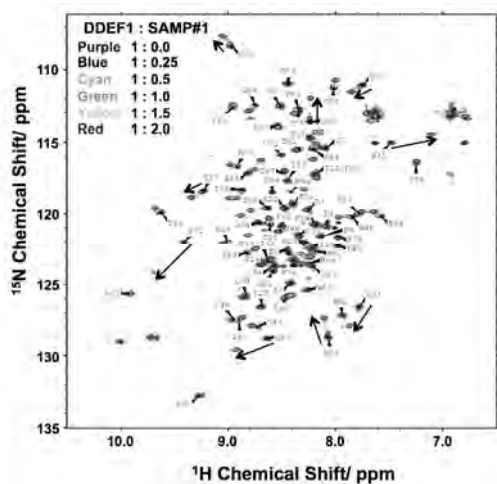


Fig.2: The result of a chemical shift perturbation experiment. A series of 2D ^1H - ^{15}N HSQC spectra of the ^{15}N -labeled SH3 domain of DDEF1 measured upon addition of the increasing concentration of a SAMP-part peptide of APC are overlapped and shown. Although the SAMP peptide contained no particular PxxP motif, it is specifically recognized by this SH3 domain.

I am currently investigating the interactions between proteins and their substrates, a hormone peptide and the associated receptors, a protein and an anticancer drug. I am especially interested in systems where a few large proteins change their interactions along with the elapse of time. The structures of their proteins in the free states are already known through X-ray crystallography, but it is rather difficult to pursue the changing mutual affinities by the method. NMR is the most suitable method by which the affinities can be detected in real-time and in an atomic resolution. Since the structures are available, NMR can be applied to such a large system by using TROSY experiments.

5. Development of NMR methodology

Further developments of NMR methodology to facilitate the above-mentioned studies are also important tasks (Fig. 3) [5]. For example, new methods for determination of much larger proteins with molecular weights of > 40 k and observation of slow dynamics by NMR should be developed more. A lot of protein structures have been solved by NMR and X-ray crystallography, but most of them are the structures of monomers. For understanding the precise mechanisms of the molecular recognition between proteins, three-dimensional structural analyses of the protein-protein complexes are required. For this purpose, a new method of revealing complex structures was developed by means of saturation transfer (SAT) and residual dipolar coupling (RDC) in hetero-nuclear NMR experiments,

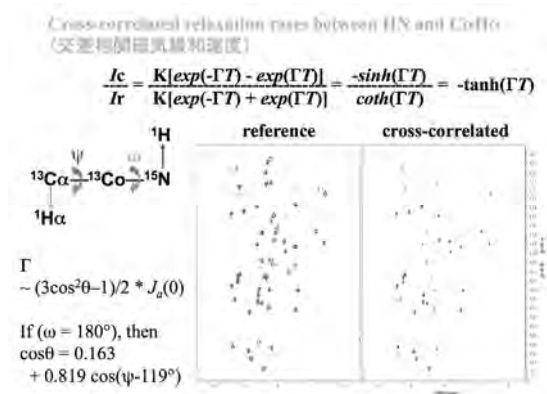


Fig.3: The relative orientation between the amide ^1H - ^{15}N bond of an amide acid and the $^{13}\text{C}\alpha$ - $^1\text{H}\alpha$ bond of the previous residue can be determined from the cross correlated relaxation rate between the dipole-dipole interactions corresponding to these two bonds. This method can be applied to determination of the structure of a ligand peptide that is particularly in an exchange equilibrium between the free form and the bound form with a large membrane receptor because the cross correlated relaxation rate increases as the molecular weight of the complex increases. Cross correlated relaxation rates also provide information on the dynamics of the related parts.

without any paired intermolecular NOE information. The SAT and RDC experiments provide the information on the interfacial residues and the relative orientations of the two protein molecules constituting a complex, respectively. Docking simulation was then performed to reconstruct a complex conformation that satisfies the SAT and RDC data obtained.

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Chemical Reaction Complex Processes Research Section

Y.H. Ogata, Professor
 T. Sakka, Associate Professor
 K. Fukami, Assistant Professor

1. Introduction

In this research section we investigate the formation of surface and interface structures, which play an important role in many photo-energy conversion processes. We utilize electrochemical methods and laser spectroscopic techniques to perform research in this subject.

In this academic year we have investigated formation of porous skeleton silicon, suppression of dendritic growth in zinc electrodeposition, particle monolayer structure at oil-water interface with two different types of particles, and the space-resolved spectroscopy of laser ablation plasma for underwater laser-induced breakdown spectroscopy.

2. Influence of alcohol in HF solutions on anodic porous silicon formation

Anodization of silicon in HF solutions results in formation of porous silicon. Of the porous structures, p-type macroporous silicon has been discussed because there are many open questions in the formation of the macroporous structure. Macropore-like structure filled with a microporous body has been known as “porous-skeleton silicon.” The morphology of porous-skeleton silicon looks very similar to macroporous silicon, except that the macropore-like structure is filled with microporous silicon. We think that understanding of the skeleton formation will lead to a much deeper understanding of macroporous silicon formation. In this year, we have studied the skeleton formation, and compared with the macroporous silicon formation.

Porous-skeleton silicon is formed in HF solutions containing bulky alcohol such as isopropanol or *tert*-butanol. In addition to this requirement, the concentration of HF should be very high like 30 wt.% and current density should be small. The effect of alcohol is common between porous-skeleton silicon and macropore formations. In contrast, macroporous silicon is formed with current densities where HF seems to be depleted in the vicinity of the pore bottom. Thus, the conditions for porous-skeleton silicon and macroporous silicon formations are very different in terms of HF concentration at the pore bottom. This difference suggests that formation of silicon oxide plays a role in macropore formation, but it is not critical for the skeleton formation.

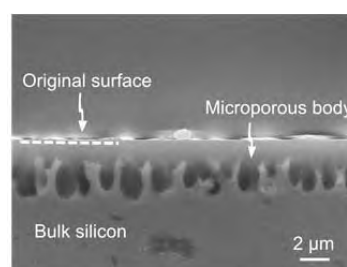


Fig. 2-1 Cross-sectional SEM image of porous-skeleton silicon. The original level of the silicon wafer is clearly observed because the microporous body still remains on the surface.

3. Suppression of dendritic growth in zinc electrodeposition using microporous silicon electrodes

Dendritic growth of metals in electrodeposition has attracted attention in view of nonlinear dynamics and spontaneous pattern formation. From an electrochemical viewpoint, such dendritic growth must be suppressed for further developments of rechargeable batteries. In this year, we have studied how the growth of zinc dendrites is suppressed especially using microporous electrodes.

Current density vs. potential curve in zinc electrodeposition shows the diffusion-limited current. In principle, dendrites grow on the electrode when zinc electrodeposition is carried out at a current density that is higher than the limiting current. However, we have found that the dendritic growth is strongly suppressed when using a microporous silicon electrode. Our results clearly showed that zinc electrodeposition is extremely enhanced within the microporous layer even at a current density higher than the limiting current. As a consequence, dendrite growth is strongly suppressed on the microporous silicon electrode (Fig. 3-1). The molecular-scale picture of the enhancement in zinc deposition within micropores is under investigation by a theoretical analysis. We think that the liquid-state within micropores might be very much different from that in the bulk phase. The concentration of zinc ions should be higher than that in the bulk, otherwise zinc electrodeposition within micropores reaches the diffusion-limited condition and results in the preferential dendritic growth on the top surface of the porous layer.

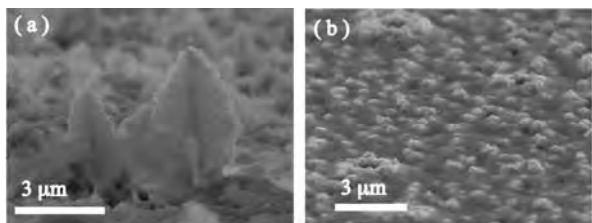


Fig. 3-1 SEM images of electrode surfaces after zinc electrodeposition at a current density higher than the limiting current. The samples (a) and (b) were prepared on a zinc plate and microporous silicon.

4. Particle monolayer structure with two different types of polystyrene spherical particles

Micrometer-sized particles can be trapped to liquid interfaces. Self-assembly of the particles at an oil-water interface can be used as the initial step for various two-dimensional structure formation. If the trapping of the particles to the interface is sufficiently strong, the structure is governed merely by interparticle interactions. It is known that a highly repulsive interparticle interaction results in a hexagonally-ordered structure with the interparticle distance being several times the particle diameter. We have confirmed this situation by using highly hydrophobic polystyrene particles with the diameter of 3.2 μm . In the present work we investigated the structure of binary system, where hydrophilic particles are added to the structure formed by hydrophobic particles.

Fig. 4-1 shows the structure obtained by dispersing the same amount of hydrophilic particles as the hydrophobic particles. The hydrophobic particles keep their interparticle distance while the hydrophilic particles occupy the interstitial sites of the hexagonal structure formed by the hydrophobic particles, and give AB_2 -type structure. Even if the amount of the particles is the same, such AB_2 structure is commonly observed, suggesting that this structure is stable. The results suggest that particles at an oil-water interface have a potential to form various ordered structures, if the interparticle interaction is appropriately controlled.

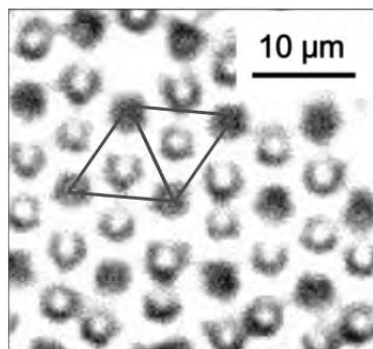


Fig. 4-1 Optical microscope image of polystyrene particles at n-decane/water interface. Two different types of particles, namely hydrophobic and hydrophilic particles, formed an AB_2 -type ordered structure at the interface.

5. Space-resolved emission spectroscopy of the plasma generated by laser ablation in water

Laser ablation plasma produced in water can be used for *in situ* spectrochemical analysis of a solid target submerged in water. This approach is a kind of laser-induced breakdown spectroscopy (LIBS) and can be used in various applications, such as submarine resource exploration. We have found that the irradiation with a 150-ns pulse (long pulse) can give clear atomic emission lines, while a short nanosecond pulse usually used in previous studies results in seriously deformed spectral lines. Underwater LIBS can also be used for the analysis of the solution covering the target. For quantitative analysis of the solution, the spatial distribution of the species from the solution should be clarified. In the present work we developed a method for space-resolved emission spectroscopy of the plasma, of which the size is as small as ~ 0.1 mm.

The experimental setup is shown in Fig. 5-1. The laser plasma generated by irradiating a submerged target with a long pulse, was imaged onto a plane, on which the edges of four optical fibers were aligned two-dimensionally. Microscope objective lens of 50 times magnification was used to obtain the image. The exit edges of the fibers were aligned at the entrance slit of a spectrograph. The spectrograph is specially designed so that the entrance slit is imaged two-dimensionally on the ICCD detector with the wavelength dispersion in the horizontal direction.

The resultant atomic spectral lines of Cu and Na suggest that Na originated from the solution is more abundant at the peripheral region than the central region, while Cu atoms, which are ablated from the target, showed opposite behavior. Such results are expected to give information to understand the mechanism of the plasma formation in liquids.

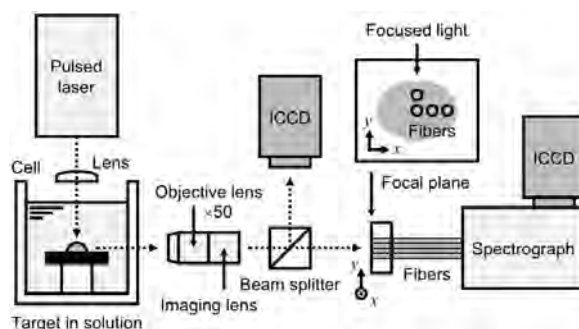


Fig. 5-1 Experimental setup for the space-resolved measurement for the spectra of a small plasma.

Financial Support

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Molecular Nanotechnology Research Section

H. Sakaguchi, Professor

T. Sagawa, Associate 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 'Electro-chemical Epitaxial Polymerization' technique which is a totally new molecular assembling technique of molecular wires on metal surface from single molecules. By the use of this technique, 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 re-search achievements in Molecular Nanotechnology Research section in the year of 2012.

2. Bottom-up massively produced grapheme nanoribbons

Graphene nanoribbon (GNR) is a promising organic electronic material. GNR can work as a semi-conductor 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 aromatic biradical species. Highly reactive organic biradicals readily diminish by trapped with impurities under the reaction conditions. Only under UHV condition, biradicals reacted inter-molecularly and afforded GNR precursor polymers.

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 radical polymerized CVD. Poly(perianthracene) can be obtained under low vacuum condition (ca. 1 Torr) from 10,10'-dibromo-9,9'-bianthryl in an extremely cleaned quartz tube as a reactor. 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,

and decreased concentrically. An atomically flat Au(111) metal surface was placed at the optimized space in a reaction tube, GNR prepolymer propagated efficiently. Further annealing process converted GNR prepolymer to conjugated GNR. The formation of poly(perianthracene) was confirmed by Raman spectrum. The reaction was applicable to the other organic monomers, for example, the narrowest GNR poly(perinaphthalene) was obtained from a mixture of 3,9-, and 3,10-dibromoperylene. 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 FET properties of bottom-up synthesized GNR films.

3. High performance of molecular wires transistor by electrochemical epitaxial polymerization

Key to realize the high performance of organic devices using conjugated polymers is how to fabricate a highly organized structure on surface at a single molecular scale. Here we have demonstrated a unique single-molecular processing-technique using electrochemistry, called 'electrochemical epitaxial polymerization' (ECEP). This technique is based on a step-by-step electropolymerization of monomer along the lattice of iodine-covered Au(111) surface to form the single conjugated-polymer wires by applying voltage-pulses into monomer electrolyte solution.

Epitaxially polymerized conjugated polymers can be successfully deposited layer by layer on I-Au(111) up to 10nm thickness. We demonstrated polymerized wires on I-Au(111) could be transferred to insulator substrates such as surface-oxidized Si, glass and various insulating polymers.

Electric double layer capacitor (EDLC) FET devices using epitaxially polymerized molecular wires showed high hole-mobility of 1 cm²V⁻¹s⁻¹. Other types of FET using different gate dielectrics

were compared with these results.

4. Benzotrithiophene polymer network prepared by electrochemical polymerization with a combination of pyrolysis

Polythiophenes are known to have well established 1D pi-conjugated system. 2D materials are desired to be fabricated on electrode using this electrochemical technique. Thiophene based molecule, which possesses C3 symmetry such as benzo[b]trithiophene (BTT) is a candidate as a precursor to form the well-developed 2D pi-conjugated thiophene network by the polymerization reaction. There is only a report with regard to the electropolymerization of BTT using cyclic voltammogram on Pt disc or ITO electrode, showing in stability of electropolymerized BTT from the results of oxidation potential varied with repeated scan. However, the detail features of these compounds are unknown. Two-step method to produce 2D conjugated polymer network on substrate, electropolymerization of BTT to form oligomers with combination of thermal conversion into 2D polymers is reported. Advantage of electropolymerization is to form BTT oligomers absorbed onto electrode surface. Formed BTT oligomers have a higher sublimation temperature than that of monomer because the monomer sublimates at temperature of 200 degrees with an atmospheric pressure of nitrogen. Therefore, thermal treatment around 500 degrees in order to develop the further conjugation by a cyclodehydrogenation reaction can be applied to BTT oligomers as second step. In conclusion, we proposed the method combined electropolymerization and thermal treatment applied for C3 symmetric BTT molecule to produce the conjugated-polymer network. Thermally treated electropolymerized BTT film at 500 degrees shows 107 times higher conductivity than before. It retains thiophene structure in spite of heating by Ra-man spectra. Absorption of heat treated electropolymerized BTT film suggests extended pi-conjugation. These results indicate the production of 2D network polymer consisted from C3 symmetric BTT.

5. Improvement of efficiencies of organic solar cells: Development of thin-film making process and novel design of device structure

Organic photovoltaics (OPVs) have been developed as new types of solar cell for next generation using conducting polymers and fullerenes as p-type (donor) and n-type (acceptor) materials. The advantages of OPVs are lightweight, large-area, flexibility and low cost roll-to-roll production by using the convenient well-developed solution-based thin film deposition technology. For the sake of highly efficient photocurrent conversion efficiencies of OPVs in terms of reduction of car-

bon dioxide emissions, we intended to (1) reform the surface of nanostructured electrodes, and (2) develop novel coating methods for thin-film making in FY2012.

(1) Effects of morphology of nanostructured ZnO and interface modification on device configuration and charge transport of ZnO/polymer hybrid solar cells: In OPV, the short exciton diffusion length of organic materials requires effective donor-acceptor heterojunction at the nanoscale. Hybrid inorganic/polymer solar cells based on ZnO nanostructures and poly(3-hexylthiophene) (P3HT) are constructed to study the effects of ZnO morphologies and wettability of the surface on the P3HT infiltration ability and charge transport mechanism. The P3HT infiltrates into ZnO nanorod (NR) more remarkably than ZnO nanoparticle (NP) substrates. Although surface modification with indoline D205 dye molecules improves the wettability (viz. enlarges the contact angle) of NP surface, the P3HT infiltration distance decreases in comparison with the pristine NP case. This leads to relatively low short-circuit current density (J_{sc}) of the NP devices in comparison with that of the NR devices, even though the surface area of NP layers are larger than that of NR one. Moreover, surface modification with squaraine dye onto the NR surface shows more significant improvement in J_{sc} than the NP case. This is due to the well-aligned morphology of the NRs, which facilitates dye modification, P3HT infiltration, and charge transport processes. These indicate that the NRs are more qualified as electron accepting substrates and transport pathway in hybrid solar cells than NPs. (2) Fast screening of an optimal ratio of conducting polymer/fullerene mixture for organic solar cells by novel coating method: Bulk heterojunction (BHJ) organic solar cells generate electrical power based on the active layer with a mixture of electron donor (D) and acceptor (A) materials. The D/A ratio is one of the critical parameters for the electrical characteristic in BHJ solar cells. Therefore, it is required to determine an optimal mixture ratio of D/A for maximum efficiency in BHJ solar cell. In this context, the modified spray or mist coating methods, which can control mixture ratio of D/A systematically and continuously, is applied. This new method is investigated whether it is appropriate for screening method, on the aspects of morphological and optical properties of OPVs based on P3HT: [6, 6]-phenyl C61 butyric acid methyl ester (PCBM). Finally, the optimum ratio of P3HT:PCBM is obtained by increasing the ratio of P3HT:PCBM gradually. This study provides a strong and practical screening method to define a critical mixture ratio among the enormous conducting polymer-fullerene combinations.

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Biofunctional Chemistry Research Section

T. Morii, Professor
 E. Nakata, Lecturer
 S. Nakano, Program Specific 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 2012.

2. DNA binding proteins for Site-Specific Protein Positioning on DNA-Origami based molecular switchboard

Structural DNA nanotechnology, which includes DNA origami, enables the rapid production of self-assembled nanostructures. One of the key features of this technology is that fully addressable nanoarchitectures of various shapes and geometries are easily designed and constructed. By taking advantage of their addressable nature, DNA nanostructures have been used as scaffolds for the site-directed assembly of functional entities, such as small molecules and nanoparticles. As well as these functional entities, proteins are a particularly interesting class of molecules to assemble because of their huge functional variability. We developed that different locations within DNA-origami structures are site-specifically and orthogonally targeted by using sequence-specific DNA-binding proteins as an adaptor, and demonstrate that adaptor-fused functional proteins are assembled at specific locations within DNA-origami structures. Last

year, we report the zinc-finger proteins (ZFPs), which is a well-studied class of sequence-specific DNA binding proteins, as the first trial of this aim. ZFPs could be used as a monomeric protein adaptor to target a specific location within molecular switchboard. Development of various types of adaptors with distinct sequence selectivity enables placing various adaptor-fused proteins on DNA origami at specific positions orthogonally, which will lead to construction of functional protein assemblies on molecular switchboard. Thus, we have developed a basic-leucine zipper (bZIP) class of protein GCN4 as a new adaptor to expand the range of target DNA sequences in this year.

Specific binding of GCN4 derivatives on DNA origami nanoarchitectures was successfully demonstrated. Analyses by AFM and gel electrophoresis confirmed specific binding of GCN4 to the address containing the specific binding site on DNA origami. And more, orthogonal targeting by GCN4 and zif268 adaptors at the respective sites on DNA origami was also confirmed by AFM and gel electrophoretic analyses. These results indicate that the adaptors for both monomeric, and homodimeric proteins of interests are now available to locate them at the specific sites on molecular switchboard with complete orthogonality.

Nature uses multiple proteins and/or enzymes in close proximity to efficiently carry out chemical reactions and signal transductions. Such assemblies of multiple proteins may be realized in vitro by using DNA-origami structures that have defined binding sites and various kinds of ZFP adaptor-fused proteins.

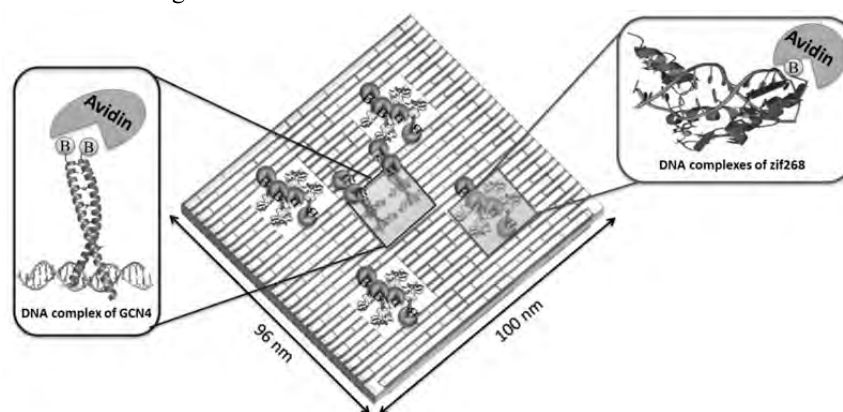


Figure 1. Conjugation of DNA origami and orthogonal adaptors fused functional domain as the molecular switchboard.

3. The sophistication of ribonucleopeptide module for fluorescent sensor

We have reported a strategy that enables isolation of fluorescent ribonucleopeptide (RNP) sensors with a variety of binding and signal-transducing characteristics, such as the ratiometric detection of target molecules and simultaneous detection of two target molecules. The strategy would provide ideal fluorescent RNP sensors for sensing biologically important molecules and events.

3-1. Construction of ratiometric fluorescent sensors

Ratiometric fluorescent sensors were constructed from RNA aptamers by generating modular ribonucleopeptide complexes. Fluorescent ribonucleopeptides containing fluorophores seminaphthorhodafluor tethered to their peptide subunit revealed a dual emission property, which permitted a ratiometric fluorescent measurement of a substrate-binding event. The strategy successfully afforded ratiometric fluorescent sensors for biologically active small ligands, tetracycline, dopamine and streptomycin.

3-2. Simultaneous Detection of ATP and GTP by Covalently Linked Fluorescent Ribonucleopeptide Sensors

A noncovalent RNA complex embedding an aptamer function and a fluorophore-labeled peptide affords a fluorescent ribonucleopeptide (RNP) framework for constructing fluorescent sensors. By taking an advantage of the noncovalent properties of the RNP complex, the ligand-binding and fluorescence characteristics of the fluorescent RNP can be independently tuned by taking advantage of the nature of the RNA and peptide subunits, respectively. Fluorescent sensors tailored for given

measurement conditions, such as a detection wavelength and a detection concentration range for a ligand of interest, can be easily identified by screening of fluorescent RNP libraries. The noncovalent configuration of a RNP becomes a disadvantage when the sensor is to be utilized at very low concentrations or when multiple sensors are applied to the same solution. We report a strategy to convert a fluorescent RNP sensor in the noncovalent configuration into a covalently linked stable fluorescent RNP sensor. This covalently linked fluorescent RNP sensor enabled ligand detection at a low sensor concentration, even in cell extracts. Furthermore, application of both ATP and GTP sensors enabled simultaneous detection of ATP and GTP by monitoring each wavelength corresponding to the respective sensor. Importantly, when a fluorescein-modified ATP sensor and a pyrene-modified GTP sensor were co-incubated in the same solution, the ATP sensor responded at 535 nm only to changes in the concentration of ATP, whereas the GTP sensor detected GTP at 390 nm without any effect on the ATP sensor. Finally, simultaneous monitoring by these sensors enabled real-time measurement of adenosine deaminase enzyme reactions.

These researches were partly supported by a Grant-in-aid for Scientific Research from Ministry of Education, Science, Sports and Culture, Japan (No. 23651215, 24121717 to T. M. and 24651150, 24107513 to E. N.) and by CREST, JST to T.M.

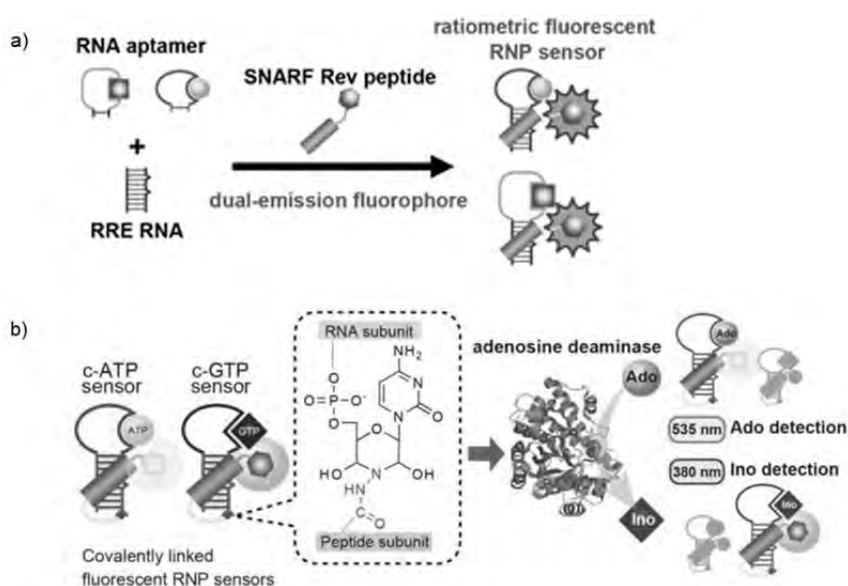


Figure 2 The sophistication of RNP module for fluorescent sensor

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Structural Energy Bioscience Research Section

M. Katahira, Professor
 T. Kodaki, Associate Professor
 T. Nagata, 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 useful to develop the way to extract energy and valuable materials that can be used as starting materials of various products from the wood biomass. Thus, we pursue to contribute to the paradigm shift from oil refinery to biorefinery.

Followings are main research achievements in the year of 2012.

2. Development of the methods to analyze wood biomass by solution NMR

We have developed new methods to quantitatively determine the amount of each component of wood biomass by solution NMR. Although HSQC spectrum has been conventionally used to estimate the amount of each component, precise quantification has not been possible due to the variation of a one-bond C-H coupling constant and a transverse relaxation constant among each component. Our new method eliminates effects of the variation and gives precise quantification that is critical information to utilize wood biomass.

We have also succeeded to establish a system in which biodegradation of wood biomass by rotting-fungi can be monitored in an NMR tube in real-time. Appearance of key metabolites for biodegradation in the course of rotting has been detected by this real-time detection system.

Atom-specific ^{13}C -labeling of lignin has also been successfully carried out in collaboration with Prof. Fukushima's group of Nagoya University (**Figure 1**). This labeling has given decisive information on the amount of various kinds of inter-unit linkages of native lignin in wood biomass.

Valuable substances that may be utilized to pro-

duce cosmetics or bioplastic have been identified in degraded wood biomass through NMR and mass analyses in collaboration with Prof. Watanabe's group of Kyoto University. Newly developed methods have been proven to be quite useful to identify and quantify such valuable substances originated from wood biomass by solution NMR.



Figure 1 Atom-specific ^{13}C -labeling of native lignin. Ginkgo shoot is supplied with atom-specifically ^{13}C -labeled lignin precursor solution (by courtesy of Professor Fukushima).

3. Molecular basis of how RNA aptamer traps prion protein and exerts its anti-disease activity

We developed an RNA aptamer that targets prion protein (PrP), which is causally related to prion diseases, and determined the mechanism of how RNA aptamer binds to and traps a full-length PrP. Our RNA aptamer forms a homodimer and each monomer simultaneously binds to the two sites of the PrP (P1 and P16). We measured the dissociation constants for bindings between RNA aptamer and either P1, P16, or the full-length PrP, and obtained the values of $\sim 10 \mu\text{M}$, $\sim 10 \mu\text{M}$, and $\sim 10 \text{nM}$, respectively. By considering the relationship between the dissociation constant of simultaneous binding, K_d , and the Gibbs free energies at the individual binding sites (**Figure 2(a)**), theoretical K_d would be 0.1nM ($= [10 \mu\text{M}]^2$) at a maximum. Since the experimental and theoretical K_d s

have similar values, it is clear that the strong binding is attributed to the simultaneous dual binding.

We then demonstrated that our RNA aptamer actually exhibits anti-prion activity by using the mouse neuronal cells that are persistently infected with the transmissible spongiform encephalopathy agent. Our molecular and cell based analyses showed that our RNA aptamer binds to PrP with a normal cellular form (PrP^C) and inhibits its conversion into an abnormal form (PrP^{Sc}) (Figure 2(b)).

Because PrP reportedly binds to amyloid- β oligomer (A β oligomer), which is thought to result in another brain disease (Alzheimer's disease), we have asked if our RNA aptamer can inhibit PrP:A β oligomer binding and prevent the disease. We have successfully produced the proteins and now the binding assay is underway.

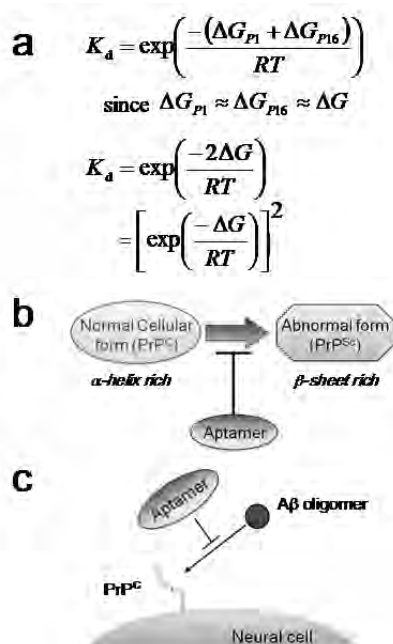


Figure 2 Our aptamer binds to two sites of the PrP^C (P1 and P16), simultaneously, to achieve strong binding (a). Roles of the aptamer are inhibition of the PrP^C to PrP^{Sc} conversion (b); and prevention of PrP^C and amyloid- β oligomer binding (c).

4. Development of intelligent enzymes that switch their activity in response to K⁺

r(GGAGGAGGAGGA) (R12) converts its single-stranded elongated form into a compact quadruplex structure in response to K⁺. In a hammerhead ribozyme, two portions of the catalytic core are linked with the stem and are located closely to exert the activity. We replaced this stem by R12 (or R11 that lacks the terminal A residue) flanked with some linker residues. In this way, we previously obtained a ribozyme that exhibits enhanced activity in response to K⁺, and so is named "quadruplex ribozyme" (Figure 3). It was suggested that the quadruplex

formation restored the active catalytic core. We have designed and constructed molecules that reduce the background nonspecific activity of the quadruplex ribozyme. As a result, our ribozyme showed activity enhancement as high as 36-fold (Figure 3). This switching capability may have therapeutic applications because the intra- and extracellular K⁺ concentrations are very different.

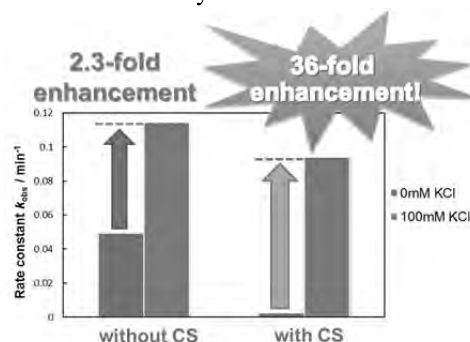


Figure 3 Sharp switching capability has been added to our intelligent K⁺-responsive ribozyme.

5. NMR study of xenotropic murine leukemia virus-related virus protease in complex with a drug

Xenotropic murine leukemia virus-related virus (XMRV) has been implicated in prostate cancer and chronic fatigue syndrome. The homodimeric protease (PR) of XMRV plays a critical role in the production of functional viral proteins and is a prerequisite for viral replication. We synthesized XMRV PR using the wheat germ cell-free expression system and carried out NMR structural analysis of XMRV PR in a complex with an inhibitor, amprevir (APV). We found that the structural heterogeneity is induced by the asymmetry of the binding of APV to the XMRV PR dimer and, more importantly, that this structural heterogeneity is transmitted to distant regions. Long-range transmission of the structural change identified for the XMRV PR complex might be utilized for the discovery of a new type of drug.

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

In this fiscal year, the more efficient xylose fermentation was achieved by overexpressing the four genes encoding the enzymes involved in the pentose phosphate pathway. These results show that the metabolic engineering is a useful strategy for development of efficient bioethanol production system.

These researches were supported by grants to M. K. from MEXT (23657072 and 24121714), JST-SENTAN, JST-CREST, and the Sumitomo Denko Foundation, those to T. K. from NEDO and MEXT (23603003), and those to T. N. from MEXT (23570146 and 24113710).

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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 investigations on the hydrophobic and hydrophilic hydrations, anomalous behavior of confined liquids, folding/unfolding mechanisms of proteins, receptor-ligand binding, prediction of the native structure of a protein, and mechanism of the 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) Structural stability of proteins in aqueous and nonpolar environments [1]

A protein folds into its native structure with the α -helix and/or β -sheet in aqueous solution under the physiological condition. The relative content of these secondary structures largely varies from protein to

protein. However, such structural variability is not exhibited in nonaqueous environment. For example, there is a strong trend that alcohol induces a protein to form α -helices, and many of the membrane proteins within the lipid bilayer consists of α -helices. Here we investigate the structural stability of proteins in aqueous and nonpolar environments using our recently developed free-energy function $F=(A-TS)/(k_B T_0)=A/(k_B T_0)-S/k_B$ ($T_0=298$ K and the absolute temperature T is set at T_0) which is based on statistical thermodynamics. $A/(k_B T_0)$ and S/k_B are the energetic and entropic components, respectively, and k_B is Boltzmann's constant. A smaller value of the positive quantity, $-S$, represents higher efficiency of the backbone and side-chain packing promoted by the entropic effect arising from the translational displacement of solvent molecules or the CH_2 , CH_3 , and CH groups which constitute nonpolar chains of lipid molecules. As for A , in aqueous solution, a transition to a more compact structure of a protein accompanies the break of protein-solvent hydrogen bonds: As the number of donors and acceptors buried without protein intramolecular hydrogen bonding increases, A becomes higher. In nonpolar solvent, lower A simply implies more intramolecular hydrogen bonds formed. We find the following. The α -helix and β -sheet are advantageous with respect to $-S$ as well as A and to be formed as much as possible. In aqueous solution, the solvent-entropy effect on the structural stability is so strong that the close packing of side chains is dominantly important, and the α -helix and β -sheet contents are judiciously adjusted to accomplish it. In nonpolar solvent, the solvent-entropy effect is substantially weaker than in aqueous solution. A is crucial and the α -helix is more stable than the β -sheet in terms of A , which develops a tendency that α -helices are exclusively chosen. For a membrane protein, α -helices are stabilized as fundamental structural units for the same reason, but their arrangement is performed through the entropic effect mentioned above.

(A-2) Characterization of native-structure models of a protein [2]

We show how to characterize the native-structure models of a protein using our free-energy function F which is based on hydration thermodynamics. Ubiquitin is adopted as an example protein. We consider models determined by the X-ray crystallography and two types of NMR model sets. A

model set of type 1 comprises candidate models for a fixed native structure, and that of type 2 forms an ensemble of structures representing the structural variability of the native state. In general, the X-ray models give lower F than the NMR models. There is a trend that as a model deviates more from the model with the lowest F among the X-ray models, its F becomes higher. Model sets of type 1 and those of type 2, respectively, exhibit two different characteristics with respect to the correlation between the deviation and F . It is argued that the total amount of constraints such as NOEs effectively taken into account in constructing the NMR models can be examined by analyzing the behavior of F . We investigate structural characteristics of the models in terms of the energetic and entropic components of F which are relevant to intramolecular hydrogen bonding and to backbone and side-chain packing, respectively.

(A-3) Entropic release of a big sphere from a cylindrical vessel [3]

Insertion and release of a solute into and from a cylindrical vessel comprising biopolymers is a fundamental function in biological systems. In earlier works, we reported that the solvent-entropy (SE) effect plays imperative roles for insertion. Here we show that release is also achievable by the SE effect: The solute can be moved from an entrance at one end of the vessel to an exit at the other end using a continuous variation of the vessel geometry. Since the SE effect is rather insensitive to the solute-solvent affinity, our result may provide a clue to the “multidrug efflux” of TolC.

(B-1) Study of bumpiness and heating position effect on fast ions using ICRF minority heating in Heliotron J

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 are 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). 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. The CX-NPA is positioned near the corner section of Heliotron J plasma. The experimental condition is as follows: the magnetic field strength is 1.25 T, the line-averaged electron density is $0.4 \times 10^{19} \text{ m}^{-3}$ and the ICRF power of 0.25–0.30 MW is injected into a target plasma produced by a 70-GHz ECH. The ion temperatures at the center of the ECH plasma are about 0.2 keV. The minority ratio is about 10%. Frequency of ICRF is 19 MHz or 23.2 MHz.

The wide range observation (about 25% in the poloidal cross section of a plasma) of fast ions by changing vertical angle from -2° to 6° of the CX-NPA is performed by changing the line of sight of the CX-NPA in two directions for three bumpinesses. For the horizontal angle, the variable range is from -0.2° to 12° . The bumpinesses (B_{04}/B_{00} , where B_{04} is the bumpy component and B_{00} is the averaged magnetic field strength) are chosen to be 0.15 (high) and 0.06 (medium) at the normalized radius of 0.67 in this study. For the quantitative comparison of the fast ion tail, the effective temperature of fast minority ions is evaluated from the energy spectrum in the range of 1 keV to 7 keV.

In this campaign, the two dimensional scan of the CX-NPA was performed for three bumpiness configurations in the on-axis heating condition. In this experiment, the asymmetry of the effective temperature of the minority protons against the magnetic axis was found for the high bumpiness configuration only. The effective temperature at 2° of the vertical angle is largest from -2° and 0° for horizontal angle. Such profile was not observed for the other configurations. The bulk deuteron temperature was also measured from the CX-NPA measurement. The profile of the deuteron temperature at the fixed horizontal angle is almost flat for all configurations. Therefore, only the fast proton profile for the high bumpiness was localized for the horizontal and vertical angles.

Monte-Carlo simulation of fast ions (protons) was performed in the energy range up to 20 keV by increasing the number of test particles. The calculated energy spectrum by the Monte-Carlo method is compared with the experimental one. The calculated spectra agree with measured ones in the experiment for three bumpiness cases. The Monte-Carlo simulation reproduces the high-energy tail up to 20 keV, which was measured only in the high bumpiness case. The change of the energy spectrum for the horizontal angle is observed. In the straight section, the number of the fast ions is small. No detectable data was obtained in the charge exchange neutral analyzer (CX-NPA) measurements for energies above 6 and 8 keV for the medium and low bumpinesses, respectively. The measured and calculated energy spectra are also identical for the medium and low bumpinesses.

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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, 花谷清, 岡田浩之, 南貴司, 小林進二, 山本聡

Stuttgart Univ. (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, 長崎百伸, 大島慎介, 佐野史道, 水内亨, 花谷清, 岡田浩之, 南貴司, 小林進二, 山本聡

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径方向電場制御, 佐野史道, 水内亨, 長崎百伸, 岡田浩之, 小林進二, 山本聡

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, 水内亨, 長崎百伸, 岡田浩之, 南貴司, 小林進二, 山本聡

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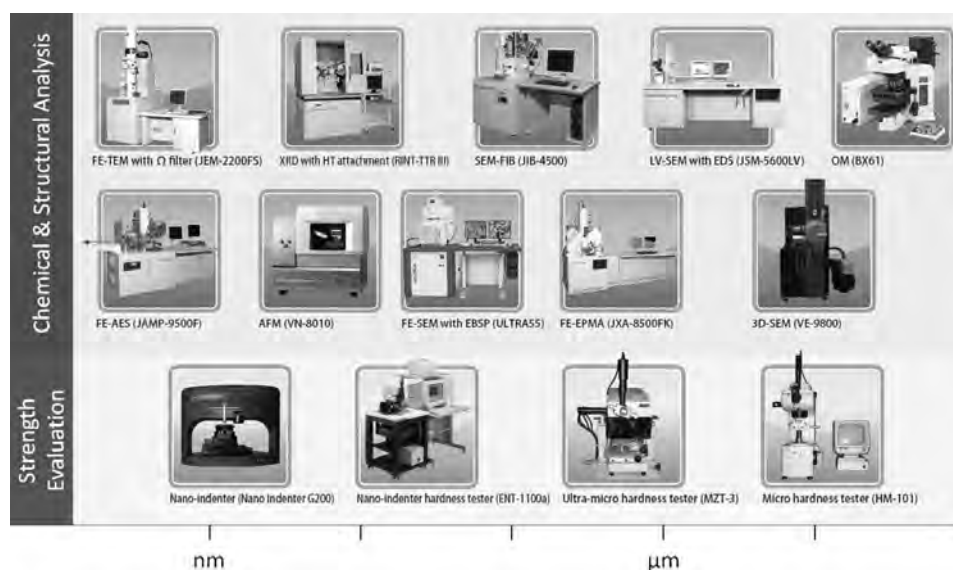


Fig. 2 Summary of the MUSTER equipment (selected).

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. 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 2012) 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 by our faculty staff.

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.

- Transmission Electron Microscope (JEOL JEM-2010): This is a 200 kV conventional TEM with a LaB₆ emitter. Point and line resolutions are 0.25 nm and 0.14 nm, respectively. This microscope is very available for material science researches. The unique holder has been developed for high temperature

in-situ observation up to 1573 K.

- Focused Ion Beam Processing Device (JEOL JIB-4500 & Micron/JEOL JFIB 2100): FIBs are mainly used for the preparation of specimens of TEM. These are able to fabricate and polish samples as well, and is available for metals, ceramics and composites. With using a micro-pick-up system, the users can choose the fabrication area anywhere on a sample.

- 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 current members providing direct support for each subject (MAR 2013).

- Akihiko Kimura, Project Leader, Professor.
- Tatsuya Hinoki, Associate Professor.
- Ryuta Kasada, Assistant Professor.
- Hideki Matsui, Specially Appointed Professor.
- Sosuke Kondo, Program-Specific Assistant Professor.
- Noriyuki Iwata, Program-Specific Assistant Professor. (will be moved to Kurume Natl. Col. Tech. at APR 2013)
- Okinobu Hashitomi, Administrator of DuET.
- Takamasa Ohmura, Administrator of MUSTER.
- Youngju Lee, Program-Specific Researcher. (will be moved to POSCO, Korea at APR 2013)
- Yasunori Hayashi, Program-Specific Researcher.
- Akiko Hasegawa, Technical Support Engineer.
- Aya Kitamura, Technical Support Engineer.
- Reine Sakamoto, Secretary.

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3-3. AWARD

Excellent Presentation Award in Asian-Core University Program on Advanced Energy Science, International Symposium on Advanced Energy System and Materials

**Advanced Atomic Energy Research Section
Sunghun Kim (D3)**

The objective of this symposium is to provide a forum to exchange latest scientific achievements, ideas and opinions on the research of advanced energy technology and the materials used for them. To provide an opportunity for young researchers and students from China, Korea and Japan to communicate with their international colleagues and have instructions from the leading researchers in the area is another major purpose.

In the symposium, I presented about the evaluation of thermal conductivity and development of UD-Cf/SiC composite as structural materials for new concept of low temperature gradient divertor. The surface of divertor is armoured with W because W has good resistance against sputtering and high thermal conductivity. However the substrate of the divertor structure, such as SiC, carries coolant in it has lower thermal conductivity. Thus it causes high thermal stress due to the high temperature gradient by lower thermal conductivity in SiC material. To reduce the high temperature gradient, the authors propose the use of UD-SiC composite with directional thermal conductivity as the divertor component. In this study, unidirectional 30vol%-C_f/SiC composite is studied as a model material to exhibit the directional thermal conductivity. The thermal conductivity of C_f/SiC composite is evaluated by using a laser flash method. All directions have higher thermal conductivity than Mono-SiC materials. These results have demonstrated convincingly that C_f/SiC composite with directional property have an enhancement effect of thermal conductivity. Particularly, thermal conductivity of the 0 degree of C_f/SiC composite was 36 W/m·K which was higher than another angle is expected to reduce temperature gradient than Mono-SiC layer against high heat flux.

Poster presentation group award in 2012 annual meeting of GCOE, for “ACCOMPLISHING JAPAN’S CO2 EMISSION REDUCTION TARGETS IN THE ABSENCE OF NUCLEAR POWER”

**Advanced Atomic Energy Research Section
Yasunori Nakai (D3)**

Given the absence of nuclear power, Japan’s strategy to reduce CO₂ emission needs to be redefined. This study explores the optimum mix of hydro, solar photovoltaic (PV), geothermal and wind power to accomplish the reductions proposed in Japan’s Kyoto Protocol (KP) and Hatoyama’s initiative. It consisted of the following steps: 1) A literature review and calculation of the land requirements, costs of construction, time of implementation and lifecycle CO₂ emissions of these alternatives. Land requirements are important given the “not-in-my-backyard” syndrome. 2) The application of an optimization model, involving the above factors and the maximum supply capacities of these energy options. 3) The estimation of Japan’s CO₂ emissions in 2011 and the amount that needs to be reduced to accomplish the two targets, including the CO₂ from these alternatives’ lifecycle.

The energy to be generated in order to meet the KP target was estimated to be 372TWh/year. Figure 1 shows the results for reaching this target according to different priorities. If the focus is to minimize investment cost (scenario 1), accomplishing the target by 2020 would require 2812 Km² and 4.7 trillion yen/year. If the priority would be sparing land (scenario 2), it would compromise 828 Km² and 5.1 trillion yen/year. Yet, minimizing cost, land and time (scenario 3), suggests that with relatively smaller differences, the target could be accomplished by 2018. This, nonetheless, is a considerable challenge.

In general, results suggest that Japan should begin tapping its small-hydro potential, followed by solar (PV), while developing its great geothermal and wind energy potentials.

Further research will scrutinize these results and include Hatoyama’s target.

Presentation award for young researchers in 9th joint meeting of the fusion energy.

**Advanced Atomic Energy Research Section
Kenzo Ibano (D3)**

Cost analysis on the biomass-fusion hybrid concept was taken. Using systems code, Cost of Product analyses for following scenarios to a fusion reactor have been taken; using a turbine to produce electricity (not a biomass hybrid), using a fuel cell to produce electricity and using an F-T process chemical plant. Comparison between these scenarios as well as biomass fuel fee consideration shows that biomass hybrid scenarios have an economical attractiveness over the conventional turbine scenario in particular for a low fusion power reactor.

GCOE Group Poster Award in 2012 Annual Meeting of GCOE for “Economic and environmental analysis”

**Advanced Atomic Energy Research Section
Gwon Hyoseong(D2),**

GCOE aims to establish an international education and research platform to foster educators, researchers, and policy makers who can develop technologies and propose policies for establishing a scenario toward a CO₂ zero-emission society no longer dependent on fossil fuels. Annual meetings of GCOE have been held every year mainly in Japan.

The 2012 annual meeting of GCOE was held at Kyoto University Clock Tower Centennial Hall. In the 2012 annual meeting of GCOE, we presented a work on economic and environmental analysis on shale gas in Japan. Japan has been stopping its operation of most of its nuclear power plants after the Fukushima accident, which occurred in March 2011. As a result, energy supply issues are seriously coming to the forefront. Natural gas is expected to serve as one of the alternatives to coal, oil, and even nuclear power in Japan due to its sufficient reserves, affordable cost, higher energy per unit weight and low CO₂ emission. In this work, we study scenarios wherein natural gas takes a larger role in the case of a zero nuclear situation and discuss the feasibility of natural gas as a main fuel resource in Japan 2030. Specifically, we focus on shale gas, an unconventional type of natural gas, which has large reserve amounts with a wide distribution all over the world. Among the scenarios studied, a notable one is the case where the electricity generation proportion of coal and oil is set to zero and that of natural gas was increased to 70% with renewable energy supplying the rest. With this, the additional natural gas demand is about 50.69 Mton and the total CO₂ emission is just 433.58 Mton, which is less than the 2009 level (449.62 Mton). The additional natural gas demand can be covered by the increases in the output of natural gas mining, which is supported by the recent success of shale gas in USA. Shale gas will be expected to be half of total natural gas production of USA in 2035. Therefore, economic feasibility of shale gas would be enough. China, Canada, Australia and Indonesia also have large amount of recoverable reserves of shale gas and have potential as exporting country to Japan. As the production of shale gas increases, we need technical developments preventing the environmental issues and the leakage of shale gas to suppress global warming effect.

Young Researcher Award of the Kansai Branch, Atomic Energy Society of Japan.

Advanced Particle Beam Energy Research Section
Taiju Kajiwara (D3)

Atomic Energy Society of Japan (AESJ) was founded in 1959 as an academic society that seeks to develop science and technology of peaceful use of nuclear energy. Two conferences have been held every year in Japan, and many other activities concerned with nuclear energy have been conducted.

In the 8th Research Meeting for Young Researchers of the Kansai Branch of AESJ, Taiju Kajiwara made a presentation on recovery of energy from electron beams in an inertial electrostatic confinement (IEC) fusion device by installation of an additional high transparent and positively biased anode grid between a central transparent cathode at a highly negative potential and a spherical vacuum chamber at a ground potential. The energy recovery technic has already been well-developed for accelerators, and it can decrease input power drastically. However, in order to apply it to IEC, there were still issues to be solved; increase of current flowing into the anode by secondary emission from the vacuum chamber surface and ionization because of relatively high gas pressure. The increase of anode current was found to cause a considerable increase of the input power.

In order to mitigate this problem, another additional high transparent grid was installed in the vicinity of the chamber. A slightly negative voltage was then applied in attempt to suppress the secondary emission and the ionization by the secondary electron.

Experimental results showed that anode current was reduced considerably by installation of the secondary emission suppressor, and the ratio of fusion rate to the input power was improved. It was also found that the ratio strongly depended on the anode voltage, and maximum of the ratio was twice as high as that of our conventional IEC which did not have the anode for the energy recovery.

As conclusions, it was found that the recovery of energy from the electrons can improve the efficiency of IEC drastically, and the suppression of secondary emission is important and necessary. Suppression of secondary emission from the suppressor itself would lead to further lower anode current and higher efficiency.

Best Student Poster Award in 14th US-Japan Workshop on Inertial Electrostatic Confinement Fusion.

Advanced Particle Beam Energy Research Section
Genki Hashimoto (M2)

Inertial Electrostatic Confinement (IEC) is a compact and high controllability process for researching the physics of nuclear fusion. Applications of IEC fusion include a novel neutron source. The 1st US-Japan IEC exchange was held at Los Alamos National Laboratory, United States in 1998 for promotion of research and development on IEC. Annual workshops have been held after the exchange. The 14th US-Japan Workshop on IEC Fusion was held in Washington, D.C., US on October 14 and 17, 2012. More than 30 including 15 students participated from US, Australia, Canada and Japan. In this workshop, I presented my work on experimental results of simultaneous X-ray and neutron radiography by use of glow discharge driven D-D IEC fusion device as a multi-radiation source, and received the best student poster award.

Demands recently grow on the extension of neutron radiography utilization. The conventional neutron sources for the radiography do not always satisfy performance requirements like compactness, portability and controllability. Since a glow discharge driven IEC fusion device has been developed well technically, the neutron radiography by use of that would be effective. Additionally, identification of materials by the simultaneous neutron and the X-ray radiography, i.e. two beam radiography is feasible in principle.

We irradiated samples with X-ray and neutrons simultaneously for 90 minutes, the neutron yield was 1.6×10^7 n/sec. Numerical thermal neutron flux density on the sample was 1.3×10^2 n/cm²/sec. Thus, the thermal neutron fluence is estimated as 7.0×10^5 n/cm² in this case. This is enough for the neutron imaging plate (IP) to provide a neutron image, which requires a fluence exceeding 10^4 n/cm².

As the result, a polyethylene and an acrylic could be distinguished from other materials by measuring the ratios between the intensities of neutrons and X-rays before and after transmission of the materials. This is because a polyethylene and an acrylic contain hydrogen that has a high ratio of the mass attenuation coefficient between X-rays and neutrons. This suggests that a material which contains hydrogen, boron or lithium for instance can be detected with a high sensitivity by the radiography of X-ray and neutron emitted from the glow discharge driven D-D IEC fusion device.

Excellent student award for research and oral presentation at 9th annual conference of the Japan Society of Maintenology

**Advance Energy Structural Materials
Yasunori Yamamoto (D2)**

The Japan society of Maintenology was founded in 2003 for establishment of advanced maintenology that systemize the science and technology required for maintaining the natural environment, artifacts, and our social civilization. Management and maintenance of fission reactors is one of the targets to be discussed in this society. Annual conferences have been held every year in Japan.

In the 9th annual conference held at Tokyo, 2012, Mr. Yamamoto presented a work on “Theoretical investigation of the oxidation process of fuel cladding material used in nuclear fission reactors”. Many participants took a great interest in his research because he uses a purely theoretical method to solve a rather practical issue occurred at fission reactors. His challenge looks very fresh to the audience and reviewers.

In his research he has employed an ab-initio calculation method that is usually used in the research field of solid-state physics. He has obtained the precise energetics of lattice defects, which is important for investigating an oxide layer on the surface of cladding material from the viewpoint of thermodynamics. With the energies thus obtained, he solved kinetic diffusion equations to understand the oxidation rate of the material. And he has finally obtained the time evolution of oxide layer thickness, which is consistent with experimental observations.

Due to his research and presentation, he received the excellent student award. His research is expected to be useful for establishment of the advanced management and maintenance of nuclear fuels.

Excellence presentation award in 14th annual meeting of The RNA Society of Japan.

**Structural Energy Bioscience Research Section
Tsukasa Mashima (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 14th annual meeting of this society was held in Tohoku University.

In the 14th annual meeting, I presented our latest work entitled "Anti-Prion activity of RNA Aptamer and its Structural Basis". Prion protein (PrP) exhibits two alternative conformational forms, a normal cellular form (PrP^C) and an abnormal form (PrP^{Sc}). The conversion from PrP^C into PrP^{Sc} is reportedly responsible for infectivity of prion diseases. In this symposium, I demonstrated how RNA aptamer, R12, recognizes and tightly binds to PrP^C. R12 folds into unique quadruplex structure and forms a homodimer conformation. Two portions within PrP, namely P1 and P16, were identified as binding sites for R12. We revealed that in the R12:PrP complex, one monomer of the R12 dimer interacts with P1 and the other with P16, simultaneously (Figure 1). This simultaneous double binding renders the high affinity to R12 against PrP. I also demonstrated that RNA aptamer, R12, actually reduces PrP^{Sc} level in prion-infected cells. R12 tightly binds to PrP^C and stabilizes the conformation of PrP^C. This results in inhibition of the conversion of PrP^C into PrP^{Sc}.

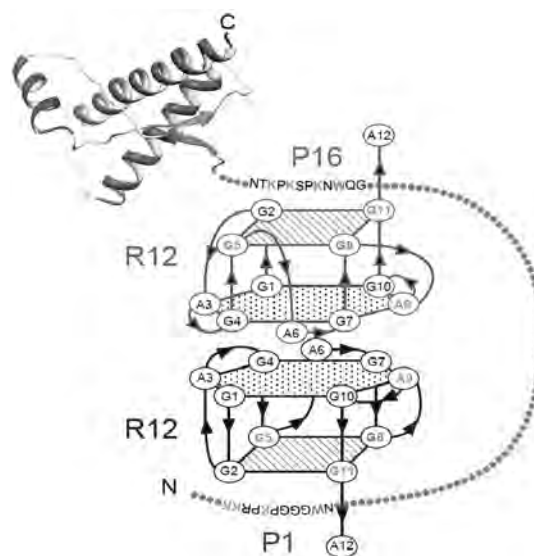


Figure 1 The overall architecture of R12:PrP complex structure.

4. JOINT USAGE/RESEARCH PROGRAM



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

It is an urgent task to get solutions against the energy and environmental problem for the sustainable development of human beings. The new energy system should be an environmentally friendly or ecological one. Here, we should consider not only the energy sources but also the efficiency in the phase of energy usage. The former should have good quality and enough quantity. The latter should be useful to realize three Rs 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 present technology is not enough. Interdisciplinary studies with innovative ideas are necessary to realize the energy system for next generation.

We propose a new ambitious concept of Zero-Emission 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. In FY 2011, we launched “Joint Usage/Research Program on Zero-Emission Energy”, which is the program authorized by the MEXT. Here, we aim to (1) promote interdisciplinary collaboration researches 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 since FY2011. Joint Usage/Research collaborations of total 79 subjects on Zero-Emission Energy were performed in FY2012 with more than 493 participants including graduate/undergraduate students from 37 all-Japan Universities and Institutions. The results of these collaborations are reported in “IAE Joint Usage/Research Program on Zero-Emission Energy 2012.” Some of them were presented and discussed in a Research Summary Session of FY2012 held at Uji Campus on March 6, 2013. If you have interest to this collection, please contact to Zero-Emission Energy Research Office (kyodo-office@iae.kyoto-u.ac.jp).

In addition to the Joint Usage/Research collaborations, we organized “the 3rd International Symposium of Advanced Energy Science ~ Toward Zero-emission Energy ~” on September 2-4, 2012 at Uji Obaku Plaza, Kyoto University. This symposium consists of one plenary session and two parallel seminars. About 170 scientists and students including four foreign and four domestic invited speakers were participated in the symposium. This kind of international symposium will be held routinely every year. In addition, several informal seminars on Zero-Emission Energy are also held irregularly.

We have also organized “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.



Fig. 1 Poster of the 3rd International Symposium

List of Zero-Emission Energy Joint Usage/Research Subjects in FY 2012

(Subject, Principal Researcher, IAE Key Person)

Structural determination of self-organizing glycoconjugates of bacterial origin aiming to heighten the added value of biomass

M. Takeda, M. Katahira

Photo-Energy Conversion System Using DNA As a Charge Transporting Material

K. Yamana, T. Morii

NMR analysis of supramolecular structure of lignin for advanced biomass utilization

K. Fukushima, M. Katahira

Phase stability in RAFM and ODS steels under ion irradiation

H. Abe, A. Kimura

Construction of a high particle and high temperature loading experiment system using the ion beam test stand, and test fusion reactor diverter system

Y. Yamamoto, T. Konishi

Enzymatic conversion of carbon dioxide to methanol using biopolymer gel matrix

N. Tanaka, T. Morii

Study of strength degradation structure by thermally aged and ion irradiation in first fission reactor material

K. Fukumoto, A. Kimura

Study on Gas Fueling and Pumping Systems for D-T Burning in Discharge Fusion Neutron Source

M. Onishi, K. Masuda

Structural analysis of lignin by ultra-high sensitivity NMR for biorefinery

T. Watanabe, M. Katahira

Property change on plasma facing materials for fusion reactor by high energy ion irradiation

K. Tokunaga, A. Kimura

Tungsten material behavior under complex fusion irradiation environment

Y. Ueda, A. Kimura

Technology development of joining between nanostructured, toughened W-TiC and ODSS alloys for blanket structures

H. Kurishita, A. Kimura

Synergistic effects of displacement damage and transmuted helium on the microstructure of fusion reactor structural materials and joints

T. Yamamoto, A. Kimura

Development of environmental-friendly low energy-loss solid surfaces nanostructured with femtosecond laser pulses

N. Yasumaru, K. Miyazaki

Microstructure evolution of ion-irradiated oxide/nitride ceramics -Role of electronic excitation and selective displacement damage-

K. Yasuda, A. Kimura

Study on photocatalytic film synthesis and biological CO₂ fixing using infrared free electron laser

Y. Hayakawa, H. Ohgaki

Development of an efficient molecular ion measurement system using intense ultra-short laser pulses

H. Niikura, K. Miyazaki

Mechanism of Radiation Resistance of Advanced Tungsten Alloys

A. Hasegawa, A. Kimura

Damage Formation Mechanism of Tungsten Under Repetitive and Pulsed High-Heat Load Conditions

K. Ezato, A. Kimura

Radiation induced hardening of pressure vessels steels due to ion irradiation

H. Watanabe, A. Kimura

Development of Green Chemical Semiconductor Materials and Visible Light Response Photocatalyst by Dual-Beam Facility for Energy Science and Technology

S. Kaoru, A. Kimura

Improvement of mechanical, corrosion and irradiation properties of low activation vanadium alloys for fusion reactor

T. Nagasaka, A. Kimura

Studies on Helical Structure in Current-Carrying Toroidal Plasmas and Their Impact on Helical Plasma Research

S. Masamune, T. Mizuuchi

Durability assessment of power plant structural material, H. Kinoshita, A. Kimura

Development of multi-pulse laser for energy enhancement of KU-FEL

- R. Kuroda, H. Ohgaki
- Heavy irradiation experiment of stainless steels under fusion condition
S. Ohnuki, A. Kimura
- High-Fluence Irradiation Behavior of Reduced Activation Fusion Reactor Materials
H. Tanigawa, T. Hinoki
- Synthesis of nano-bubble/particle dispersion strengthened alloys and evaluation of radiation effect on the microstructure
S. Ukai, A. Kimura
- Evaluation of radiation damages and helium effect on ODS ferritic steels
M. Ando, A. Kimura
- Hybrid Solar Energy Research suitable for Rural Electrification
W. Hew, H. Ohgaki
- Zero-emission energy system-challenge design and development of low-carbon boron tracing molecules
H. Hori, E. Nakata
- Development of iron-base composite materials with high thermal conductivity
N. Hashimoto, A. Kimura
- R&D of Diverter Element for Fusion Reactor Using Explosion Welding
K. Hokamoto, R. Kasada
- Research on enzymatic hydrolysis of plant biomass
S. Sawayama, T. Kodaki
- Studies on DNA Nanowire Transistor
K. Yamana, T. Morii
- Build-Up Strategy of ultra-thin carbon wire for Energy Conservation Devices
T. Nakae, H. Sakaguchi
- A fluorescent peptide probe for imaging of energy metabolism in cells
S. Sato, T. Morii
- Design of functional protein nano-fiber and its application to the cell culture plate
N. Tanaka, T. Morii
- Development of small molecular organic thin-film solar cells
M. Hiramoto, T. Sagawa
- Study of role of symmetry in collisional transport in toroidal plasma
M. Kikuchi, K. Nagasaki
- Probing the intrinsic electrical and optical properties of high-quality carbon nanotubes by microscopic spectroscopy
Y. Miyata, K. Matsuda
- Development of Radiation Detection Method Emitted from IEC Device
T. Misawa, K. Masuda
- Phase measurement of Vacuum-Ultraviolet pulse and control of electronic states
R. Itakura, T. Nakajima
- Study of neutral transport in high-temperature plasmas
Y. Nakashima, S. Kobayashi
- Study of Simultaneous X ray/Neutron Radiography by IEC D-D Fusion Device
H. Osawa, K. Masuda
- Fabrication of functional organic thin-films and evaluation of their PL and PV properties
H. Ihara, T. Sagawa
- Generation of high-intensity fs vacuum ultraviolet pulses by using harmonic radiation
M. Kaku, K. Miyazaki
- In vivo analysis of environmental sensitive fluorescent probes for tumor imaging
H. Harada, E. Nakata
- High power harmonic beam line to characterize useful materials for zero-emission
T. Sekikawa, T. Nakajima
- Phase relaxation mechanism of excitons in doped carbon nanotubes
S. Konabe, K. Matsuda
- Safety assessment of nuclear power plants and future energy education
H. Iwakiri, K. Morishita
- Highly efficient photochemical reactions induced by optimal laser pulses
Y. Ohtsuki, T. Nakajima
- Production of novel clusters with femtosecond laser ablation of solid materials
T. Kobayashi, T. Nakajima
- Flow analysis from a nozzle for SMBI

N. Nishino, T. Mizuuchi

Correlation measurement of electron cyclotron emission signals at two toroidal positions in torus plasmas

Y. Yoshimura, K. Nagasaki

Modeling of microstructural development in irradiated materials for fusion applications

Y. Watanabe, K. Morishita

Detection of deuterium trapping site of deuterium-charged tungsten

K. Sato, A. Kimura

Research of fracture toughness behavior of structural materials using small specimens

E. Wakai, A. Kimura

Development of Organic-Inorganic Hybrid Film toward High-Performance Organic Thin-Film Solar Cells

T. Akiyama, H. Sakaguchi

Development of a steerable ring-type millimeter wave launcher

H. Shidara, K. Nagasaki

Preparation of silicone resin with micro-rod structure and development of self-cleaning materials

T. Yamauchi, K. Fukami

Assembly of membrane transporters on the DNA nano-structure

Y. Mori, T. Morii

Evaluation of Deformation and Fracture Behavior of Plasma Facing Material

S. Nogami, T. Hinoki

Research and development of advanced optical devices with brilliant and high conversion efficiency by metallic nano particle dispersed oxide materials by ion irradiation technique

T. Shibayama, T. Hinoki

Fundamental study and applications of electrical properties of graphene nanostructures using optical spectroscopy

J. Haruyama, K. Matsuda

Development of single-electron irradiation technique for microscopic track structure study

Y. Uozumi, H. Ohgaki

Theoretical study on thermal disintegration of hydrogen clusters trapped by vacancies in metals

D. Kato, K. Morishita

The role of organic solvents in the formation of porous semiconductors by electrochemical methods

E. Tsuji, K. Fukami

Diagnostics of plasma turbulence by using micro-wave

S. Inagaki, K. Nagasaki

2-dimensional imaging of fluctuations by fast cameras using a sheet-shaped super sonic molecular beam

M. Takeuchi, T. Mizuuchi

Theoretical study on atomistic modeling for interactions between hydrogen/oxygen atoms and additive elements in zirconium alloys

Y. Kaneta, K. Morishita

The effects of ion irradiation on microstructure of pyrolytic carbon interphase in advanced SiC/SiC composites

K. Ozawa, T. Hinoki

Biochemical Analysis of Molecular Interactions by Human Intrinsically Disordered Proteins

Y. Aizawa, T. Morii

Studies of visualization based on computer tomography of three dimensional high temperature plasmas

S. Ohdachi, S. Yamamoto

Applicability study of ion beam induced luminescence measurements for evaluation of irradiation damages in SiC materials

T. Tanaka, T. Hinoki

Study of the effect of crystallographic orientation on the thermal and electric conductivities in SiC

T. Suzuki, T. Hinoki

Evaluation on High Temperature Strength and Corrosion Properties of Dissimilar Friction Stir Welded RAF steels

H. Sakasegawa, A. Kimura

Creation of functional proteins toward regulation and elucidation of cellular events

M. Imanishi, T. Morii

Boundary diagnostics and rf heating in Heliotron J-II

K. Uehara, T. Mizuuchi

5. COLLABORATION WORKS IN THE LABORATORY FOR COM- PLEX 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 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 2012.

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 30 were applied and applications of 29 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 32

		category A			B	total
		A1	A2	A3		
Kibann *1	inside	1	1	1	0	3
	outside	0	0	0	0	0
Syorei/Kikaku-chosa *2	inside	3	11	10	1	25
	outside	0	1	0	0	1

“inside” or “outside” : Numbers applied by the inside or outside of the Institute

The individual research subjects are as follows, *1 and *2 mean the “Kiban” and “Syorei”/“Kikaku-chosa’ co-operative research theme, respectively,

The individual research subjects are as follows.

A1,

“International Collaborative Research on Advanced Energy Materials Science and Technology”

- (1) M.J. Fluss
- (2) G.R. Odette
- (3) S.T. Zinkle
- (4) F.M. Tabassoli
- (5) C. Zhang
- (6) J. Jang
- (7) A. Kimura, K. Morishita, O. Hashitomi, T. Ohmura
- (1) *Laurence Livermore National Laboratory, USA*
- (2) *Dept. of Mechanical Engineering, University of California Santa Barbara, USA*
- (3) *Oakridge National Lab Inst. High Temperature*
- (4) *Korea Institute of Science and Technology*
- (5) *Institute of Modern Physics, Chinese Academy of Science Landu, China*
- (6) *Korea Atomic Energy Research Institute ,Daejon Korea*
- (7) *Institute of Advanced Energy, Kyoto University*

A2,

“Development of Advanced Plasma and Quantum Energy Studies”

- (1) K. Nagasaki, R. Kasada, S. Ohshima, Shi nan, S. Konishi, T. Minami, H.Okada, S. Kobayashi S. Yamamoto, F. Sano, T. Mizuuchi, S. Konoshima C. Takahashi
- (2) H. Lee, Z. Linge, K. Ibane
- (3) K. Tanaka, K. Mukai
- (1) *Institute of Advanced Energy, Kyoto University*
- (2) *Graduate School of Energy Science, Kyoto University*
- (3) *National Institute for Fusion Science*

A3

“Research on establishment of Photo-Energy Nano Science”

- (1) H. Ohgaki, Member of Photo-Energy Nano-Science
- (1) *Institute of Advanced Energy, Kyoto University*

A1

“Multiscale modeling of fusion reactor material's behavior during irradiation”

- (1) Y. Kaneta
- (2) Y. Watanabe
- (3) D. Kato
- (4) S. Ohnuki
- (5) X. Qui, T. Yoshiie
- (6) Y. Yamamoto
- (7) K. Morishita, A. Kimura
- (1) *Akita National College of Technology Japan*
- (2) *Japan Atomic Energy Agency*
- (3) *National Institute for Fusion Science*
- (4) *Graduate School of Engineering, Hokkaido University*
- (5) *Kyoto University Research Reactor Institute*
- (6) *Graduate School of Energy Science, Kyoto University*
- (7) *Institute of Advanced Energy, Kyoto University*

“Advanced maintenance technology for nuclear power plant safety”

- (1) K. Morishita, A. Kimura
- (2) Y. Yamamoto
- (3) S. Ishino
- (4) H. Abe
- (5) H. Muta
- (6) H. Iwakiri
- (1) *Institute of Advanced Energy, Kyoto University*
- (2) *Graduate School of Energy Science, Kyoto University*
- (3) *University of Tokyo*
- (4) *School of Engineering, Tohoku University*
- (5) *Graduate School of Engineering, Osaka University*
- (6) *Development Education, University of Ryuky*

“Numerical Simulation of DC/Pulsed Magnetron Discharge”

- (1) K. Masuda
- (2) M. Bilek, J. Kipritidis
- (3) T. Kajiwara
- (1) *Institute of Advanced Energy, Kyoto University*
- (2) *The School of Physics, the University of Sydney*

(3) *Graduate School of Energy Science, Kyoto University*

A2

“Computational Study of Twisted-Tape-Induced Swirl Flow Turbulent Heat Transfer in a Short Circular Tube under Velocities Controlled (Part Effect of Swirl Velocity on Thermal Boundary Layer Thickness)”

- (1) K. Hata
- (2) Y. Shirai
- (3) T. Masuzaki
- (4) M. Hamura
- (1) *Institute of Advanced Energy, Kyoto University*
- (2) *Graduate School of Energy Science, Kyoto University*
- (3) *National Institute for Fusion Science*
- (4) *Concentration Heat and Momentum Ltd*

“Observation of Stereoscopic Image for Edge Plasma Turbulence”

- (1) T. Mizuuchi
- (2) N. Nishino
- (3) Z. Linge, S. Mengyu
- (1) *Institute of Advanced Energy, Kyoto University*
- (2) *Graduate School of Engineering, Hiroshima University*
- (3) *Graduate School of Energy Science, Kyoto University*

“Materials-system integration study for innovative divertor device”

- (1) R. Kasada, S. Konishi, Y. Takeuchi, K. Noborio
- (2) H. Gwon, K. Wada
- (1) *Institute of Advanced Energy, Kyoto University*
- (2) *Graduate School of Energy Science, Kyoto University*

“Stabilization of MHD Instabilities by Control of Rotational Transform”

- (1) K. Nagasaki, K. Sakamoto, F. Sano, T. Mizuuchi, T. Minami, H. Okada, K. Masuda, S. Kobayashi, S. Yamamoto, S. Konoshima, S. Ohshima
- (2) Y. Nakamura
- (3) Y. Yoshimura, G. Motojima, K. Mukai
- (4) N. Marushchenko
- (5) A. Cappa, T. Estrada
- (1) *Institute of Advanced Energy, Kyoto University*
- (2) *Kyoto University Pioneering Research Unit for Next Generation, Kyoto University*
- (3) *Graduate School of Energy Science, Kyoto University*
- (4) *National Institute for Fusion Science*
- (5) *Max Plank Institute, Germany*
- (6) *CIEMAT, Spain*

“Control of TF/Helical Combined Ripple by the Placement of Ferritic Steel Plates”

- (1) A. Kimura, K. Nagasaki, O. Hashitomi, T. Ohmura

(1) *Institute of Advanced Energy, Kyoto University*

“The Mechanism of Mn Effects based on the Annihilation Behavior of Frankel Pairs among Cascade Damage Structures”

- (1) A. Kimura, H. Ohgaki, T. Kii, R. Kasada O. Hashitomi, T. Ohmura
- (2) K. Yabuuchi
- (1) *Institute of Advanced Energy, Kyoto University*
- (2) *Graduate School of Energy Science, Kyoto University*

“Development of High Speed AD Converter for High Resolution Nd:YAG Thomson Scattering measurement.”

- (1) T. Minami
- (2) H. Funaba, K. Yamada, H. Nakanishi
- (3) T. Hatae
- (1) *Institute of Advanced Energy, Kyoto University*
- (2) *National Institute for Fusion Science*
- (3) *Japan Atomic Energy Association*

“Studies of anomalous loss mechanism of energetic ion in Heliotron J plasmas.”

- (1) S. Yamamoto, H. Okada, F. Sano, T. Minami, T. Mizuuchi, S. Kobayashi, K. Nagasaki, S. Ohshima, S. Konoshima
- (2) Y. Nakamura
- (3) M. Isobe, K. Nagaoka, K. Ogawa
- (1) *Institute of Advanced Energy, Kyoto University*
- (2) *Graduate School of Energy Science, Kyoto University*
- (3) *National Institute for Fusion Science*

“Energies of Coincidence Boundaries in Si”

- (1) K. Ishihara
- (2) A. Ohtsuki
- (1) *Graduate School of Energy Science, Kyoto University*
- (2) *Institute of Advanced Energy, Kyoto University*

“Study of edge plasma behavior caused from fast ion driven MHD instability”

- (1) S. Ohshima, K. Nagasaki, F. Sano, T. Mizuuchi, H. Okada, S. Kobayashi, S. Yamamoto, Shi Nan, S. Konoshima
- (1) *Institute of Advanced Energy, Kyoto University*

“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, T. Mizuuchi, K. Nagasaki, F. Sano, S. Ohshima
- (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) *Plasma Research Center, University of Tsukuba*
- (5) *Graduate School of Engineering, Hiroshima University*

“Experimental study on relationship between particle transport coefficients and turbulent fluctuation-Radial structure of particle and turbulent transport under strong electron heating conditions-”

- (1) S. Kobayashi, T. Minami, T. Mizuuchi, K. Nagasaki, H. Okada, S. Yamamoto, S. Konoshima, F. Sano K. Tohshi, K. Sakamoto
- (2) Y. Nakamura, H.Y. Lee, Y. Nagae, T. Harada
- (3) Y. Suzuki, K. Nagaoka, Y. Takeiri, S. Okamura, K. Tanaka, K. Mukai
- (4) T. Ohishi
- (5) Y. Nakashima
- (6) S. Murakami
- (7) S. Kado
- (8) T. Estrada
- (1) *Institute of Advanced Energy, Kyoto University*
- (2) *Graduate School of Energy Science, Kyoto University*
- (3) *National Institute for Fusion Science*
- (4) *Faculty of Engineering, Nagoya University*
- (5) *Plasma Research Center, University of Tsukuba*
- (6) *Graduate School of Engineering, Kyoto University*
- (7) *School of Engineering, The University of Tokyo*
- (8) *CIEMAT, Spain*

A3

“Single-shot measurement of the KUFEL spectra using nonlinear frequency conversion”

- (1) T. Nakajima, H.Zen, T. Kii, T. Sakka, H. Ohgaki X. Wang
- (1) *Institute of Advanced Energy, Kyoto University*

“Interface design and evaluations of photovoltaic properties of bulk heterojunction organic thin-film solar cells”

- (1) T. Sagawa
- (2) H. Kaji
- (1) *Institute of Advanced Energy, Kyoto University*
- (2) *Institute for Chemical Research Kyoto University*

“Preparation and characterization of metal oxide nanofiber”

- (1) T. Sagawa
- (2) Y. Tsujii
- (3) T. Sato
- (1) *Institute of Advanced Energy, Kyoto University*
- (2) *Institute for Chemical Research Kyoto University*
- (3) *Tsuruoka national College of Technology*

“Formation of binary particle-layers by various kinds of particles at liquid-liquid interfaces an”

- (1) T. Sakka, T. Nakajima, K. Fukami, Y. Ogata
- (2) G. Oye
- (3) Y. Suzuki
- (1) *Institute of Advanced Energy, Kyoto University*
- (2) *Norwegian University of Science and Technology*
- (3) *Uyemura & Co.,Ltd.*

“Development of a highly efficient bioethanol production yeast by metabolic engineering”

- (1) T. Kodaki, M. Katahira
- (2) S. Sawayama
- (1) *Institute of Advanced Energy, Kyoto University*
- (2) *Graduate School of Agriculture, Kyoto University*

“A Turing-type instability observed in electrochemical dissolution of silicon”

- (1) K. Fukami, T. Sakka, Y. Ogata
- (2) K. Krischer
- (3) Y. Suzuki,
- (1) *Institute of Advanced Energy, Kyoto University*
- (2) *Technical University of Munich*
- (3) *Uyemura Co. Ltd*

“Development of Photocathode RF Gun for Intense Mid Infrared Free Electron Laser”

- (1) H. Zen, H. Ohgaki, K. Masuda. T. Kii
- (2) K. Shimahashi
- (1) *Institute of Advanced Energy, Kyoto University*
- (2) *Graduate School of Engineering, Kyoto University*

“Construction of High-efficient material conversion system by using DNA nanostructure”

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

“Fabrication and Property Measurement of MgB2 for Bulk Superconducting Undulator”

- (1) T. Kii, H. Ohgaki, H. Zen
- (1) *Institute of Advanced Energy, Kyoto University*

“Nanograting Formation on Wide-gap semiconductor surface with ultraviolet femtosecond laser pulses”

- (1) G. Miyaji, K. Miyazaki
- (2) A.E. Kaplan
- (3) J. Reif
- (1) *Institute of Advanced Energy, Kyoto University*
- (2) *Johns Hopkins University*
- (3) *Brandenburgische Technische Univ.*

“Molecular mechanisms of the translational repression complex that maintains the self-renewal or tumorigenic potential of the cells”

- (1) T. Nagata, M. Katahira, T. Morii, E. Nakata
- (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. In 2012, three regular meetings and the annual meeting for the cooperative research results were held with following theme.

1. The regular meeting
 - (1) The First Meeting, July 6, 2012
H. Ono, "Initial Event Analysis of the Fukushima Daiichi Nuclear Power Plant Accident -Until a Core Melts-", "Validity Evaluation of the long-term cooling technique in the Fukushima Daiichi Nuclear Power Plant" *Japan Nuclear Energy Safety Organization*
 - (2) The Second Meeting, September 11, 2012,
K. Muraoka, "Requirements for commercial fusion reactors in the future energy system", *Professor emeritus, Kyusyu University*
 - (3) The Third Meeting, October 10, 2012
H. Ikehira, "Recent topics on the organic electro-luminescence polymers" *Sumitomo Chemical Co., Ltd. Fellow Laboratory*
2. The Annual Meeting for the Cooperative Research Results, April 5, 2013
 - (1) A. Kimura, "International Collaborative Research on Advanced Energy Materials Science and Technology", *Institute of Advanced Energy, Kyoto University*
 - (2) K. Morishita, "Advanced maintenance technology for nuclear power plant safety" *Institute of Advanced Energy, Kyoto University*
 - (3) E. Nakata, "Construction of High-efficient material conversion system by using DNA nanostructure", *Institute of Advanced Energy, Kyoto University*
 - (4) H. Ohgaki, "Research on establishment of Photo-Energy Nano Science", *Institute of Advanced Energy, Kyoto University*
 - (5) K. Fukami, "A Turing-type instability observed in electrochemical dissolution of silicon", *Institute of Advanced Energy, Kyoto University*
 - (6) T. Nakajima, "Single-shot measurement of the KUFEL spectra using nonlinear frequency conversion", *Institute of Advanced Energy, Kyoto University*
 - (7) K. Nagasaki, "Development of Advanced Plasma and Quantum Energy Studies", *Institute of Advanced Energy, Kyoto University*
 - (8) K. Hata, "Computational Study of Twisted-Tape-Induced Swirl Flow Turbulent Heat Transfer in a Short Circular Tube under Velocities Controlled", *Institute of Advanced Energy, Kyoto University*
 - (9) S. Ohshima, "Study of edge plasma behavior caused from fast ion driven MHD instability", *Institute of Advanced Energy, Kyoto University*

6. PROJECTS WITH OTHER UNIVERSITIES AND ORGANIZATIONS

Asian CORE (Center Of Research and Education) program, 2008-2012

The Asian CORE (Center Of Research and Education) program for the “Advanced Energy Science” between Japan, Korea and China was granted by the JSPS (Japan Society for the Promotion of Science) of 5 year collaboration has completed its entire 5 year program. In this program, Japan and core institutes in Eastern Asian nations established the network of research and education in the advanced and important fields of energy science by the extensive collaboration of mutually equal contribution, The Institute of Advanced Energy played the role of the hub institute in Japan to represent universities and research institutes, with Prof. Yukio Ogata as the representative and Prof. Satoshi Konishi as the Program Coordinator. Counterparts were Prof. Hangyu Joo in Seoul National University in Korea and Prof. Kan Wang in Tsinghua University in China.

Advanced energy science and technology are of common interests in these countries where industrial application of energy is extensive. This program supported the exchanges of scientists and students in the field of advanced energy research, for collaboration, workshops and other research activities. This program was operated by equal contribution basis, and it requires “matching fund” from counterpart countries, and Korea and China have different types of funding to send and accept approximately same level of exchanges. In this 5 years, situations on energy technology and circumstances in these three countries has been changed drastically. Particularly, Great Eastern Japan earthquake, tsunami, and nuclear accidents in Japan had a significant impact not only in Japan, but also these neighboring countries. This

program has assisted the information exchange on the studies of advanced nuclear energy and renewable energies, that have important position in the future energy supply in the area and the world.

Subtasks on five technical areas were agreed for the collaboration as follows.

Task 1 Advanced Nuclear Energy Systems: liquid metal technology, high temperature nuclear energy conversion, neutronics, and fusion technology.

Task 2 Fusion Plasma Science: plasma physics, simulation and theory, heating and current drive, diagnostics and plasma wall interaction.

Task 3 Bioenergy: Synthesis of biofuel from biomass materials and energy production systems.

Task 4 Advanced Energy Materials: nuclear materials for high temperature use, ODS and ceramics, irradiation, and microscopy.

Task 5 Application of Quantum Radiation: electron beam, accelerator technology, free electron laser, tera hertz wave and its application.

In the fiscal year 2012, we have conducted the exchanges in these areas as summarized in the fig.1. Some difficult situations in the politics between the countries has not affected due to the strong relations established by the previous collaborations.

In this year summer school was held in Aomori in August 2012 with the contributions from R-1, R-2, and R-4. Figure 2 shows the group photo of the participants at this seminar. Future possible collaborations to succeed this Asian CORE are planned and discussed.

	J→K	K→J	J→C	C→J
SCM	0/0	0/0	0/0	0/0
Task-1	5/33	6/35	2/14	3/9
Task-2	1/5	0/0	2/10	0/0
Task-3	7/21	0/0	0/0	0/0
Task-4	11/43	1/4	2/10	2/14
Task-5	8/26	2/10	1/4	1/30
Seminar	0/0	18/72	0/0	9/45
subtotal	32/128	27/121	7/38	15/98
Total	81/385			

Fig.1 Conducted exchanges in 2012 under the Asian CORE program.(man/man-day)



Fig.2 Asian CORE seminar held in Aomori, Japan in Aug, 2012.

Global COE Program “Energy Science in the Age of Global Warming – Toward CO2 Zero-emission Energy System –”

Securing energy and conservation of the environment are the most important issues for the sustainable development of human beings. Until now, people have relied heavily on fossil fuels for their energy requirements and have released large amounts of Greenhouse gases such as carbon dioxide (abbreviated to CO₂ below). CO₂ has been regarded as the main factor in climate change in recent years. It is becoming a pressing issue in the world how to control over the CO₂ release. The energy problem cannot be simply labeled as a technological one, as it is also deeply involved with social and economic elements. It is necessary to establish the “Low carbon energy science” in the interdisciplinary field adding the social science and the human science to the natural science.

From FY2008, four departments of Kyoto University, Graduate School of Energy Science, Institute of Advanced Energy, Department of Nuclear Engineering, Research Reactor Institute have joined together, and also with the participation from Institute of Economic Research have been engaging in "Energy Science in the Age of Global Warming - Toward a CO₂ Zero-emission Energy System " for a Global COE Program of the Ministry of Education, Culture, Sports, Science and Technology under the full faculty support taking advantage of characteristics of the university. This program aims to establish an international education and research platform to foster educators, researchers, and policy makers who can develop technologies and propose policies for establishing a scenario toward a CO₂ zero-emission society no longer dependent on fossil fuels, by the year 2100.

In the course of implementing the Global COE, we placed the GCOE Unit for Energy Science Education at the center, and we proceed from the Scenario Planning Group, the Advanced Research Cluster to the Evaluation, forming mutual associations as we progress. The Scenario Planning Group sets out CO₂ zero emission technology roadmap and proposed several CO₂ zero emission scenarios in Japan, Middle-East, and ASEAN region. The Advanced Research Cluster, as an education platform based on research, promotes the socio-economic study of energy, study of new technologies for solar energy and biomass energy, and research for advanced nuclear energy by following the scenarios

proposed by the Scenario Planning Group. Evaluation is conducted by exchanging ideas among advisors inside and outside of the university and from abroad, to gather feedback on the scenario, education, and research.

For education activities, we establish “the GCOE Unit for Energy Science Education” and select students from the doctoral course, and foster these human resources. The students plan and conduct interdisciplinary group research containing both the social and the human science and the natural science toward CO₂ zero emission at the initiative of the students themselves. The students will acquire the faculty to survey the whole “energy system” through participation in scenario planning and interaction with researchers from other fields, and apply it to their own research. This approach should become the major methodology of human resources cultivation. We will strive to foster young researchers not only who will be able to employ their skills and knowledge with a wide international perspective as well as expertise in their field of study in order to respond to the needs of the society in terms of the variety of energy and environmental problems, but who will also lead people to a 21st century full of vitality and creativity, working towards harmony between the environment and mankind.

In FY2012, which is the last year of this program, we carried on finalizing activities of the GCOE the education programs and promoting the Zero-Emission Scenario Planning and the Advanced Researches. In order to report the developments and to discuss the post-GCOE activities internationally, we held the 4th International Symposium of the Global COE titled “Zero-Carbon Energy 2012” in May, 2012 in cooperation with The Joint Graduate School of Energy and Environment, King Mongkut’s University of Technology Thonburi, Thailand, and the annual symposium of the Global COE on January, 2013. We also made a strong effort to the international exchange promotion activities such as co-hosting SEE (Sustainable Energy and Environment) forums held in Brunei on November, 2012 and other related seminars and symposiums, as well as the AUN-KU International Symposium in May.

As a post-GCOE program, the “Re-Inventing Japan Program” has been adopted from October, 2012, in cooperation between AUN member universities.

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) instability suppression by controlling magnetic configuration, (3) ECH/EBW heating physics, (4) toroidal current control, (5) fueling control and exhaust control of heat and particles, and (6) development of the FIR measurement system and so on. The results of several subjects are described below.

Study of MHD instability driven by energetic ions

[1, 2]: Alpha particles generated in fusion plasmas excite MHD fluctuation during their slowing process resonantly coupling with Alfvén wave or sound waves. These MHD activities possibly enlarge transport loss of alpha particles. In NBI plasmas of Heliotron J, the MHD instability induced by energetic ions is often observed. The mode of this instability is found to be $m/n=2/1$ coherent mode with the frequency of 50~95 kHz. The theoretical prediction of density dependence of the instability frequency almost agrees with the experimental one. Both indicate $1/n_e^{1/2}$ dependence. The iota dependence of the frequency of the instability in the experiment is identical with that from the theoretical shear Alfvén spectrum taking account of toroidal plasma current effect. In the experiment, the mode below 50 kHz was not observed. The frequency may become higher from the combination of shear Alfvén wave and acoustic wave.

Stabilization of MHD mode driven by energetic ions using ECCD [3]:

Using the second harmonic electron cyclotron current drive, the control of instability is studied for the suppression of the bulk plasma confinement deterioration or energetic ion loss. The aim of this study is the suppression of the coherent MHD fluctuation (EPM) with more than 30 kHz of frequency observed in the NBI plasma in Heliotron J. ECCD is performed in the condition of the balanced NB injection. The line averaged electron density is $0.5 \times 10^{19} \text{ m}^{-3}$ for this experiment. The EC beam deflection is small and local heating is expected. The EPM fluctuation is observed in the MP signal without ECCD. This mode is $m/n=4/2$ and 80 kHz in frequency. The ECCD is applied and the 2kA of toroidal current is generated. Then, the fluctuation is sufficiently suppressed. It is considered that the generated magnetic shear is effective for the MHD fluctuation suppression.

Control of particle fueling [4]:

In order to optimize particle fueling for the good plasma confinement, supersonic molecular beam injection (SMBI) and intense gas puff (HIGP) are investigated. SMBI is considered to be an effective method for density increase and profile control. The achieved plasma stored energy for SMBI is 4.5 kJ, about 20% higher than that for HIGP under the same line-averaged density condition in the NBI heated plasma with 1.2 MW injection power. The electron and ion temperature in the plasma core region is also higher. The peaked density profile is observed in the core region as well.

References

- [1] S. Yamamoto, et al., "Studies of Energetic-ion-driven MHD Instabilities in Helical Plasmas with Low Magnetic Shear", 24th IAEA Fusion Energy Conference, San Diego, USA, 8-13 Oct. 2012, EX/5-2.
- [2] S. Ohshima, et al., "Edge Plasma Response to Beam-driven MHD Instability in Heliotron J", 24th IAEA Fusion Energy Conference, San Diego, USA, 8-13 Oct. 2012, EX/P4-17.
- [3] T. Mizuuchi, et al., "Study of Fuelling Control for Confinement Experiments in Heliotron J", 24th IAEA Fusion Energy Conference, San Diego, USA, 8-13 Oct. 2012, EX/P3-07.
- [4] K. Nagasaki, et al., "Stabilization of Energetic-Ion-Driven MHD Mode by ECCD in Heliotron J", 24th IAEA Fusion Energy Conference, San Diego, USA, 8-13 Oct. 2012, EX/P8-10.

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 "Open Advanced Facilities to Industry" 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 as well as 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 a fixed term, i.e. 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 relatively simple 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 one year 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



DuET, the dual-ion beam irradiation facility

user may be kept undisclosed if the user so requests.

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

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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 京都府宇治市五ヶ庄
TEL 0774-38-3400 FAX 0774-38-3411