ISSN 1342-3177
IAE-AR-2022

Institute of Advanced Energy
Kyoto University

ANNUAL REPORT
2021

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

ANNUAL REPORT

2021

Institute of Advanced Energy
Kyoto University

Gokasho, Uji, Kyoto 611-0011
Japan

CONTENTS

FOREWORD

The Institute of Advanced Energy (IAE) was established in May 1996 to explore the energy systems for next generation by going back to the basic principles of nature, and to create new energy theories for the next generation and advanced technologies to lead and realize these theories. Currently, faculty members belonging to the Faculty Consort of Advanced Energy in the Natural Science Platform are engaged in 14 research sections in three divisions, each of which investigates one of the following three basic processes of energy: generation, conversion, and utilization. The institute has set up the Laboratory for Complex Energy Processes with five research sections, which supports and stimulates collaborative research to address issues related to complex energy processes.

The two core research areas of the institute are “Plasma and Quantum Energy Science” and “Soft Energy Science”. The former aims to realize nuclear fusion to generate solar energy on earth. The latter aims to achieve highly efficient energy utilization and conversion based on the principles of materials science and energy use by living organisms, which have built the biosphere on earth with solar energy. In addition to actively promoting the internationalization of research and the return of research results to society through industry–academia–government collaboration, we educate students of Liberal Arts and Science Courses and the Graduate School of Energy Science as the Cooperating Chair, foster young researchers in a front-line research environment.

The institute has been certified as a “Zero-Emission Energy” Joint Usage/Research Center by the Ministry of Education, Culture, Sports, Science and Technology (MEXT) in 2011, and has held this status for the third time, starting from the fiscal year of 2022. As the research hub of Zero-Emission Energy, we collaborate with domestic and overseas researchers over a broad spectrum of academic fields, as well as promote the share-use of cutting-edge research equipment to strengthen the foundation of academic research and to accelerate novel scientific research.

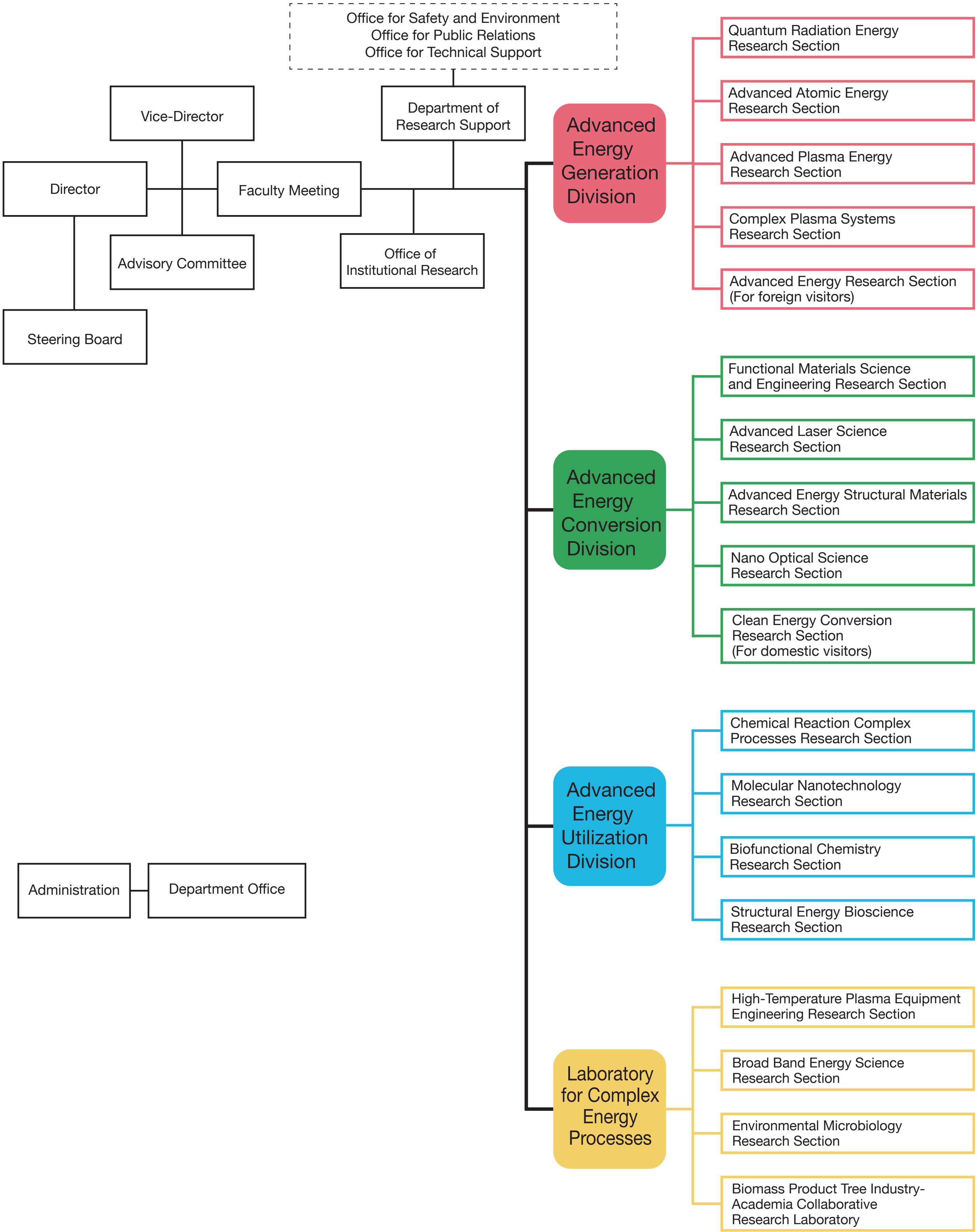
In Japan, too, the goal of “virtually eliminating greenhouse gas emission by 2050” has been set, and carbon neutrality is now a goal for societies worldwide. IAE has been committed to pursue a wide range of research aimed at Zero-Emission Energy, which will play an increasingly important role in achieving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

This annual report summarizes the key research findings at each research section of IAE for FY2021 (April 2021-March 2022). I hope you enjoy the ongoing research of our institute in a wide array of scientific disciplines that will certainly create innovative solutions to satisfy the demands to realize carbon neutrality.

March 2022

Takashi MORII
Director
Institute of Advanced Energy
Kyoto University

2. ORGANIZATION CHART



3. RESEARCH ACTIVITIES

3-1. RESEARCH ACTIVITIES IN 2021

Quantum Radiation Energy Research Section

H. Ohgaki, Professor
T. Kii, Associate Professor
H. Zen, Assistant Professor
Jordi Cravioto Caballero, Program-Specific Assistant Professor

1. Introduction

Coherent-radiation energy with a wide wavelength tunability and a high power is an indispensable tool for exploiting cutting-edge science. The research in this section aims at generating and application of new quantum-radiation energy. Free-electron laser (FEL) is one of such radiation. We have been developing a mid-infrared FEL, KU-FEL. To extend study field wider wavelength region, a coherent A compact THz source, high Tc undulator for X-ray generation, and Laser Compton Gamma-ray (LCS) for isotope imaging have been carried out. Transdisciplinary research on renewable energy has also been promoted through international collaborations.

2. Free-electron Laser

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

2.1 KU-FEL

The target wavelength of KU-FEL is MIR (Mid infra-red) regime, from 5 to 20 μm, with high-power and turnability for basic researches on energy materials. Figure 1 shows a schematic drawing of the KU-FEL system. The KU-FEL consists of a 4.5-cell thermionic RF gun, a 3-m travelling wave accelerator tube, a beam transport system, and a 1.8-m undulator and a 5-m optical resonator. The FEL device now can cover the wavelength range from 3.4 to 28 μm. The maximum macro-pulse energy which can provide is around 40 mJ in a 2-μs macro-pulse at the wavelength of 4.9 μm. The FEL is routinely operated and opened for internal and external users.

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

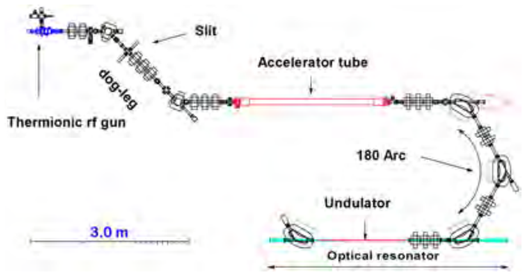


Fig. 1 Schematic drawing of the KU-FEL

2.2 THz Coherent Undulator Radiation Source

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

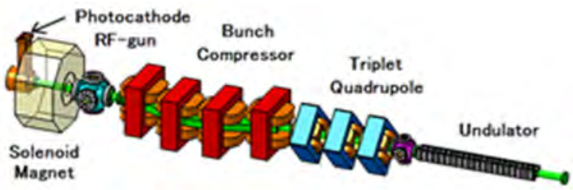


Fig. 2 3D image of THz coherent undulator radiation source.

The 1.6 cell RF gun used for the THz-CUR was replaced with an energy chirping cell attached RF gun for improving its performance under collaboration with Dr. Sakaue, Tokyo University. The gun utilizes a velocity bunching scheme for generating ultra-short electron bunch. A commissioning experiment has been done and the saturation of THz peak power due to the space charge effect can be successfully suppressed.

The polarization control method of the THz-CUR has been developed under collaboration with Dr. Kashiwagi, Tohoku University. The polarization state of the THz-CUR can be easily controlled from linear to left-handed circular and right-handed circular without significant power loss.

2.3 Application of MIR-FEL and THz-CUR

Many application researches of MIR-FEL and THz-CUR have been performed under the Joint Usage/Research Center for Zero Emission Energy Research of our Institute. In JFY2020, 14 external user groups used KU-FEL.

3. Bulk HTSC Staggered Array Undulator

An undulator with strong magnetic field will play an important role in future synchrotron light sources and FELs. We have developing a new undulator which consists of stacked bulk high critical temperature superconductors array and a solenoid magnet. As a next prototype of this type of undulator, we have developed new prototype consists of a new solenoid whose maximum field was 6 T and GM cryocooler. Periodic magnetic field using bulk MgB_2 array was demonstrated and better field uniformity than that of REBCO array was observed as shown in fig. 3.

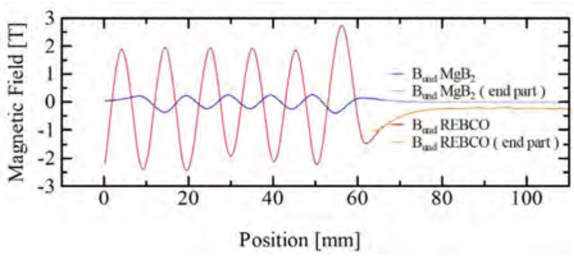


Fig. 3 Unduloator field using the MgB2 array and the REBCO array were demonstrated. Although the measured field amplitude of the MgB2 array was smaller than that of the REBCO, the field uniformity for the MgB2 array was better than that of the REBCO.

4. Isotope Imaging for Nuclear Safety and Security

A Nuclear Resonance Fluorescence (NRF) method is a powerful tool for an isotope selective

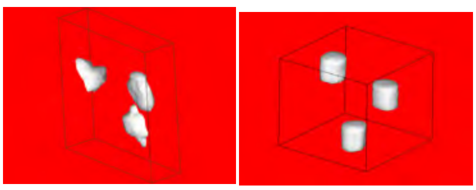


Fig. 4 Original isotope selective 3D image (left) and the fusion visualization image (right).

imaging. In 2021, we improved the image quality of the isotope selective 3D image by using a fusion visualization technique in combination with the NRF based rough CT image which provides the isotope distribution and a gamma-ray CT image which gives a high-resolution image of the CT target. A proof-of-principle experiment has been carried out at BL1U LCS beamline in UVSOR. The image quality of the original isotope (^{208}Pb) selective 3D image (Fig.4 left) was dramatically improved by the fusion visualization technique, as shown in Fig. 4 right.

5. Social aspects of energy use

Electrification projects using renewables are essential to achieve SDG7. These projects can positively influence poverty eradication and community development. Our group investigates the effects of electrification on quality of life in rural contexts of ASEAN by comparing the process and outcomes of different electrification systems (Fig. 5).

Fig. 5 Rural electrification survey sites 2016-2022

In urban contexts of ASEAN, our group also conducts analyses on household roles in connection with efficient appliance purchasing using survey data and quantitative methods. Finally, in the context of Latin America, we also study geographical and socio-cultural characterizations of household energy services.

Acknowledgment

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

Collaboration Works

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

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

大垣英明，NSTDA（タイ），JASTIP「日 ASEAN 科学技術イノベーション共同研究拠点－持続可能開発研究の推進」

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

大垣英明，Cravioto Jordi，University of Malaya（マレーシア），Fundamental Research Grant Scheme（マレーシア）

Financial Support

1. Grant-in-Aid for Scientific Research

大垣英明，基盤研究(B)，F-LCS レーザーコンプトン散乱γ線による同位体イメージングの高度化に関する研究

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

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

Cravioto Jordi，基盤研究(B)，包括的 QoL 評価法の確立：東南アジアの僻地電化における幸福度と不公平

Cravioto Jordi，若手研究，Comparative studies of culturally-based characterisation of energy services（期間延長）

2. Others

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

大垣英明，科学技術振興機構，サトウキビ収穫廃棄物の統合バイオリファイナリー

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

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

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

大垣英明，理化学研究所，次世代アンジュレータのための高温超伝導体の評価研究

Cravioto Jordi，（公財）村田学術振興財団，ＱｏＬ評価法の提案：東南アジアの僻地電化における幸福度とエネルギーの評価

Publications

A. Khaled, H. Zen, H. Ohgaki, T. Kii, T. Hayakawa, T. Shizuma, M. Katoh, Y. Taira, M. Fujimoto, H. Toyoka-wa, Fusion Visualization Technique to Improve a Three-Dimensional Isotope-Selective CT Image Based on Nuclear Resonance Fluorescence with a Gamma-CT Image, Applied Sciences, 11, 24, 11866, 2021

H. Negm, H. Zen, H. Ohgaki, Comprehensive simula-tion study on CT isotope imaging beyond the experi-ment on the 208Pb based on nuclear resonance fluores-cence, Journal of Nuclear Science and Technology, 2022

N. Sei, H. Zen, H. Ohgaki, Peak Shift of Coherent Edge Radiation Spectrum Depending on Radio Frequency Field Phase of Accelerator, Applied Sciences, 12, 2, 626, 2022

Y. Tanaka, M. Hashida, C. Hosokawa, H. Zen, T. Na-gashima, N. Ozaki, S. Inoue, S. Sakabe, Mid-infrared free electron laser induced periodic surface structures on semiconductors, Laser Applications in Microelectronic and Optoelectronic Manufacturing (LAMOM) XXVI，11673, 116730U, 2021

全炳俊，紀井俊輝，大垣英明，京都大学小型中赤外自由電子レーザ施設の開発とその利用展開，放射光，34，3，144-151，2021

全炳俊，共振器型赤外自由電子レーザーの引き出し効率とその向上，加速器，18，2，54-62，2021

全炳俊，第 8 回研究奨励賞受賞論文紹介 中赤外自由電子レーザの高性能化とその利用推進，日本赤外線学会誌，31，2，99-101，2022

Shizuma, H. Toyokawa, M. Fujimoto, Y. Taira, M. Katoh, Three-Dimensional Nondestructive Iso-tope-Selective Tomographic Imaging of 208Pb Distribu-tion via Nuclear Resonance Fluorescence, Applied Sci-ences, 11, 8, 3415, 2021

R. Garcia-Ochoa, D.I. Avila-Ortega, J. Cravioto, The Geography of unequal access to energy services in Mexican households, Terra Digitalis, 5, 1, 1, 7, 2021

J. Cravioto, E. Yamasue, D.Q. Nguyen, T.D. Huy, Benefits of a regional co-processing scheme: The case of steel/iron and cement industries in Vietnam, Laos, and Cambodia, Journal of Cleaner Production, 312, 127702, 2021

J. Cravioto, A. Mosqueda, Local Culture and Urban Retrofit: Reflections on Policy and Preferences for Wall and Roof Materials, Frontiers in Sustainable Cities, 3, 63, 2021

R. Akasegawa, H. Zen, K. Hachiya, K. Yoshida, T. Goto, T. Sagawa, H. Ohgaki, Mode-selective excitation of an infrared-inactive phonon mode in diamond using mid-infrared free electron laser, Japanese Journal of Applied Physics, 60, 10, 102001, 2021

H. Zen, H. Ohgaki, Study of the origin of the complex beam profile of a hole-coupled free electron laser oscil-lator, Journal of the Optical Society of America A-Optics Image Science and Vision, 38, 11, 1656, 1661, 2021

Presentations

H. Zen, H. Ohgaki, R. Hajima, Record High Extraction Efficiency of Free Electron Laser Oscillator, IPAC2021, Online, 2021.5.28

全炳俊， 中赤外自由電子レーザの高性能化とその利用推進，日本赤外線学会第 89 回定例研究会, Online, 2021.6.4

K. Ali, H. Ohgaki, H. Zen, T. Kii, T. Hayakawa, T. Shi-zuma, H. Toyokawa, Y. Taira, M. Fujimoto, M. Katoh, Proposal study for the fused visualization technique of 3D NRF-CT and a high-resolution gamma-CT image, 3rd International Conference on Nuclear Photonics (NP2020), Online, 2021.6.9

T. Hayakawa, H. Zen, K. Kawase, M. Fujimoto, T. Shi-zuma, J. K. Koga, R. Hajima, T. Kii, H. Ohgaki, M. Katoh, Delbruck scattering using linearly polarized gamma-rays generated by laser Compton scattering at UVSOR-III, 3rd International Conference on Nuclear Photonics (NP2020), Online, 2021.6.9

Anugerah Yuka Asmara, AR. Rohman Taufik Hidayat, H. Ohgaki, T. Mitsufuji, J. Cravioto Caballero, Utilization of Solar and Wind Energy to Increase Quality of Life for Rural Communities in Blora Regency - Indonesia: From Triple Helix to Quadruple Helix, 5th International Con-ference on Planning in the Era of Uncertainty, "Rural Urban Connectivity, Online, 2021.7.19

J. Cravioto, On The Use of Hard Data in Energy-Related Research from Social Science and Humanities, 未踏科学研究ユニット報告会 2021, Online, 2021.7.24

Jordi Cravioto，大垣英明，Mark Napao，Joseph Quinones, Household lighting and quality of life in rural Philippines:the effect of PV lamps use in non-electrified communities of Tanay，第 40 回エネルギー･資源学会研究発表会, Online, 2021.8.3

Chansatya Meas，大垣英明，Jordi Cravioto, Gender Inequality in Renewable Energy Policy，第 40 回エネルギー・資源学会研究発表会, Online, 2021.8.3

全炳俊， 常伝導加速器を用いた共振器型赤外自由電子レーザの引き出し効率向上に関する研究， 第 18 回日本加速器学会年会, Online, 2021.8.11

宮島司，全炳俊，高富俊和，福田将史，梶田駿汰，島田美帆，大垣英明，羽島良一，高効率極短 FEL パルス生成のための 1.6 セル高周波電子銃の開発，第 18 回日本加速器学会年会, Online, 2021.8.11

全炳俊，大垣英明，羽島良一，京都大学小型中赤外自由電子レーザからの数サイクルパルス発生とその計測，第 18 回日本加速器学会年会，Online, 2021.8.12

全炳俊，紀井俊輝，大垣英明, 京都大学自由電子レーザ施設の現状，第 18 回日本加速器学会年会，Online, 2021.8.12

B.J.Y. Hnin, H. Zen, R. Akasegawa, K. Hachiya, K. Yoshida, H. Ohgaki, Mode-Selective Phonon Excitation Of SrTiO3 By MIR-FEL With Anti-Stokes Hyper Raman Scattering Spectroscopy, IRMMW-THz2021, Online, 2021.9.2

全炳俊，自由電子レーザ引き出し効率のリアルタイム計測に向けた二次電子放出型電荷分布モニタ開発，日本原子力学会 2021 年秋の大会，Online, 2021.9.8

K. Ali, H. Ohgaki, H. Zen, T. Kii, T. Hayakawa, T. Shi-zuma, H. Toyokawa, M. Katoh, M. Fujimoto, Y. Taira, Fused CT imaging technique to improve 3D iso-tope-selective NRF-CT image, 日本原子力学会 2021 年秋の大会, Online, 2021.9.8

J.Y.H. Bo, H. Zen, R. Akasegawa, K. Hachiya, K. Yoshida, H. Ohgaki, Anti-Stokes Hyper-Raman Scattering Spectroscopy of Strontium Titanate for Mode-Selective Phonon Excitation Using Mid-Infrared Free Electron Laser, 第 30 回（2021 年度）日本赤外線学会研究発表会, Online, 2021.10.21

清紀弘，小川博嗣，早川恭史，境武志，住友洋介，田中俊成，早川建，高橋由美子，野上杏子，山添亮，木下耀，大谷昭仁，川島雄介，金田隆，全炳俊，大垣英明，高強度コヒーレントエッジ放射光源の開発及び利用研究，第 30 回（2021 年度）日本赤外線学会研究発表会, Online, 2021.10.22

K. Ali, Y. Ogino, T. Sakamoto, C. Meas, T. Sakabe, A.Eladl, O. Eladl, J. Cravioto, K. Mukai, C. Qu, H. Ohgaki, S. Konishi, Alternative strategies for the car-bon-neutral transition to advance renewable energy sup-ply in specific Japanese manufacturing sectors, 2021 Ajou – Kyoto – Zhejiang Joint Symposium on Energy Science, Online, 2021.11.29

K. Ali, Non-destructive Inspection for the hidden isotopes using Laser Compton scattering gamma rays, 2021 Ajou – Kyoto – Zhejiang Joint Symposium on Energy Science, Online, 2021.11.29

R. Akasegawa, H. Zen, K. Yoshida, K. Hachiya, T. Goto, T. Sagawa, H. Ohgaki, Selective phonon-mode excitation with mid-infrared freeelectron laser probed by hyper-Raman scattering spectroscopy, 2021 Ajou – Kyoto – Zhejiang Joint Symposium on Energy Science, Online, 2021.11.29

H. Ohgaki, Global Energy Situation and Carbon Neutral Strategy in Japan, AUN/SEED-Net Joint Regional Conferences in Transportation, Energy and Mechanical Manufacturing Engineering, Online, 2021.12.10

H. Ohgaki, Realizing Sustainable Carbon Neutral Society 5.0, Japan case: The 6th Strategic Energy Plan & McKinsey Report, International Multidisciplinary Symposium on Contemporary Global Issues 2021, Kumamoto, 2021.12.11

J.Y.H. Bo, Hyper-Raman scattering spectroscopy of the phonons of Strontium Titanate, 2nd Japan ASEAN Collaboration Education Program (JACEP) Research Forum and Workshop, Online, 2021.12.20

H. Ohgaki, Present Status of KU-FEL and Appilcation of MIR-FEL, PCELL/CMU Meeting, Chiang Mai University, 2021.12.27

全炳俊，大垣英明，羽島良一, KU-FEL高効率発振時のパルス構造測定，第 35 回放射光学会年会放射光科学合同シンポジウム，オンライン開催, 2022.1.8

"J. Cravioto, L. Seniorita, S.M.G. Dumlao, K-K. Krishna-Murthy, C. Qu, H. Ohgaki, Household roles and efficient appliances purchasing in Indonesia and The Philippines, 第 38 回エネルギーシステム・経済・環境コンファレンス，オンライン開催, 2022.1.25

C. Meas, J. Cravioto, H. Ohgaki, Women's Leadership in Energy Transition: Cambodia's Perspectives, 第 38 回エネルギーシステム・経済・環境コンファレンス，オンライン開催, 2022.1.26

J. Cravioto, Household roles and efficient appliances purchasing in urban Indonesia and The Philippines, DASU2021 年度年度末ワークショップ，オンライン開催, 2022.3.2

H. Ohgaki, WP5: Briefing of WP5 2021 JFY, -Asia WP5 Group Workshop Integrated Biorefinery of Sugarcane Trash, Online, 2022.3.8

Ju Yoon Hnin Bo, Hyper-Raman Scattering Spectroscopy of Selective Phonon Excitation of Strontium Titanate Using Mid-Infrared Free Electron Laser, 第 28 回 FEL と High-Power Radiation 研究会, Online, 2022.3.9

全炳俊，移設先直線部における UVSOR-FEL の再立ち上げと Intracavity Laser Compton Scattering によるガンマ線発生，第 28 回 FEL と High-Power Radiation 研究会, Online, 2022.3.10

Zhao Yuhao, Simulation of a new Photocathode RF Gun in KU-FEL, 第 28 回 FEL と High-Power Radiation 研究会, Online, 2022.3.10

羽島良一，全炳俊，大垣英明, 長波長赤外 FEL パルスによるガスの放電発光，日本物理学会第 77 回年次大会，オンライン開催, 2022.3.15

柏木茂，全炳俊，坂上和之, 光共振器を用いたアンジュレータ超放射の電場重畳による高強度 THz パルス発生，日本物理学会第 77 回年次大会，オンライン開催, 2022.3.16

紀井俊輝，バルク超伝導体アンジュレータにおけるバルクソーティングによるピーク磁場強度調整，日本物理学会第 77 回年次大会，オンライン開催, 2022.3.16

H. Ohgaki, Current biogas-to electricity status, pilot case and funding opportunities, BIOGAS-TO-ELECTRICITY FOCUS GROUP DISCUSSION (FGD) IN ASEAN, オンライン開催, 2022.3.17

全炳俊，電子ビームからの超放射，日本物理学会第 77 回年次大会，オンライン開催, 2022.3.19

H. Ohgaki, Socioeconomic analysis of the integrated process, e-ASIA Workshop Integrated Biorefinery of Sugarcane Trash, Online, 2022.3.30

Advanced Atomic Energy Research Section

S. Konishi, Professor
J. Yagi, Junior Associate Professor
K. Mukai, Assistant Professor
K. Sakamoto, Specially Appointed Professor
M. Bakr, Distinguished Visiting Associate Professor

1. Introduction

Main objective of our research section is to realize advanced energy systems for the sustainable development under global environmental constraints. We have shown a Zero-emission energy scenario based on fusion energy with biomass-based recycling system where biomass waste is converted into liquid fuel or hydrogen. And further we now propose an innovative Negative emission scenario. to isolate CO_2 in the atmosphere by a carbonization process. Our research section focuses on development of hydrogen isotopes fuel circulation system, breeding blankets, fusion material R&D, feasibility study for fusion-biomass hybrid power system, conversion of biomass waste, and fusion neutron generation/measurement. Followings are main research achievements in the fiscal year of 2021.

- Hydrogen permeation quantification through a structure material and the effect of the existence of ceramic breeding material.
- Development and successful operation of liquid lithium lead droplet system for efficient recovery of hydrogen isotope using a heat and mass-transfer loop.
- Development of hydrogen isotope pumping system using proton conducting ceramics for the divertor exhaust in a fusion system.
- Upgrade of a compact fusion neutron source for radiography

2. Hydrogen permeation through structural material

Understanding the permeation behavior of tritium from a pebble bed breeding blanket is essential for establishing a self-sufficient fuel cycle in a nuclear fusion reactor. It is known that double corrosion layers forms on reduced activation ferritic-martensitic (RAFM) steel surface by gas release from a ceramic breeder material, however, its effect on hydrogen permeation behavior has not been elucidated. In-situ measurement of hydrogen permeation through an F82H RAFM wall of a ceramic breeder pebble bed was performed using a new experimental set-up (Fig. 1). The corrosion layer formed on the F82H sample had a dense microstructure, which reduced hydrogen permeation flux at least by one order of magnitude. The permeation reduction factors were 20–50 at the water-coolant temperature of a blanket. A self-repairing ability is expected for the surface oxide layer as the corrosion occurs spontaneously inside a breeding blanket.

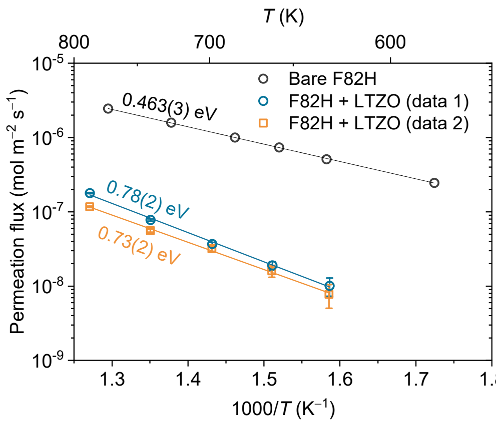


Fig. 1 Hydrogen permeation fluxes through the bare and corroded F82H samples.

3. Development of liquid lithium lead droplet system

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

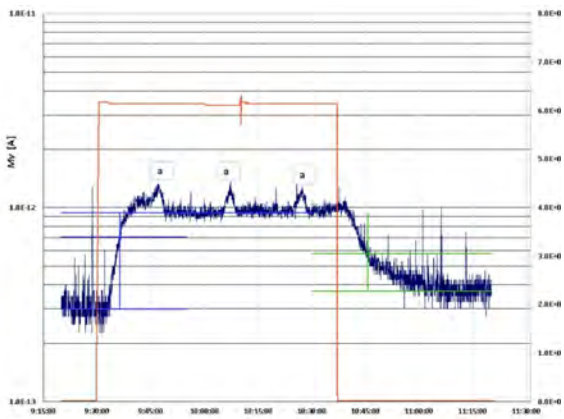


Fig.2: The hydrogen isotope recovery by VST.

loss. The vacuum sieve tray (VST) method, tritium recovery from the liquid droplet surface falling in vacuum, is a candidate developed in this section. This fiscal year, on a collaboration work with National Institute for Fusion Science (NIFS) a VST test device (multiple nozzles system) was integrated to Oroshhi-2 (Pb-Li test loop) at NIFS and the continuous operation campaign was performed in the next fiscal year. One of the recovery result for deuterium is shown in Figure 2. The deuterium fed to the loop system was successfully recovered at the VST test section.

4. Electrochemical transport of hydrogen isotopes for the diverter exhaust development

Hydrogen isotopes pumping system using a proton conducting electrolyte (ceramic) is a candidate diverter exhaust pump for a nuclear fusion system, which can selectively exhaust hydrogen isotopes (D and T) without He, reducing the tritium inventory in the tritium fuel cycle system.

BYCO ($BaCe_{0.8}Y_{0.2}O_{3-\alpha}$) plate with Pt electrodes were fabricated and the hydrogen isotopes transport behavior through the plate was investigated. The experimental setup is shown in Fig.3. H_2 and D_2 containing Ar gas was fed to the outer surface of the BYCO plate, and the inner surface was wept by pure Ar gas, whose H and D concentration was monitored afterward.

The mass flux result obtained at 500℃, changing the feeding gas concentration applying 1 V, is shown in the Figure 4. The current efficiency is assumed to be around 70%, and transport of D was found to be less than that of H.

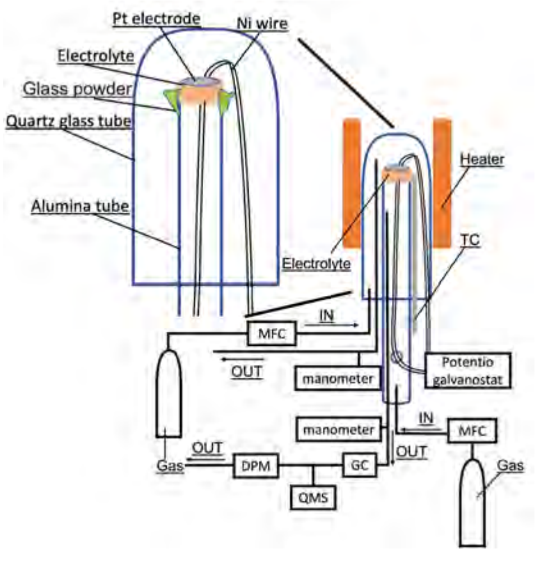


Fig.4: The experimental setup of the hydrogen isotopes pumping system using BYCO plate.

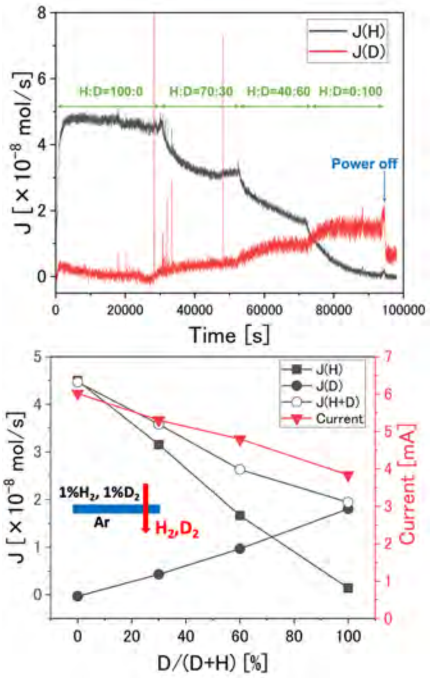


Fig.4: The H and D transport behavior at 500 ℃ trend (upper) and the quasi-steady state analysis (lower)

5. Compact fusion neutron source for radiography

Development of a compact neutron source with a higher neutron production rate is of importance for a wide range of its application, including radiography and boron neutron capture therapy (BNCT). A three-stage feedthrough system is employed in the developed compact IEC to address this contradiction. A feedback control system was developed and applied to the input and output parameters. Characterization of the developed system was performed by scanning the neutron yield as a function of applied voltage and cathode current. To date, a maximum neutron yield of 9.2×10^7 $n \cdot s^{-1}$ at 6.4 kW (80 kV and 80 mA) has been obtained. Neutron images (Fig. 5) showed there was good a contrast between the sample and the background. The results suggest that optimization of the experimental parameters is needed to perform higher accuracy neutron radiography.

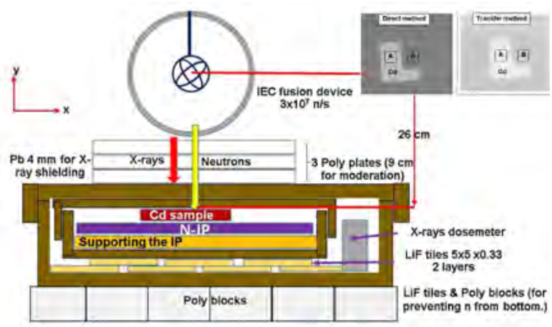


Fig.5 Experimental layout and neutron images by direct method and transfer method.

Collaboration Works

小西哲之，八木重郎，核融合科学研究所・LHD 計画共同研究，ヘリカル炉液体ブランケットトリチウム回収プロセスの基礎工学研究

八木重郎，University of California San Diego（アメリカ），SiC/SiC 複合材料で製作した配管試験体を流動液体金属（PbLi）に曝露し、その腐食特性を調べる

八木重郎，向井啓祐，小西哲之，核融合科学研究所・一般共同研究，高融点鉛リチウム金属間化合物を用いた水素移行に関する基礎研究

八木重郎，量子科学技術研究開発機構・原型炉開発共同研究，液体リチウム流動ループにおける窒素回収

向井啓祐，小西哲之，八木重郎，核融合科学研究所・一般共同研究，LHD 本体室における中性子線量の制御による核融合炉ブランケットの高性能化

Financial Support

1. Grant-in-Aid for Scientific Research

八木重郎，基盤研究(B)，核融合炉ブランケットにおける水素・腐食・照射相乗効果の解明と機能性材料設計（分担金）

向井啓祐，若手研究，核融合ブランケットの中性子輸送と燃料生産性の実験評価

向井啓祐，基盤研究(B)，特殊な電圧プロファイル下の電気透析による６リチウム同位体濃縮技術の研究（分担金）

向井啓祐，基盤研究(B)，核融合炉ブランケットにおける水素・腐食・照射相乗効果の解明と機能性材料設計（分担金）

荻野靖之，特別研究員奨励費，核融合炉ブランケットの中性子輸送とトリチウム増殖現象の実験解析の研究

2. Others

小西哲之，核融合科学研究所，高速応答原型炉燃料サイクルとプロトンポンプフロントエンド

小西哲之，京都フュージョニアリング（株），原子力エネルギー変換装置の設計と解析

小西哲之，京都フュージョニアリング（株），マイクロ波を用いたバイオマスガス化技術開発

八木重郎，量子科学技術研究開発機構，液体リチウム流動ループ中での窒素トラップの健全性評価

向井啓祐，科学技術振興機構，精製・リサイクルの循環型サプライチェーンの導入により想定される国際経済波及効果、並びに資源・環境影響評価に関する国立大学法人京都大学による研究開発

Publications

S. Miura, K. Nakamura, E. Akahoshi, S. Kano, J. Yagi, Y. Hishinuma, T. Tanaka, T. Chikada, Lithium-lead corrosion behavior of zirconium oxide coating after heavy-ion irradiation, Fusion Engineering and Design, 170, 112536, 2021

K. Kubo, K. Katayama, M. Oya, K. Tsukahara, S. Fukada, T. Tanaka, A. Sagara, J. Yagi, Y. Iinuma, Tritium release behavior from neutron-irradiated FLiNaBe mixed with titanium powder, Fusion Engineering and Design, 171, 112558, 2021

Y. Ogino, K. Mukai, S. Konishi, Simulations for practical measurement methods of spatial neutron distribution inside blanket mock-up irradiated with DT neutrons, Fusion Engineering and Design, 168, 112417, 2021

H. Matsuura, T. Suganuma, Y. Koga, M. Naoi, K. Katayama, T. Otsuka, M. Goto, S. Nakagawa, S. Hamamoto, E. Ishitsuka, K. Tobita, S. Konishi, R. Hiwatari, Y. Someya, Y. Sakamoto, The T-containment properties of a Zr-containing Li rod in a high-temperature gas-cooled reactor as a T production device for fusion reactors, Fusion Engineering and Design, 169, 112441, 2021

M. Bakr, K. Mukai, K. Masuda, J. Yagi, S. Konishi, Characterization of an ultra-compact neutron source based on an IEC fusion device and its prospective applications in radiography, Fusion Engineering and Design, 167, 112346, 2021

R. Omura, J. Yagi, K. Mukai, M. Oyaidzu, K. Ochiai, A. Kasugai, S. Konishi, Analysis of nitrogen distribution in iron-titanium alloys after nitrogen trapping in liquid lithium by using soft X-ray emission spectroscopy, Fusion Engineering and Design, 170, 112548, 2021

T. Chikada, M.H.H. Kolb, H. Fujita, K. Nakamura, K. Kimura, M. Rasinski, Y. Hishinuma, K. Mukai, R. Knitter, Compatibility of tritium permeation barrier coatings with ceramic breeder pebbles, Corrosion Science, 182, 109288, 2021

M.M. Islam, M. Bakr, J.N. Aboa, F.A. Selim, New thermally stimulated emission spectrometer for the detection of ultra-shallow low-density traps, Journal of Applied Physics, 130, 3, 33104, 2021

X. Wu, S. Kondo, H. Yu, Y. Okuno, M. Ando, H. Kurotaki, S. Tanaka, K. Hokamoto, R. Ochiai, S. Konishi, R. Kasada, Bonding strength evaluation of explosive welding joint of tungsten to ferritic steel using ultra-small testing technologies, Materials Science and Engineering A-Structural Materials Properties Microstructure and Processing, 826, 141995, 2021

H. Nam, S. Konishi, K.W. Nam, Comparative analysis of decision making regarding nuclear policy after the Fukushima Dai-ichi Nuclear Power Plant Accident: Case study in Germany and Japan, Technology in Society, 67, 101735, 2021

S. Kenjo, Y. Ogino, K. Mukai, M. Bakr, J. Yagi, S. Konishi, Employing of ZrCo as a fuel source in a discharge-type fusion neutron source operated in self-sufficient mode, International Journal of Hydrogen Energy, 47, 5, 3054-3062, 2022

K. Mukai, S. Kenjo, N. Iwamatsu, B. Mahmoud, T. Chikada, J. Yagi, S. Konishi, Hydrogen permeation from F82H wall of ceramic breeder pebble bed: The effect of surface corrosion, International Journal of Hydrogen Energy, 47, 9, 6154-6163, 2022

S. Miura, K. Nakamura, E. Akahoshi, S. Kano, J. Yagi, Y. Hishinuma, T. Tanaka, T. Chikada, The synergy of heavy-ion irradiation and lithium-lead corrosion on deuterium permeation behavior of ceramic coating, Nuclear Materials and Energy, 30, 101109, 2022

Y. Koga, H. Matsuura, K. Katayama, T. Otsuka, M. Goto, S. Hamamoto, E. Ishitsuka, S. Nakagawa, K. Tobita, S. Konishi, R. Hiwatari, Y. Someya, Y. Sakamoto, Effect of nuclear heat caused by the 6Li(n,α)T reaction on tritium containment performance of tritium production module in High-Temperature Gas-Cooled reactor for fusion reactors, Nuclear Engineering and Design, 386, 111584, 2022

小西哲之，CO2 はどこへ行くのか？ 炭素循環から考える気候変動，ＰＨＰ研究所，2021

Presentations

Y. Urano, K. Hata, R. Orito, S. Kurosawa, K. Fushimi, S. Konishi, M. Bakr, K. Mukai, Measurement of scintillation response by fast neutron, 第 12 回エネルギー理工学研究所国際シンポジウム, Online, 2021.9.7

K. Ali, A. Eladl, Y. Ogino, T. Sakamoto, C. Meas, T. Sakabe, O. Eladl, J. Cravioto, K. Mukai, C. Qu, K. Ueda, S. Konishi, H. Ohgaki, Carbon-neutral transitions: An evaluation of industrial strategies to advance renewable energy supply in some sectors of the Japanese manufacturing, 第 12 回エネルギー理工学研究所国際シンポジウム, Online, 2021.9.7

S. Takayama, K. Mukai, J. Yagi, Development of a method for compsiting Li_2TiO_3 and nanocarbon by microwave irradiation, 第 12 回エネルギー理工学研究所国際シンポジウム, Online, 2021.9.7

K. Sasaki, K. Mukai, K. Shin-mura, H. Takahashi, R. Tokuyoshi, I. Takahashi, R. Kasada, Analysis of element distribution changes in solid lithium electrolyte generated by electrodialysis using rf-GD-OES, 第 12 回エネルギー理工学研究所国際シンポジウム，Online, 2021.9.7

I. Takahashi, E. Kaji, T. Watanabe, K. Sasaki, K. Mukai, Study of material development and interface design for all-solid- state Li ion battery, 第 12 回エネルギー理工学研究所国際シンポジウム, Online, 2021.9.7

A. Miyashita, K. Mukai, S. Ohshima, R. Matoike, B.J. Peterson, S. Kobayashi, H. Okada, S. Kado, T. Minami, T. Mizuuchi, S. Konoshima, K. Nagasaki, First Application of Infrared Imaging Video Bolometer to Neutral Beam Injected Plasma in Heliotron J, 第12回エネルギー理工学研究所国際シンポジウム, Online, 2021.9.7

S. Konishi, R. Pearson, T. Hinoki, K. Mukai,d T. Nagao, Development of self–cooled SiC composite–LiPb high temperature blanket system, 20th International Conference on Fusion Reactor Materials (ICFRM-20), Online, 2021.10.24-29

K. Mukai, R. Knitter, T. Hoshino, T. Terai, S. Kenjo, N. Iwamatsu, T. Chikada, J.o Yagi, S. Konishi, Structural analysis and chemical behavior of tritium breeding materials, 20th International Conference on Fusion Reactor Materials (ICFRM-20), Online, 2021.10.24-29

J. Yagi, R. Omura, K. Mukai, M. Oyaidzu, K. Ochiai, A. Kasugai, S. Konishi, Nitrogen trapping in flowing liquid lithium using Fe-Ti alloy pebble, 20th International Conference on Fusion Reactor Materials (ICFRM-20), Online, 2021.10.24-29

S. Kenjo, Y. Ogino, K. Mukai, M. Bakr, J. Yagi, S. Konishi, Self–sufficient system for a compact discharge–type fusion neutron source using ZrCo as a fuel source, 20th International Conference on Fusion Reactor Materials (ICFRM-20), Online, 2021.10.24-29

小西哲之，向井啓祐，八木重郎，山口修平，世古圭, 原型炉ダイバータのためのトリチウム排気ポンプシステム, 第 38 回 プラズマ・核融合学会 年会, オンライン開催, 2021.11.22-25

坂本慶司, 平田洋介, 小田靖久, 高橋良和, 西正孝, リチャード・ピアソン, 世古圭, 今井隆志, 長尾 昂, 小西哲之, 京都フュージョニアリングにおけるジャイロトロン開発, 第 38 回 プラズマ・核融合学会年会 , オンライン開催, 2021.11.22-25

坂部俊郎，見城俊介，荻野靖之，向井啓祐，マハムド バクル，八木重郎，小西哲之, 核融合放電中性子源の電極コーティングが中性子発生率に及ぼす影響, 第 38 回プラズマ・核融合学会年会，オンライン開催, 2021.11.22-25

松尾拓海，見城俊介，向井啓祐，八木重郎，小西哲之，燃料閉じ込め式放電型核融合中性子源における水素同位体交換挙動の分析，第 38 回 プラズマ・核融合学会年会，オンライン開催, 2021.11.22-25

法月亮介，田中照也，能登裕之，八木重郎，菱沼良光，芦川直子，近田拓未, セラミックー鉄接合被覆の重水素透過挙動およびリチウム鉛中腐食挙動, 第 38 回プラズマ・核融合学会年会，オンライン開催, 2021.11.22-25

三浦颯太，中村和貴，赤星江莉加，八木重郎，菱沼良光，田中照也，近田拓未, 機能性セラミックス被覆の重水素透過挙動に対する照射ー腐食相乗効果, 第 38 回 プラズマ・核融合学会年会，オンライン開催, 2021.11.22-25

S. Konishi, K. Mukai, J. Yagi, S. Yamaguch, K. Sakamoto, K. Seko, T. Imai, R. Pearson,T. Nagao, Development of Tritium Compatible Pumping Train for Plasma Exhausts, 29th IEEE Symposium on Fusion Engineering (SOFE), Online, 2021.12.12-16

K. Sakamoto, Y. Hirata, Y. Oda, S. Hara, T. Yoshida, M. Okada, A. Takeshima, Y. Takahashi, M. Nishi, K. Mukai, R. Pearson, K. Seko, T. Nishino, Y. Yoshioka, T. Imai, T. Nagao, S. Konishi, Activities of gyrotron development at Kyoto Fusioneering in Japan, 29th IEEE Symposium on Fusion Engineering (SOFE), Online, 2021.12.12-16

Y. Ogino, S. Kenjo, T. Sakabe, K. Mukai, M. Bakr, J. Yagi, S. Konishi, Measurements of neutron spatial distribution divided into specific energy regions inside a blanket mock-up, 29th IEEE Symposium on Fusion Engineering (SOFE), Online, 2021.12.12-16

T. Sakabe, S. Kenjo, Y. Ogino, K. Mukai, M. Bakr, J. Yagi, S. Konishi, Effects of metal hydride coatings on neutron production rate at electrodes surface in a discharge-type fusion neutron source, 29th IEEE Symposium on Fusion Engineering (SOFE), Online, 2021.12.12-16

Y. Murata, J. Yagi, K. Mukai, S. Konish, Solubility of Bi in Li-Pb eutectic alloy between 508 and 623 K, 29th IEEE Symposium on Fusion Engineering (SOFE), Online, 2021.12.12-16

S. Yamaguchi, K. Mukai, J. Yagi, S. Konishi, Evaluation of hydrogen isotope transport performance using proton conductor for divertor pumping system, 29th IEEE Symposium on Fusion Engineering (SOFE), Online, 2021.12.12-16

M. Bakr, T. Sakabe, J-. Wulfkuehler, K. Mukai, T. Wallace-Smith, Y. Ogino, M. Tajmar, T. Scott, S. Konishi, Influence of electrodes geometrical properties on the neutron production rate of a discharge fusion neutron source, 29th IEEE Symposium on Fusion Engineering (SOFE), Online, 2021.12.12-16

R. Pearson, C. Baus, S. Konishi, K. Mukai, T. Imai, T. Nagao, K. Sakamoto, K. Seko, S. Takeda, Overview of Kyoto Fusioneering's SCYLLA© (Self-Cooled Yuryo Lithium-Lead Advanced) blanket for commercial fusion reactors, 29th IEEE Symposium on Fusion Engineering (SOFE), Online, 2021.12.12-16

向井啓祐, SXES による核融合材料の分析, 第 4 回 SXES スクール日本電子㈱, オンライン開催, 2022.1.19

S. Konishi, T. Hinoki, K. Mukai, R. Pearson, C. Baus, T. Nagao, Fusion Blanket systems based on advanced SiCf/SiC composite with LiPb for near term commercial fusion reactors, 46th International Conference and Expo on Advanced Ceramics and Composites (ICACC2022), Online, 2022.1.24-28

荻野靖之，核融合ブランケット模擬体系内部における放射化箔・イメージングプレートを用いた中性子空間分布計測手法の研究，日本原子力学会関西支部「第 17 回若手研究者による研究発表会」，オンライン開催, 2022.3.10

坂部俊郎，放電型核融合中性子源の電極コーティングが中性子発生率に及ぼす影響，日本原子力学会関西支部「第 17 回若手研究者による研究発表会」, オンライン開催, 2022.3.10

向井啓祐，八木重郎，小西哲之,，パルスレーザーを用いたリチウムセラミックス微小球の製造，日本セラミックス協会 2022 年年会，オンライン開催, 2022.3.10-12

田宮裕之，八木重郎，向井啓祐，小西哲之， 高山定次，二酸化チタン共存下におけるセルロースのガス化におけるマイクロ波効果，日本セラミックス協会 2022 年年会，オンライン開催, 2022.3.10-12

小西哲之，京都フュージョニアリング株式会社による核融合産業化，日本原子力学会 2022 年春の年会，オンライン開催, 2022.3.16-18

興野文人，浜地志憲，田中照也，八木重郎，小西哲之，液体金属テストループ(オロシー2)によるリチウム鉛からのトリチム連続回収試験結果報告，日本原子力学会 2022 年春の年会，オンライン開催, 2022.3.16-18

松田洋樹，萩原雅之，竹内章博，糸賀俊朗，小西哲之，3GeV 次世代放射光施設における放射光による遮蔽設計，日本原子力学会 2022 年春の年会，オンライン開催, 2022.3.16-18

興野文人，浜地志憲，田中照也，八木重郎，小西哲之，液体金属テストループ(オロシー2)によるリチウム鉛からの水素同位体連続回収試験結果報告，NIFS 研究会「原型炉に向けた炉内機器・材料・システム統合研究会」「横断的研究のための COE 共同研究プラットフォーム・Oroshhi-2 の利用検討会」共同研究会，オンライン開催, 2022.3.18

村田勇斗，八木重郎，向井啓祐，小西哲之，核融合炉液体ブランケット材料 Li–Pb における Bi 不純物の溶解挙動に関する研究, NIFS 研究会「原型炉に向けた炉内機器・材料・システム統合研究会」「横断的研究のための COE 共同研究プラットフォーム・Oroshhi-2 の利用検討会」共同研究会，オンライン開催, 2022.3.18

Advanced Plasma Energy Research Section

K. Nagasaki, Professor
S. Kobayashi, Associate Professor

1. Introduction

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

In this report, a remarkable result obtained in the Heliotron J experimental study in FY2020 is reported focusing on transport characteristics regarding magnetic configurations, including the magnetic island effect, especially in (1) characteristics of edge plasmas inside the magnetic island, (2) measurement of radial electric field and its dependence on rotational transform profile and (3) development of beam emission spectroscopy for turbulent fluctuation measurement.

2. Characteristics of edge plasmas inside magnetic island based on Langmuir Probe measurements

Plasma transport in the magnetic island is gaining importance in stellarator/heliotron and tokamak devices. Heliotron J can control the width and the position of magnetic islands by controlling the rotational transformation. Therefore, the effects of the magnetic island structure on transport and turbulent fluctuations can be systematically investigated.

We measured a magnetic island around the last closed flux surface (LCFS) with a Langmuir probe. The connection length of the magnetic field in the measurement range of the probe and the electron temperature profiles are shown in Figure 1(a) and (b). The horizontal axis is the distance from the LCFS. In the case without the magnetic island, the electron temperature decreases monotonically as the connection length decreases outside the LCFS. However, in the case of the magnetic island, there is a peak in the electron temperature profile in the magnetic island region outside the LCFS, where the connection length is in the same order of the confinement region.

To investigate the effect of the magnetic island on the heat transport, the ECH was modulated (frequency of 100 Hz and modulation amplitude of 30%), and the response was observed. As shown in Figure 1(c), the phase inside the magnetic island, determined from the response time to the pre-programmed modulation heating, is delayed compared to the outer edge of the island. This may reflect the closed magnetic field line structure in the magnetic island region, which inhibits the propagation of heat into the island. It was shown that the magnetic island structure in the edge region affects the heat transport in the edge region and that heating modulation is a useful tool for investigating the magnetic field structure outside the LCFS.

3. Measurement of radial electric field using Doppler reflectometer and its dependence on rotation transform profile

The radial electric field structure has a significant effect on the performance of the plasma confinement. The shear of the radial electric field E_r at the peripheral region causes $\boldsymbol{E}_r \times \boldsymbol{B}$ drift, and flow generated by the drift may suppress turbulence by tearing off large vortices in the plasma. Because the plasma confinement in Heliotron J has been dependent on the rotational transform, it is important to investigate the relationship between the radial electric field and the confinement. In this study, we investigated the dependence of

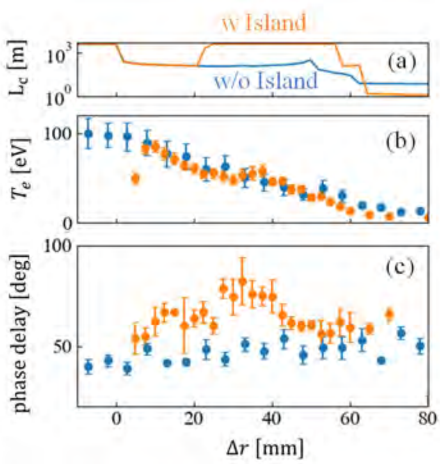


Fig. 1 Profiles of (a) connection length, (b) electron temperature and (c) phase delay with and without the magnetic island.

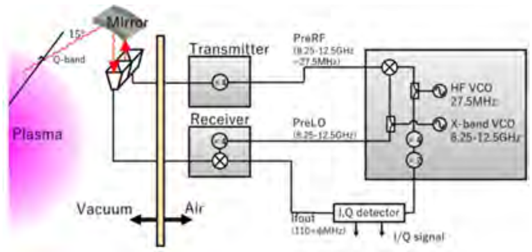


Fig. 2. Schematic diagram of the reflectometer system.

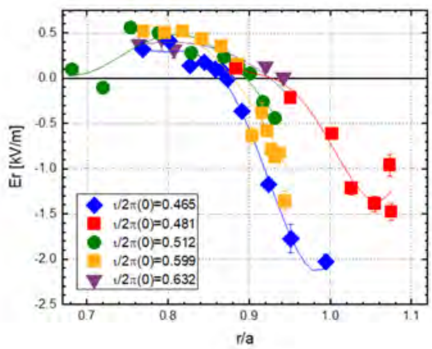


Fig. 3. Radial electric field and its dependence on rotational transform profile.

the spatial profile of the radial electric field contributing to the confinement performance on the magnetic field configuration in ECH plasmas by scanning the rotational transform. We used a microwave Doppler reflectometer to measure the radial electric field. A schematic diagram is shown in Fig. 2.

The spatial profile of the radial electric field for each rotational transformation obtained by reflectometer is shown in Fig. 3. The horizontal axis represents the normalized minor radius of the torus, and the vertical axis represents the radial electric field. Almost all configurations, a positive radial electric field with a flat profile can be seen inside r/a = 0.9, while a significant radial electric field shear is generated at the peripheral region. The position of the radial electric field shear shifts significantly outward at $\iota/2\pi(0)$ = 0.481. Since it is known that magnetic islands are generated at the peripheral plasma region in the magnetic configuration, the existence of the magnetic island may affect the radial electric field structure at the peripheral region.

4. Development of beam emission spectroscopy for turbulent fluctuation measurement in peripheral region

The transport by fluctuations is considered one of the key factors that deteriorate the plasma confinement performance. The density fluctuations have been measured in Heliotron J using beam emission spectroscopy (BES). The BES has been a great advantage for understanding the physics of MHD activities and long-wavelength plasma turbulence. In the numerical calculation for the turbulent transport of Heliotron J, the intensity of turbulent fluctuations is considered to be in the order of $\tilde{n}/n \sim 0.1\%$. The previous studies have shown that detectable intensity level of the density fluctuation was in the order of 1%, and it requires the BE intensity up to three times higher than the current system. This study aims to construct a new BES system that can measure turbulent fluctuations. Since the intensity of turbulent fluctuations outside the torus is expected to be higher and the new sightlines are nearer observation area, the new BES system are expected to measure turbulent fluctuations.

To investigate the favorable sightlines for Heliotron J configuration, we have simulated the BE intensity using a numerical model calculation. This code can calculate the spatial and spectral profile of the beam emission deduced from the collisional excitation model between the electrons/ions and the neutral beam atoms in plasmas deduced from the beam trajectory analysis using Monte Carlo method. The new BES sightlines are shown in Fig. 4(a). The sightlines are 5(radial) × 4(poloidal) = 20 channel. The spatial pitch between sightlines is 10 mm. The measurable wave number range $k_\perp\rho$ is estimated to be smaller than 0.42 in the standard parameter of Heliotron J plasmas. Fig. 4(b) shows the radial profile of beam emission intensity. As a result, higher beam intensity can be expected at the peripheral area using new sightlines.

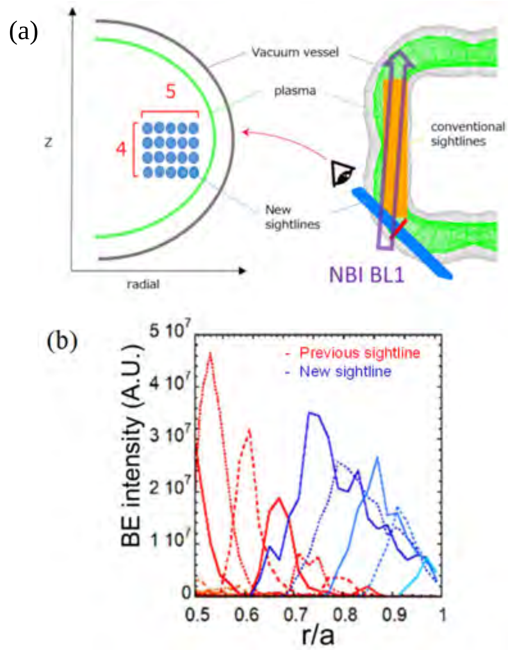


Fig. 4. (a) Schematic illustration of the BES sightlines. The new sightlines are designed to observe density fluctuations at peripheral region. (b) Radial profile of the calculated BE intensity.

Collaboration Works

長﨑百伸，小林進二，南貴司，大島慎介，Univ. Wisconsin（アメリカ），Oak Ridge National Laboratory（アメリカ），Max Plank Institute（ドイツ），Stuttgart Univ（ドイツ），CIEMAT（スペイン），Australian National Univ.，（オーストラリア），Kharkov Institute（ウクライナ），Southwest Institute of Physics（中国），先進ヘリカルシステムにおける周辺プラズマ・ダイバータ研究

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

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

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

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

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

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

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

門信一郎，小林進二，核融合科学研究所・双方向型共同研究，磁場閉じ込めプラズマにおける複合粒子補給制御を用いた高密度化（GAMMA 10/PDX における複合粒子制御法を用いた ELM 模擬）

Financial Support

1. Grant-in-Aid for Scientific Research

長﨑百伸，基盤研究(B)，高密度プラズマ輸送解析に向けた電子バーンスタイン放射計測に関する研究

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

2. Others

長﨑百伸，日本学術振興会研究拠点形成事業（A），磁場の多様性が拓く超高温プラズマダイナミクスと構造形成の国際研究拠点形成

長﨑百伸，（株）日立製作所，核融合研究に対する研究助成

長﨑百伸，自然科学研究機構，2021 年度双方向型共同研究

Publications

S. Ohshima, P. Zhang, H. Kume, C. Deng, A. Miyashita, S. Kobayashi, H. Okada, T. Minami, S. Kado, P. Adulsiriswad, D. Qiu, M. Luo, R. Matoike, T. Suzuki, S. Konoshima, T. Mizuuchi, K. Nagasaki, Development of a multi-channel 320 GHz interferometer for high density plasma measurement in Heliotron J, Review of Scientific Instruments, 92, 053519, 2021

S. Kobayashi, S.T.A. Kumar, F.S.B. Anderson, C.B. Deng, K.M. Likin, J.N. Talmadge, S. Ohshima, D.T. Anderson, Development of beam emission spectroscopy in the helically symmetric experiment stellarator, Review of Scientific Instruments, 92, 063503, 2021

A. Miyashita, K. Mukai, S. Ohshima, R. Matoike, B.J. Peterson, S. Kobayashi, H. Okada, S. Kado, T. Minami, T. Mizuuchi, S. Konoshima, K. Nagasaki, First Application of an InfraRed Imaging Video Bolometer to Heliotron J Plasma, Plasma and Fusion Research, 16, 1202079, 2021

S. Kobayashi, K. Nagasaki, K. Hada, T. Stange, H. Okada, T. Minami, S. Kado, S. Ohshima, K. Tokuhara, Y. Nakamura, A. Ishizawa, Y. Suzuki, M. Osakabe, T. Murase, S. Konoshima, T. Mizuuchi, Role of pre-ionization in NBI plasma start-up of Heliotron J using non-resonant microwave heating, Nuclear Fusion, 11, 11, 116009, 2021

P. Adulsiriswad, Y. Todo, S. Kado, S. Yamamoto, S. Kobayashi, S. Ohshima, H. Okada, T. Minami, Y. Nakamura, A. Ishizawa, S. Konoshima, T. Mizuuchi, K. Nagasaki, Numerical investigation of the peripheral energetic particle driven MHD modes in Heliotron J with free boundary hybrid simulation, Nuclear Fusion, 61, 11, 116065, 2021

R. Matoike, G. Kawamura, S. Ohshima, Y. Suzuki, M. Kobayashi, S. Masuzaki, S. Kobayashi, S. Kado, T. Minami, H. Okada, T. Mizuuchi, S. Konoshima, Y. Feng, H. Frerichs, K. Nagasaki, Numerical analysis of heat load distribution in Heliotron J with magnetic field tracing and plasma transport modeling, Plasma Physics and Controlled Fusion, 63, 11, 115002, 2021

M. Yoshikawa, J. Kohagura, N. Ezumi, T. Iijima, K. Nojiri, A. Terakado, Y. Nakashima, T. Kariya, T. Numakura, M. Hirata, R. Minami, M. Sakamoto, M. Ichimura, M.S. Islam, Y. Shima, R. Yasuhara, I. Yamada, H. Funaba, T. Minami, N. Kenmochi, D. Kuwahara, H.J. van der Meiden, Study of detached plasma profile in the divertor simulation experimental module of tandem mirror GAMMA 10/PDX, AIP Advances, 11, 12, 125231, 2021

K. Nagasaki, Y. Kato,,Y. Oka, H. Igami,T. Minami, S. Kado, S. Kobayashi, S. Ohshima, Y. Nakamura, A. Ishizawa, T. Mizuuchi, H. Okada, S. Konoshima, R. Matoike, A. Iwata, M.Luo, P. Zhang, C. Wang, Y. Kondo, N. Marushchenko, Electron temperature measurement using electron bernstein emission in Heliotron J, 47th EPS Conference on Plasma Physics, EPS 2021, 2021-June, 1016, 1019, 2021

Presentations

K. Nagasaki, S. Ohshima, T. Minami, M. Miyoshi, S. Yamamoto, H. Okada, S. Kado, S. Kobayashi, S. Konoshima, T. Mizuuchi, Y. Kishimoto, Y. Nakamura, A. Ishizawa, P. Adulsiriswad, D. Qiu, M. Luo, Á. Cappa, K. Wang, N. Smith, Effect of Magnetic Configuration on Energy Confinement and Energetic-Particle-Driven MHD Modes in Heliotron J, 28th IAEA Fusion Energy Conference, Online, 2021.5.10-15

S. Ohshima, H. Okada, S. Kobayashi, T. Minami, S. Kado, P. Adulsiriswad, D. Qiu,M. Luo, R. Matoike, S. Yamamoto, Y. Nakamura, S. Konoshima, T. Mizuuchi, K. Nagasaki, Turbulent Properties Against Hydrogen Isotope Ratio and Zonal Flow Activities in Heliotron J, 28th IAEA Fusion Energy Conference, Online, 2021.5.10-15

S. Kobayashi, K. Nagasaki, K. Hada, T. Stange, K. Tokuhara, S. Ohshima, H. Okada,T. Minami, S. Kado, H. Ohgaki, T. Kii, H. Zen, Y. Nakamura, A. Ishizawa,Y. Suzuki, M. Osakabe, T. Murase, Y. Kishimoto, S. Konoshima, T. Mizuuchi, Study of NBI plasma start-up assisted by seed-plasma generation using non-resonant microwave heating in Heliotron J, 28th IAEA Fusion Energy Conference, Online, 2021.5.10-15

M. Osakabe, H. Takahashi, K. Mukai, H. Yamada, T. Kobayashi, K. Ida, S. Ohdachi, K. Ogawa, M. Kobayashi, S. Kamio, S. Murakami, S. Inagaki, K. Tanaka, M. Sakamoto, S. Masuzaki, K. Nagasaki, Y. Suzuki, M. Isobe, T. Morisaki and LHD experiment group, Recent results of Deuterium Experiment on the Large Helical Device and its contribution to the fusion reactor development, 28th IAEA Fusion Energy Conference, Online, 2021.5.10-15

T. Kariya, R. Minami, T. Imai, T. Numakura, F. Motoyoshi, Y. Endo, H. Idei,T. Onchi, S. Kojima, K. Hanada, T. Shimozuma, S. Kubo, M. Ono, K. Nagasaki, T. Eguchi, Y. Mitsunaka, M. Sakamoto, Development of 28/35 GHz Dual-Frequency and 14 GHz Gyrotrons for Advanced Fusion Devices, 28th IAEA Fusion Energy Conference, Online, 2021.5.10-15

H. Takahashi, H. Yamada, K. Ida, K. Nagasaki, K. Tanaka, K. Mukai, K. Ogawa,M. Kobayashi, M. Osakabe, M. Isobe, M. Sakamoto, S. Murakami, S. Ohdachi,S. Inagaki, S. Kamio, S. Masuzaki, T. Kobayashi, T. Morisaki, Y. Suzuki, Recent results of Deuterium Experiment on the Large Helical Device and its contribution to the fusion reactor development, 28th IAEA Fusion Energy Conference, Online, 2021.5.10-15

Y. Kondo, S. Ohshima, K. Nagasaki, D. Kuwahara, K. Inoshita, T. Fukuda, T. Minami, S. Kado, S. Kobayashi, S. Konoshima, T. Mizuuchi, H. Okada, T. Tomita, Development of Dual X-mode Doppler Reflectometer system in Heliotron J, ECPD(European Conference on Plasma Diagnostic)2021, Online, 2021.6.7-10

K. Nagasaki, H. Igami, Y. Oka, H. Okada, T. Minami, S. Kado, S. Kobayashi, S. Ohshima, T. Mizuuchi, S. Konoshima, Y. Nakamura, A. Ishizawa, D. Qiu, R. Matoike, M. Luo, N. Marushchenko, F. Volpe, Electron Temperature Measurement Using Electron Bernstein Emission in Heliotron J, 47th EPS Conference on Plasma Physics, Online, 2021.6.21-25

J. Varela, K. Nagasaki, K. Nagaoka, S. Yamamoto, D. Spong, L. Garcia, A. Cappa, K.Y. Watanabe, Theoretical analysis of the ECH effect on the energetic particle driven modes stability in Heliotron J, 47th EPS Conference on Plasma Physics, Online, 2021.6.21-25

小林進二，永岡賢一，長﨑百伸，徳原圭一，大垣英明，紀井俊輝，全炳俊，岡田浩之，福嶋亮人，大島慎介，門信一郎，南貴司，木島滋，水内亨，ヘリオトロン型磁場配位における非共鳴波動加熱を利用した統計加速，日本物理学会 2021 年秋季大会，オンライン開催, 2021.9.20-23

加藤悠，長﨑百伸，伊神弘恵，岡佑旗，小林進二，大島慎介，門信一郎，南貴司，中村祐司，石澤明宏，木島滋，水内亨，岡田浩之，的池遼太，Heliotron J における B-X-O モード変換を用いた電子バーンシュタイン放射計測，日本物理学会 2021 年秋季大会，オンライン開催，2021.9.20-23

近藤恭斗，大島慎介，長﨑百伸，桑原大介，井下圭，福田武司，南貴司，門信一郎，小林進二，木島滋，水内亨，岡田浩之，富田剛士，ヘリオトロン J における径電場分布の回転変換依存性，日本物理学会 2021 年秋季大会，オンライン開催，2021.9.20-23

茶谷智樹，四竈泰一，上野陽平，門信一郎，川染勇人，南貴司，小林進二，大島慎介，岩田晃拓，的池遼太，石澤明宏，中村祐司，岡田浩之，木島滋，水内亨，長﨑百伸，ヘリウム原子輝線のゼーマン効果高感度計測を利用した分光と輸送計算の局所比較，日本物理学会 2021 年秋季大会，オンライン開催，2021.9.20-23

P. Adulsiriswad, Y. Todo, S. Kado, S. Yamamoto, S. Kobayashi, S. Ohshima, T. Minami, H. Okada, A. Ishizawa, Y. Nakamura, S. Konoshima, T. Mizuuchi, K. Nagasaki, Study of the Interaction between Peripheral Energetic Particle Mode and Energetic Particles in Heliotron J with MEGA, a Hybrid MHD Simulation with Free Boundary Condition, 日本物理学会 2021 年秋季大会，オンライン開催，2021.9.20-23

K. Nagasaki, S. Ohshima, R. Matoike, T. Minami, S. Kado, S. Kobayashi, Y. Nakamura, A. Ishizawa, S. Konoshima, T. Mizuuchi, H. Okada, P. Adulsiriswad, A. Iwata, D. Qiu, M. Luo, P. Zhang, C. Wang, Y. Kondo, K. Inoshita, A. Miyashita, N. Kenmochi, G. Motojimab,c, N. Marushchenkod, N. Smith, Physics Study Using 3-D Magnetic Configuration Flexibility in Heliotron J, The 30th International Toki Conference on Plasma and Fusion Research, Online, 2021.11.16-19

P. Adulsiriswad, Y. Todo, S. Kado, S. Yamamoto, S. Kobayashi, S. Ohshima, T. Minami, H. Okada, A. Ishizawa, Y. Nakamura, S. Konoshima, T. Mizuuchi, K. Nagasaki, First Achievement of Free-Boundary Kinetic-Magnetohydrodynamic Hybrid Simulation of Energetic-Particle Driven Modes in Heliotron J, プラズマ・核融合学会第 38 回年会，オンライン開催，2021.11.22-25

K. Nagasaki, High-Temperature Plasma Dynamics and Structure Formation Based on Magnetic Field Diversity（磁場の多様性が開く超高温プラズマダイナミクスと構造形成），プラズマ・核融合学会第 38 回年会，オンライン開催，2021.11.22-25

馮超，門信一郎，岡野竜成，岩田晃拓，森敦樹，南貴司，大島慎介，小林進二，岡田浩之，木島滋，水内亨，長﨑百伸，鈴木琢土，川向泰生，ヘリオトロン J のネオンガス入射実験における真空紫外スペクトル空間分布の時間発展，プラズマ・核融合学会第 38 回年会，オンライン開催，2021.11.22-25

伊神弘恵，長﨑百伸，加藤悠，福山淳，下妻隆，吉村泰夫，西浦正樹，高橋裕己，辻村享，釼持尚輝，矢内亮馬，LHD 低磁場放電における電子バーンシュタイン波放射計測，プラズマ・核融合学会第 38 回年会，オンライン開催，2021.11.22-25

南貴司，釼持尚輝，Dechuan 邱德川，篠塚凌我，戸羽佑輔，松谷遼，門信一郎，大島慎介，小林進二，木島滋，岡田浩之，水内亨，長﨑百伸，Heliotron J における電子内部輸送障壁形成への電子サイクロトロン波電流駆動の影響，プラズマ・核融合学会第 38 回年会，オンライン開催，2021.11.22-25

小林進二，永岡賢一，長﨑百伸，徳原圭一，大垣英明，紀井俊輝，全炳俊，岡田浩之，伊藤龍志，福嶋亮人，大島慎介，門信一郎，南貴司，木島滋，水内亨，閉じ込め磁場配位における非共鳴マイクロ波を用いた統計加速と実験室シミュレーションへの展開，プラズマ・核融合学会第 38 回年会，オンライン開催，2021.11.22-25

清野智大，高橋宏幸，飛田健次，長﨑百伸，福山淳，前川孝，水平入射および上部入射における ECCD 電流駆動効率の入射パワー依存性，プラズマ・核融合学会第 38 回年会，オンライン開催，2021.11.22-25

宮下顕，大島慎介，的池遼太，鈴木琢土，小林進二，岡田浩之，門信一郎，南貴司，水内亨，木島滋，長﨑百伸，静電プローブによるヘリオトロン J 周辺部磁気島内の局所計測，プラズマ・核融合学会第 38 回年会，オンライン開催，2021.11.22-25

的池遼太，大島慎介，河村学思，宮下顕，鈴木琢土，小林進二，門信一郎，南貴司，岡田浩之，水内亨，木島滋，長﨑百伸，ヘリオトロン J 磁場の回転変換スキャンによる周辺磁気島構造制御，プラズマ・核融合学会第 38 回年会，オンライン開催，2021.11.22-25

辻政裕，小田靖久，下元一輝，中井優汰，坂本欣三，長﨑百伸，ECH 伝送系上パワー測定のためのダミーロードの開発，プラズマ・核融合学会第 38 回年会，オンライン開催，2021.11.22-25

鈴木琢土，大島慎介，森敦貴，的池遼太，宮下顕，本島厳，門信一郎，南貴司，小林進二，長﨑百伸，西野信博，水内亨，岡田浩之，木島滋，ペレット溶発過程に観測されたフィラメント状揺動の特性, プラズマ・核融合学会第 38 回年会, オンライン開催, 2021.11.22-25

C. Wang, S. Kobayashi, K. Nagasaki, D. Qiu, M. Luo, R. Fukushima, P. Zhang, R. Matoike, A. Miyashita, Y. Kondo, K. Inoshita, T. Minami, S. Kado, S. Ohshima, H. Okada, S. Konoshima, T. Mizzuchi, Analysis of ion temperature profile in high intensity gas puffing experiments of Heliotron J, プラズマ・核融合学会第 38 回年会, オンライン開催, 2021.11.22-25

M. Luo, K. Nagasaki, D. Qiu, A. Miyashita, K. Inoshita, T.Minami, S. Kado, S. Kobayashi, S. Ohshima, S. Konoshima, T. Mizuuchi, H. Okada, Improvement of Energy confinement with HIGP in Heliotron J, プラズマ・核融合学会第 38 回年会, オンライン開催, 2021.11.22-25

D. Qiu, T. Minami, R. Shinotsuka, M. Luo, C. Wang, P. Zhang, N. Kenmochi, S. Kado, C. Takahashi, S. Ohshima, H. Okada, S. Kobayashi, T. Mizuuchi, S. Konoshima, R. Yasuhara, K. Nagasaki, Present Status of Double Pockels cells Multi-pass Thomson Scattering System on Heliotron J, プラズマ・核融合学会第 38 回年会, オンライン開催, 2021.11.22-25

P. Zhang, S. Ohshima, H. Zhao, S. Kobayashi, H. Okada, T. Minami, S. Kado, S. Konoshima, T. Mizuuchi, K. Nagasaki, Development and construction of 320 GHz interferometer system for Heliotron J, プラズマ・核融合学会第 38 回年会, オンライン開催, 2021.11.22-25

井下圭, 大島慎介, 桑原大介, 近藤恭斗, 小林進二, 岡田浩之，門信一郎，南貴司，水内亨，木島滋，長﨑百伸，ヘリオトロン J におけるドップラー反射計を用いた径電場の回転変換依存性計測，プラズマ・核融合学会第 38 回年会，オンライン開催，2021.11.22-25

近藤恭斗, 大島慎介, 長﨑百伸, 桑原大介, 井下圭, 南貴司，門信一郎，小林進二，木島滋，水内亨，岡田浩之，ヘリオトロン J におけるゾーナルフロー探索を目的としたデュアルドップラー反射計システムの開発，プラズマ・核融合学会第 38 回年会，オンライン開催, 2021.11.22-25

福嶋亮人, 小林進二, 長﨑百伸, 門信一郎, 南貴司, 大島慎介, 王晨宇, 岡田浩之, 小林達哉, 中村祐司, 石澤明宏, 木島滋, 水内亨, 永岡賢一, 村上定義, ビーム放射分光法を用いたヘリオトロン J プラズマの密度揺動二次元計測, プラズマ・核融合学会第 38 回年会, オンライン開催, 2021.11.22-25

森敦樹，門信一郎，本島厳，岡田浩之，南貴司，大島慎介，小林進二，木島滋，水内亨，長﨑百伸，岩田晃拓，馮超，鈴木琢土，川向泰生, ヘリオトロン J における 2 次元高速分光計測器を用いた水素ペレット溶発雲の計測, プラズマ・核融合学会第 38 回年会, オンライン開催, 2021.11.22-25

篠塚凌我，南貴司，Dechuan Qiu，戸羽佑輔，松谷遼，釼持尚輝，門信一郎，岡田浩之，大島慎介，小林進二，木島滋，水内亨，長﨑百伸, ヘリオトロン J における Nd:YAG レーザマルチパストムソン散乱計測装置の性能向上, プラズマ・核融合学会第 38 回年会, オンライン開催, 2021.11.22-25

三瓶明希夫，比村治彦，井上孟流，稲垣秦一郎，高岡亮太，小嶋夏葵，二宮貴哉，新元美晴，佐々木貴弘，政宗貞男，長﨑百伸，大舘暁, 三次元プラズマ発光分布の一方向からの推定, プラズマ・核融合学会第 38 回年会, オンライン開催, 2021.11.22-25

清野智大, 高橋宏幸, 飛田健次, 福山淳, 長﨑百伸, 前川孝, 上部入射 ECCD における電流駆動効率の入射パワー依存性, 日本物理学会第 77 回年次大会, オンライン開催, 2022.3.15-19

岩田晃拓，門信一郎，本島厳，森敦樹，岡田浩之，南貴司, 大島慎介, 小林進二, 石澤明宏, 中村祐司, 木島滋，水内亨，長﨑百伸，馮超，鈴木琢土，四竈泰一，荼谷智樹, ヘリオトロン J におけるペレット溶発雲の近赤外スペクトル計測, 日本物理学会第 77 回年次大会, オンライン開催, 2022.3.15-19

羅茂原，長﨑百伸，Dechuan Qiu，Chengyu Wang, 井下圭，南貴司，門信一郎，小林進二，大島慎介, 木島滋, 水内亨, 岡田浩之, Heliotron J における HIGP を用いたコア電子熱輸送の改善, 日本物理学会第 77 回年次大会, オンライン開催, 2022.3.15-19

宮下顕, 大島慎介, 的池遼太, 鈴木琢土, 小林進二, 岡田浩之，門信一郎，南貴司，水内亨，木島滋，長﨑百伸，ラングミュアプローブによるヘリオトロン J 周辺部磁気島内の局所計測, 日本物理学会第 77 回年次大会, オンライン開催, 2022.3.15-19

小林進二，永岡賢一，長﨑百伸，伊藤龍志，大垣英明，紀井俊輝，全炳俊，岡田浩之，福嶋亮人，Wang Chenyu，大島慎介，門信一郎，南貴司，木島滋，水内亨，ヘリオトロン型磁場配位において非共鳴波動加熱中に観測される高エネルギーX 線スペクトルの特徴，日本物理学会第 77 回年次大会，オンライン開催, 2022.3.15-19

Complex Plasma Systems Research Section

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

1. Introduction

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

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

Results in FY2021 featured in this report are about the diagnostic upgrade which is regarded as a key issue for characterizing the transport properties in fusion-relevant magnetic confinement plasmas.

2. Development of Multi-path Thomson Scattering System on Heliotron J

Nd:YAG-Laser Thomson scattering diagnostics is a powerful tool to measure electron temperature and density having high spatial resolution. Our system in Heliotron J, employing dual laser system, can operate at 100 Hz.

Due to the small scattering cross section, however, the scattered light signal produced from an ECH plasma (n_e~0.5×10^{19}m^{-3}) needs to be accumulated for many shots to yield better signal-to noise ratio.

We have developed a double-pass and multi-path system with signal accmulation technique in multi-path Thomson scattering system (MPTS) on Heliotron J.

An anisotropic electron temperature measurement, as shown in Fig.1, requires analyzing signal separately, for reaching a better understanding of transport mechanism of super-thermal electrons. The scattered light signals, corresponding to two adjacent beam incidences having 160º and 20º scattering angles respectively, overlap with each other completely due to an insufficient length of optical path caused by limited room providing for layout of Thomson scattering system.

To solve this problem, a MPTS with signal separation function is proposed using double-pockels cells. Design of optical path for the double pockels-cells system is given out based on Gaussian beam analysis, which determines the specific position of each optical component, by maintaining spot size and power density evolution of laser beam under the limit of entry diameter, exit diameter and power threshold of each component.

We have performed a signal detection of the MPTS , in following order:

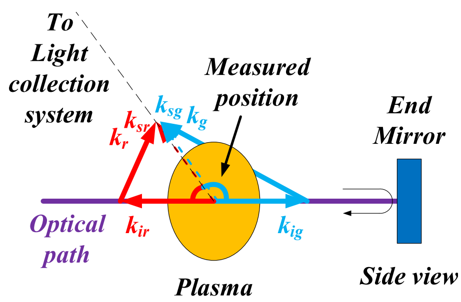


Fig.1 Going(g) and returning(r) wave vectors in reciprocating probe beam.

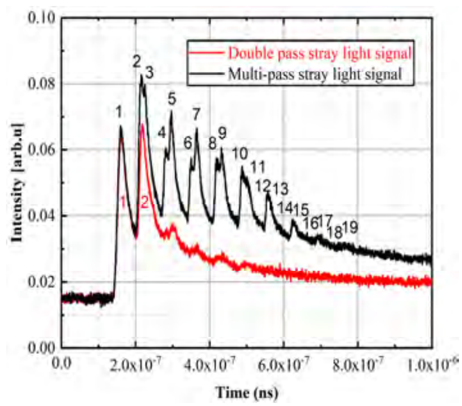


Fig. 2 Comparison of stray light signal between multi-pass system and double-pass system.

1) stray-light produced by the diffuse reflection from the mirror in the beam path,
2) Raman scattering using 300 Torr Nitrogen gas, and
3) Thomson scattering signal in plasma experiment.

We confirmed up to at least 16 reciprocating scattering signals in 1), as in Fig.2, showing the successful optical configuration and trigger synchronization.

3. Upgrade of the EUV Spectroscopy System for the Spatial Distribution Measurement of Impurity Spectra in Heliotron J

Highly charged impurity ions in the fuel gases, deuterium and tritium, can lead to a considerable amount of plasma energy loss, making the critical conditions for fusion reactions more difficult to achieve. This situation becomes more significant in high density and high temperature plasmas where considerable fraction of plasma radiation is in extreme ultraviolet (EUV) region. Therefore, EUV spectroscopy would be an important method to study those impurities [1].

In Heliotron J experiment, we have used micro-channel plate (MCP) system combined with the phosphor-screen and linear sensor for EUV spectroscopy for many years. In this study, we replaced the MCP system with a new Soft-X ray (SX-) CCD detector. The SX-CCD can be operated in full vertical binning (FVB) mode, in which full image area is binned to a direction of the shift register to improve the time resolution.

Figure 3 shows the spectra obtained for both detectors using the reproducible discharge condition of the magnetic configuration and the electron density. Impurity spectral intensity was not perfectly but fairly close to each other.

The signal was normalized to the spectral peak at around O V at 17.22 nm ($1s^2 2s^2\ {}^1S_0 - 1s^2 2s3p\ {}^1P^o{}_1$). Note, however, that the quantum efficiency for both detectors could be different. One can see that the root-mean-square noise for SX-CCD has much better than MCP system by more than 7 times.

The other specifications compared are listed in Table 1. SX-CCD, with the compatible flange, has a little wide measurement region, giving more pixels per instrumental function, full-with at half maximum (FWHM).

One concern we encountered in the application of SX-CCD was the malfunction under the time-varying dominantly vertical magnetic field up to 30 mT at the location of the detector, since all electrical circuit are built-in in the detector. To reduce this magnetic field, a magnetic shield made of soft iron 6 mm in thickness was installed.

The vertical magnetic field inside the shield was reduced down to about 0.15 mT. Even though the horizontal component of 3 mT was remained, we confirmed the appropriate operation of the detector.

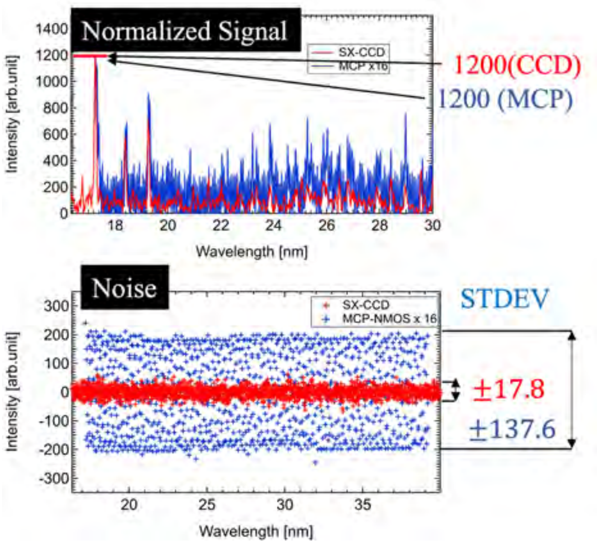


Fig. 3 S/N acescent for #78218 (MCP) and #81829 (CCD). Signal (up) was normalized to both detectors and noise component, before the plasma discharge, (down) was compared.

	MCP system	SX-CCD
Region	17.215 ~ 39.21 nm	16.345 ~ 39.98 nm
Pixels in FWHM	5.56~4.00	9.00~6.42
Resolution(around 34.61nm)	0.10 nm	0.09 nm
S/N	8.7:1	67.4:1
Reciprocal linear dispersion	0.018 ~ 0.025 nm/pixel	0.010 ~ 0.014 nm/pixel

Table. 1 Comparisons of both detectors.

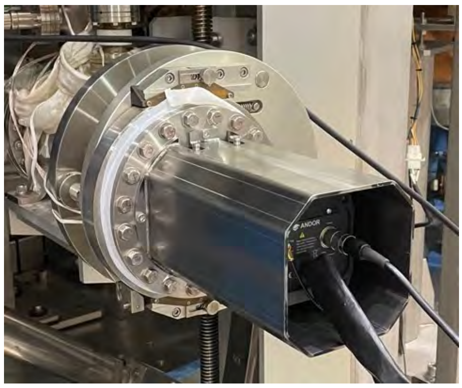


Fig. 4 Magnetic shield structure for the SX-CCD.

1) C. Dong, S. Morita et al., PFR, volume 6, 2402078 (2011)

Collaboration Works

長崎百伸，小林進二，南貴司，大島慎介，Univ. Wisconsin（アメリカ），Oak Ridge National Laboratory（アメリカ），Max Plank Institute（ドイツ），Stuttgart Univ（ドイツ），CIEMAT（スペイン），Australian National Univ.，（オーストラリア），Kharkov Institute（ウクライナ），Southwest Institute of Physics（中国），先進ヘリカルシステムにおける周辺プラズマ・ダイバータ研究

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

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

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

片平正人，永田崇，BIOTEC，NSTDA （タイ），LIPI（インドネシア），NUOL （ラオス），e-ASIA
大島慎介，西南物理研究所（中国），新しい非線形結合に関する揺動解析手法に関する共同研究

門信一郎，林祐貴，核融合科学研究所・双方向型共同研究，定常高密度プラズマのミラー磁場への入射特性評価

門信一郎，江角直道，核融合科学研究所・双方向型共同研究，GAMMA10/PDX ダイバータ模擬プラズマを用いたダイバータスロット形状効果に関する研究

門信一郎，小林進二，核融合科学研究所・双方向型共同研究，磁場閉じ込めプラズマにおける複合粒子補給制御を用いた高密度化（GAMMA 10/PDX における複合粒子制御法を用いた ELM 模擬）

門信一郎，坂本瑞樹，核融合科学研究所・双方向型共同研究，大電力ジャイロトロン開発と原型炉開発へ向けた開放端磁場構造を活かした境界プラズマ研究

門信一郎，山本聡，核融合科学研究所・双方向型共同研究，Heiliotron J における固体水素ペレット運転領域の拡張

門信一郎，鈴木康浩，核融合科学研究所・双方向型共同研究，Heliotron J 装置における新古典輸送および高速イオン閉じ込め最適化とその実験的検証

門信一郎，西村伸，核融合科学研究所・双方向型共同研究，燃焼炉心プラズマ研究に向けた高エネルギー粒子物理と熱化粒子新古典理論の統合

門信一郎，田村直樹，核融合科学研究所・双方向型共同研究，レーザーブローオフ法を用いたヘリオトロン J プラズマにおける不純物輸送研究

門信一郎，桑原大介，核融合科学研究所・双方向型共同研究，ヘリオトロン J における X-mode 多チャンネル反射計の開発

門信一郎，黒田賢剛，核融合科学研究所・双方向型共同研究，Heliotron J における高速カメラ観測と磁気プローブ計測によるプラズマ解析

門信一郎，向井清史，核融合科学研究所・双方向型共同研究，先進ヘリカル磁場配位における境界プラズマの実験・シミュレーション間比較研究

門信一郎，本島厳，核融合科学研究所・双方向型共同研究，ヘリオトロン J における固体水素ペレットの溶発機構理解を目指した分光学的研究

門信一郎，吉川正志，核融合科学研究所・双方向型共同研究，磁場閉じ込めプラズマにおける複合粒子補給制御を用いた高密度化（ヘリオトロン J における高密度プラズマ生成と輸送特性）

門信一郎，小田靖久，核融合科学研究所・双方向型共同研究，伝送系途上での RF パワー計測法の研究

門信一郎，長崎百伸，核融合科学研究所・双方向型共同研究，磁場分布制御を活用したプラズマ構造形成制御とプラズマ輸送改善

門信一郎，松浦寛人，核融合科学研究所・双方向型共同研究，プラズマ熱流束計測に置ける電磁ノイズの抑制と信号補償

門信一郎，釼持尚輝，核融合科学研究所・双方向型共同研究，電子内部輸送障壁に対する磁場の三次元効果の解明

門信一郎，花田和明，核融合科学研究所・双方向型共同研究，ＱＵＥＳＴにおける粒子制御と高電力入射による定常運転の実現

門信一郎，四竈泰一，核融合科学研究所・LHD 計画共同研究，近赤外ゼーマン分光法を用いた SOL 電子温度密度の空間分布計測

門信一郎，田中謙治，核融合科学研究所・LHD 計画共同研究，トロイダルプラズマにおける新古典輸送と乱流駆動輸送の包括的な理解

門信一郎，長崎百伸，核融合科学研究所・LHD 計画共同研究，捕捉粒子制御による高エネルギー励起 MHD 不安定性の励起・減衰

Financial Support

Grant-in-Aid for Scientific Research

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

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

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

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

Publications

S. Ohshima, P. Zhang, H. Kume, C. Deng, A. Miyashita, S. Kobayashi, H. Okada, T. Minami, S. Kado, P. Adulsiriswad, D. Qiu, M. Luo, R. Matoike, T. Suzuki, S. Konoshima, T. Mizuuchi, K. Nagasaki, Development of a multi-channel 320 GHz interferometer for high density plasma measurement in Heliotron J, Review of Scientific Instruments, 92, 053519, 2021

A. Miyashita, K. Mukai, S. Ohshima, R. Matoike, B.J. Peterson, S. Kobayashi, H. Okada, S. Kado, T. Minami, T. Mizuuchi, S. Konoshima, K. Nagasaki, First Application of an InfraRed Imaging Video Bolometer to Heliotron J Plasma, Plasma and Fusion Research, 16, 1202079, 2021

K. Mukai, B.J. Peterson, N. Ezumi, N. Shigematsu, S. Ohshima, A. Miyashita, R. Matoike, Sensitivity improvement of infrared imaging video bolometer for divertor plasma measurement, Review of Scientific Instruments, 92, 063521, 2021

A. Miyashita, K. Mukai, S. Ohshima, R. Matoike, B.J. Peterson, S. Kobayashi, H. Okada, S. Kado, T. Minami, T. Mizuuchi, S. Konoshima, K. Nagasaki, First Application of an InfraRed Imaging Video Bolometer to Heliotron J Plasma, Plasma and Fusion Research, 16, 1202079, 2021

S. Kobayashi, K. Nagasaki, K. Hada, T. Stange, H. Okada, T. Minami, S. Kado, S. Ohshima, K. Tokuhara, Y. Nakamura, A. Ishizawa, Y. Suzuki, M. Osakabe, T. Murase, S. Konoshima, T. Mizuuchi, Role of pre-ionization in NBI plasma start-up of Heliotron J using non-resonant microwave heating, Nuclear Fusion, 11, 11, 116009, 2021

P. Adulsiriswad, Y. Todo, S. Kado, S. Yamamoto, S. Kobayashi, S. Ohshima, H. Okada, T. Minami, Y. Nakamura, A. Ishizawa, S. Konoshima, T. Mizuuchi, K. Nagasaki, Numerical investigation of the peripheral energetic particle driven MHD modes in Heliotron J with free boundary hybrid simulation, Nuclear Fusion, 61, 11, 116065, 2021

R. Matoike, G. Kawamura, S. Ohshima, Y. Suzuki, M. Kobayashi, S. Masuzaki, S. Kobayashi, S. Kado, T. Minami, H. Okada, T. Mizuuchi, S. Konoshima, Y. Feng, H. Frerichs, K. Nagasaki, Numerical analysis of heat load distribution in Heliotron J with magnetic field tracing and plasma transport modeling, Plasma Physics and Controlled Fusion, 63, 11, 115002, 2021

T. Nishizawa, M. Griener, R. Dux, G. Grenfell, D. Wendler, S. Kado, P. Manz, M. Cavedon, ASDEX Upgrade team, Linearized spectrum correlation analysis for thermal helium beam diagnostics, Review of Scientific Instruments, 92, 103501, 2021

M. Yoshikawa, J. Kohagura, N. Ezumi, T. Iijima, K. Nojiri, A. Terakado, Y. Nakashima, T. Kariya, T. Numakura, M. Hirata, R. Minami, M. Sakamoto, M. Ichimura, M. S. Islam, Y. Shima, R. Yasuhara, I. Yamada, H. Funaba, T. Minami, N. Kenmochi, D. Kuwahara, H.J. van der Meiden, Study of detached plasma profile in the divertor simulation experimental module of tandem mirror GAMMA 10/PDX, AIP Advances, 11, 125231, 2021

K. Nagasaki, Y. Kato,Y. Oka, H. Igami,T. Minami, S. Kado, S. Kobayashi, S. Ohshima, Y. Nakamura, A. Ishizawa, T. Mizuuchi, H. Okada, S. Konoshima, R. Matoike, A. Iwata, M.Luo, P. Zhang, C. Wang, Y. Kondo, N. Marushchenko, Electron temperature measurement using electron bernstein emission in Heliotron J, 47th EPS Conference on Plasma Physics, EPS 2021, 2021-June, 1016-1019, 2021

Presentations

K. Nagasaki, S. Ohshima, T. Minami, M. Miyoshi, S. Yamamoto, H. Okada, S. Kado,S. Kobayashi, S. Konoshima, T. Mizuuchi, Y. Kishimoto, Y. Nakamura, A. Ishizawa, P. Adulsiriswad, D. Qiu, M. Luo, Á. Cappa, K. Wang, N. Smith, Effect of Magnetic Configuration on Energy Confinement and Energetic-Particle-Driven MHD Modes in Heliotron J, 28th IAEA Fusion Energy Conference, Online, 2021.5.10-15

S. Ohshima, H. Okada, S. Kobayashi, T. Minami, S. Kado, P. Adulsiriswad, D. Qiu,M. Luo, R. Matoike, S. Yamamoto, Y. Nakamura, S. Konoshima, T. Mizuuchi, K. Nagasaki, Turbulent Properties Against Hydrogen Isotope Ratio and Zonal Flow Activities in Heliotron J, 28th IAEA Fusion Energy Conference, Online, 2021.5.10-15

S. Kobayashi, K. Nagasaki, K. Hada, T. Stange, K. Tokuhara, S. Ohshima, H. Okada,T. Minami, S. Kado, H. Ohgaki, T. Kii, H. Zen, Y. Nakamura, A. Ishizawa,Y. Suzuki, M. Osakabe, T. Murase, Y. Kishimoto, S. Konoshima, T. Mizuuchi, Study of NBI plasma start-up assisted by seed-plasma generation using non-resonant microwave heating in Heliotron J, 28th IAEA Fusion Energy Conference, Online, 2021.5.10-15

M. Osakabe, H. Takahashi, K. Mukai, H. Yamada, T. Kobayashi, K. Ida, S. Ohdachi, K. Ogawa, M. Kobayashi, S. Kamio, S. Murakami, S. Inagaki, K. Tanaka, M. Sakamoto, S. Masuzaki, K. Nagasaki, Y. Suzuki, M. Isobe, T. Morisaki and LHD experiment group, Recent results of Deuterium Experiment on the Large Helical Device and its contribution to the fusion reactor development, 28th IAEA Fusion Energy Conference, Online, 2021.5.10-15

M. Yoshikawa, J. Kohagura, N. Ezumi, T. Iijima, K. Nojiri, A. Terakado,Y. Nakashima, T. Kariya, T. Numakura, M. Hirata, R. Minami, M. Sakamoto, M. Ichimura, T. Imai, M. S. Islam, Y. Shima, S. Suto, T. Mouri, T. Hara, R. Yasuhara, I. Yamada, H. Funaba, T. Minami, N. Kenmochi, D. Kuwahara, andH. J. van der Meiden, Study of detached plasma profile in the divertor simulation experimental module of GAMMA 10/PDX, 28th IAEA Fusion Energy Conference, Online, 2021.5.10-15

T. Tsujimura, R. Yanai, K. Tanaka, Y. Yoshimura, T. Tokuzawa, M. Nishiura, R. Sakamoto, G. Motojima, S. Kubo, T. Shimozuma, H. Igami, H. Takahashi, M. Yoshinuma, S. Ohshima, Improved Performance of ECRH by Real-Time Deposition Location Control and Perpendicular Injection in LHD, 28th IAEA Fusion Energy Conference, Online, 2021.5.10-15

U. Losada, B. Liu, D. Fernández Ruiz, T. Kobayashi, S. Ohshima, B. van Milligen, Á. Cappa, M. Liniers, B. López-Miranda, G. Guedes Grenfell, C. Silva, and C. Hidalgo, Isotope Effect, Operational Limits and Zonal Flows in the TJ-II Stellarator, 28th IAEA Fusion Energy Conference, Online, 2021.5.10-15

L. Zang, S. Ohshima, Y. Qu, P. Shi, W. Zhong, L. Yan, D. Yu, Z. Shi, Y. Liu, Q. Yang, Analysis of Nonlinear Mode-Mode Interaction using Hilbert Transform on HL-2A, 28th IAEA Fusion Energy Conference, Online, 2021.5.10-15

K. Nagasaki, H. Igami, Y. Oka, H. Okada, T. Minami, S. Kado, S. Kobayahi, S.Ohshima, T. Mizuuchi, S. Konoshima, Y.Nakamura, A. Ishizawa, D. Qiu, R. Matoike, M. Luo, N. Marushchenko, F. Volpe, Electron Temperature Measurement Using Electron Bernstein Emission in Heliotron J, 47th EPS Conference on Plasma Physics, Online, 2021.6.21-25

U. Losada, B. Liu, D. Fernández, T. Kobayashi, S. Ohshima, A. Cappa, B. van, Milligen, M. Liniers, B. López-Miranda, G. G. Grenfell, C. Silva, C. Hidalgo, TJ-II team, On the physics of isotope effect, operational limits and Zonal Flows in the TJ-II stellarator, 47th EPS Conference on Plasma Physics, Online, 2021.6.21-25

T. Minami, N. Kenmochi, C. Takahashi, S. Kobayashi, H. Okada, S. Kado, S. Ohshima, S. Konoshima, G. Weir, T. Mizuuchi, K. Nagasaki, Effect of magnetic field structure on electron internal transport barrier formation in Heliotron J, 5th Asia Pacific Conference on Plasma Physics, Online, 2021.9.26-10.1

小林進二，永岡賢一，長崎百伸，徳原圭一，大垣英明，紀井俊輝，全炳俊，岡田浩之，福嶋亮人，大島慎介，門信一郎，南貴司，木島滋，水内亨，ヘリオトロン型磁場配位における非共鳴波動加熱を利用した統計加速，日本物理学会 2021 年秋季大会，オンライン開催, 2021.9.20-23

加藤悠，長崎百伸，伊神弘恵，岡佑旗，小林進二，大島慎介，門信一郎，南貴司，中村祐司，石澤明宏，木島滋，水内亨，岡田浩之，的池遼太, Heliotron J における B-X-O モード変換を用いた電子バーンシュタイン放射計測，日本物理学会 2021 年秋季大会，オンライン開催, 2021.9.20-23

近藤恭斗，大島慎介，長崎百伸，桑原大介，井下圭，福田武司，南貴司，門信一郎，小林進二，木島滋，水内亨，岡田浩之，富田剛士，ヘリオトロン J における径電場分布の回転変換依存性，日本物理学会 2021 年秋季大会，オンライン開催, 2021.9.20-23

茶谷智樹，四竈泰一，上野陽平，門信一郎，川染勇人，南貴司，小林進二，大島慎介，岩田晃拓，的池遼太，石澤明宏，中村祐司，岡田浩之，木島滋，水内亨，長﨑百伸，ヘリウム原子輝線のゼーマン効果高感度計測を利用した分光と輸送計算の局所比較, 日本物理学会 2021 年秋季大会，オンライン開催, 2021.9.20-23

P. Adulsiriswad, Y. Todo, S. Kado, S. Yamamoto, S. Kobayashi, S. Ohshima, T. Minami, H. Okada, A. Ishizawa, Y. Nakamura, S. Konoshima, T. Mizuuchi, K. Nagasaki, Study of the Interaction between Peripheral Energetic Particle Mode and Energetic Particles in Heliotron J with MEGA, a Hybrid MHD Simulation with Free Boundary Condition, 日本物理学会 2021 年秋季大会，オンライン開催, 2021.9.20-23

A. Iwata, S. Kado, N. Tamura, T. Minami, S. Ohshima, S. Kobayashi, Y. Nakamura, A. Ishizawa, H. Okada, S. Konoshima, T. Mizuuchi, K. Nagasaki, Applicability Evaluation of Laser Blow-off Spectroscopy System in Heliotron J, The 30th International Toki Conference on Plasma and Fusion Research, Online, 2021.11.16-19

T. Shikama, S. Kado, Y. Ueno, T. Chatani, H. Kawazome, T. Minami, S. Kobayashi, S. Oshima, H. Okada, A. Iwata, R. Matoike, T. Oishi, A. Ishizawa, Y. Nakamura, S. Konoshima, T. Mizuuchi, K. Nagasaki, M. Hasuo, Development of a near-infrared Stokes spectropolarimetry system for the spatially resolved measurements of atomic emissivity and velocity distribution in the scrape-off-layer of Heliotron J, The 30th International Toki Conference on Plasma and Fusion Research, Online, 2021.11.16-19

X.N. Bui, H. Matsuura, R. Matoikea, S. Ohshima, Divertor heat flux sensor upgrade using small thermocouple, The 30th International Toki Conference on Plasma and Fusion Research, Online, 2021.11.16-19

P. Adulsiriswad, Y. Todo, S. Kado, S. Yamamoto, S. Kobayashi, S. Ohshima, T. Minami, H. Okada, A. Ishizawa, Y. Nakamura, S. Konoshima, T. Mizuuchi, K. Nagasaki, First Achievement of Free-Boundary Kinetic-Magnetohydrodynamic Hybrid Simulation of Energetic-Particle Driven Modes in Heliotron J, プラズマ・核融合学会第 38 回年会，オンライン開催, 2021.11.22-25

馮超，門信一郎，岡野竜成，岩田晃拓，森敦樹，南貴司，大島慎介，小林進二，岡田浩之，木島滋，水内亨，長﨑百伸，鈴木琢土，川向泰生, ヘリオトロン J のネオンガス入射実験における真空紫外スペクトル空間分布の時間発展, プラズマ・核融合学会第 38 回年会，オンライン開催, 2021.11.22-25

南貴司，釼持尚輝，Dechuan 邱德川，篠塚凌我，戸羽佑輔，松谷遼，門信一郎，大島慎介，小林進二，木島滋，岡田浩之，水内亨，長﨑百伸, Heliotron J における電子内部輸送障壁形成への電子サイクロトロン波電流駆動の影響, プラズマ・核融合学会第 38 回年会，オンライン開催, 2021.11.22-25

小林進二，永岡賢一，長﨑百伸，徳原圭一，大垣英明，紀井俊輝，全炳俊，岡田浩之，伊藤龍志，福嶋亮人，大島慎介，門信一郎，南貴司，木島滋，水内亨，閉じ込め磁場配位における非共鳴マイクロ波を用いた統計加速と実験室シミュレーションへの展開, プラズマ・核融合学会第 38 回年会，オンライン開催, 2021.11.22-25

宮下顕, 大島慎介, 的池遼太, 鈴木琢土, 小林進二, 岡田浩之，門信一郎，南貴司，水内亨，木島滋，長﨑百伸，静電プローブによるヘリオトロン周辺部磁気島内の局所計測，プラズマ・核融合学会第 38 回年会，オンライン開催, 2021.11.22-25

的池遼太, 大島慎介, 河村学思, 宮下顕, 鈴木琢土, 小林進二，門信一郎，南貴司，岡田浩之，水内亨，木島滋，長﨑百伸，ヘリオトロン J 磁場の回転変換スキャンによる周辺磁気島構造制御, プラズマ・核融合学会第 38 回年会，オンライン開催, 2021.11.22-25

鈴木琢土，大島慎介，森敦貴，的池遼太，宮下顕，本島厳，門信一郎，南貴司，小林進二，長﨑百伸，西野信博，水内亨，岡田浩之，木島滋, ペレット溶発過程に観測されたフィラメント状揺動の特性, プラズマ・核融合学会第 38 回年会, オンライン開催, 2021.11.22-25

C. Wang, S. Kobayashi, K. Nagasaki, D. Qiu, M. Luo, R. Fukushima, P. Zhang, R. Matoike, A. Miyashita, Y. Kondo, K. Inoshita, T. Minami, S. Kado, S. Ohshima, H. Okada, S. Konoshima, T. Mizzuchi, Analysis of ion temperature profile in high intensity gas puffing experiments of Heliotron J, プラズマ・核融合学会第 38 回年会，オンライン開催, 2021.11.22-25

M. Luo, K. Nagasaki, D. Qiu, A. Miyashita, K. Inoshita, T.Minami, S. Kado, S. Kobayashi, S. Ohshima, S. Konoshima, T. Mizuuchi, H. Okada, Improvement of Energy confinement with HIGP in Heliotron J, プラズマ・核融合学会第 38 回年会，オンライン開催, 2021.11.22-25

D. Qiu, T. Minami, R. Shinotsuka, M. Luo, C. Wang, P. Zhang, N. Kenmochi, S. Kado, C. Takahashi, S. Ohshima, H. Okada, S. Kobayashi, T. Mizuuchi, S. Konoshima, R. Yasuhara, K. Nagasaki, Present Status of Double Pockels cells Multi-pass Thomson Scattering System on Heliotron J, プラズマ・核融合学会第 38 回年会, オンライン開催, 2021.11.22-25

P. Zhang, S. Ohshima, H. Zhao, S. Kobayashi, H. Okada, T. Minami, S. Kado, S. Konoshima, T. Mizuuchi, K. Nagasaki, Development and construction of 320 GHz interferometer system for Heliotron J, プラズマ・核融合学会第 38 回年会, オンライン開催, 2021.11.22-25

井下圭, 大島慎介, 桑原大介, 近藤恭斗, 小林進二, 岡田浩之, 門信一郎, 南貴司, 水内亨, 木島滋, 長﨑百伸, ヘリオトロン J におけるドップラー反射計を用いた径電場の回転変換依存性計測, プラズマ・核融合学会第 38 回年会, オンライン開催, 2021.11.22-25

近藤恭斗, 大島慎介, 長﨑百伸, 桑原大介, 井下圭, 南貴司, 門信一郎, 小林進二, 木島滋, 水内亨, 岡田浩之, ヘリオトロン J におけるゾーナルフロー探索を目的としたデュアルドップラー反射計システムの開発, プラズマ・核融合学会第 38 回年会, オンライン開催, 2021.11.22-25

福嶋亮人, 小林進二, 長﨑百伸, 門信一郎, 南貴司, 大島慎介, 王晨宇, 岡田浩之, 小林達哉, 中村祐司, 石澤明宏, 木島滋, 水内亨, 永岡賢一, 村上定義, ビーム放射分光法を用いたヘリオトロン J プラズマの密度揺動二次元計測, プラズマ・核融合学会第 38 回年会, オンライン開催, 2021.11.22-25

森敦樹, 門信一郎, 本島厳, 岡田浩之, 南貴司, 大島慎介, 小林進二, 木島滋, 水内亨, 長﨑百伸, 岩田晃拓, 馮超, 鈴木琢土, 川向泰生, ヘリオトロン J における 2 次元高速分光計測器を用いた水素ペレット溶発雲の計測, プラズマ・核融合学会第 38 回年会, オンライン開催, 2021.11.22-25

篠塚凌我, 南貴司, Dechuan Qiu, 戸羽佑輔, 松谷遼, 釼持尚輝, 門信一郎, 岡田浩之, 大島慎介, 小林進二, 木島滋, 水内亨, 長﨑百伸, ヘリオトロン J における Nd:YAG レーザマルチパストムソン散乱計測装置の性能向上, プラズマ・核融合学会第 38 回年会, オンライン開催, 2021.11.22-25

岩田晃拓, 門信一郎, 本島厳, 森敦樹, 岡田浩之, 南貴司, 大島慎介, 小林進二, 石澤明宏, 中村祐司, 木島滋, 水内亨, 長﨑百伸, 馮超, 鈴木琢土, 四竈泰一, 茶谷智樹, ヘリオトロン J におけるペレット溶発雲の近赤外スペクトル計測, 日本物理学会 2022 年年会, オンライン開催, 2022.3.15-19

羅茂原, 長﨑百伸, Dechuan Qiu, Chengyu Wang, 井下圭, 南貴司, 門信一郎, 小林進二, 大島慎介, 木島滋, 水内亨, 岡田浩之, Heliotron J における HIGP を用いたコア電子熱輸送の改善, 日本物理学会 2022 年年会, オンライン開催, 2022.3.15-19

宮下顕, 大島慎介, 的池遼太, 鈴木琢土, 小林進二, 岡田浩之, 門信一郎, 南貴司, 水内亨, 木島滋, 長﨑百伸, ラングミュアプローブによるヘリオトロン J 周辺部磁気島内の局所計測, 日本物理学会 2022 年年会, オンライン開催, 2022.3.15-19

小林進二, 永岡賢一, 長﨑百伸, 伊藤龍志, 大垣英明, 紀井俊輝, 全炳俊, 岡田浩之, 福嶋亮人, Wng Chenyu, 大島慎介, 門信一郎, 南貴司, 木島滋, 水内亨, ヘリオトロン型磁場配位において非共鳴波動加熱中に観測される高エネルギーX 線スペクトルの特徴, 日本物理学会 2022 年年会, オンライン開催, 2022.3.15-19

門信一郎, 高校数学に基づく新型コロナ感染症流行曲線の簡易分析, 日本物理学会 2022 年年会, オンライン開催, 2022.3.15-19

Functional Materials Science and Engineering Research Section

Y. Miyauchi, Professor
T. Nishihara, Assistant Professor

1. Introduction

Our research section focuses on the physical properties, functions, and energy applications of quantum materials that exhibit significant quantum mechanical effects, such as carbon nanotubes (CNT) and recently discovered topological materials. The aim is to create new technologies for highly efficient use of solar light/thermal energy that will contribute to the realization of a sustainable energy society. To understand the unique physical properties of these materials from the fundamental principles and extract superior functions that exceed the limits of conventional materials, we are promoting interdisciplinary research that covers basic sciences, including condensed matter physics and materials synthesis, as well as thermal, mechanical, electronic, and optical engineering along with the fabrication of integrated nanomaterials. Followings are main research achievements in the year of 2021.

2. Development of theory of exciton thermal radiation in semiconducting single-walled carbon nanotubes

As one of the advanced application technologies of thermal radiation, thermophotovoltaic power generation technology is under development. In this power generation method, thermal radiation generated from a hot object is used as an input to a photovoltaic cell to generate electricity (Figure 1a). In principle, the energy conversion efficiency is high when the radiation energy is concentrated in the near-infrared wavelength region near the band gap of the photovoltaic cell, and therefore, materials with high emissivity only in the near-infrared region and high thermal stability are suitable as materials for thermal radiation generating components called wavelength selective emitters.

Single-walled carbon nanotubes (SWCNTs), which are nanoscale materials (nanomaterials) composed of a single layer of graphene sheet rolled up into a cylindrical shape with a diameter of the order of 1 nm, are promising materials with such characteristics. Previously, we revealed that SWCNTs show significantly narrow-band near-infrared thermal radiation in the near infrared wavelength range (Figure 1b) [1] based on the direct observation of the thermal radiation from an individual suspended SWCNTs heated to temperatures above 1000 K using dark-field microscopy in vacuum. Recently, we have theoretically clarified that this narrow bandwidth is a consequence of

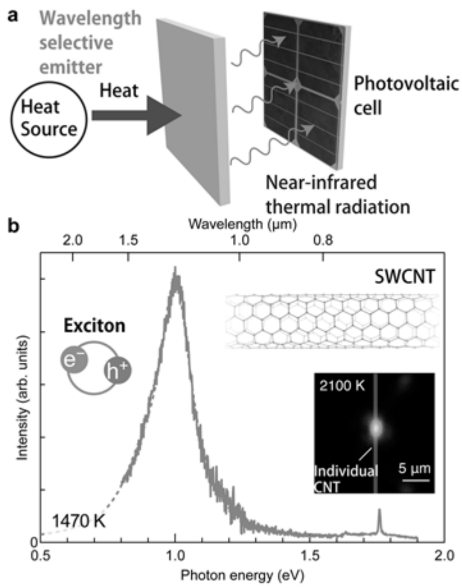


Fig. 1 (a) Schematic of thermophotovoltaic power generation. (b) Thermal radiation spectrum of a single suspended SWCNT. Inset shows an example of an SWCNT structure (top) and microscopy image of the thermal radiation at 2100 K from an individual SWCNT.

the very strong Coulomb interaction between electrons (negative charge) and holes (positive charge) in SWCNTs. Unlike in conventional materials, the electrons and holes are bound to each other and move in a correlated manner in SWCNTs. Therefore, thermal excitation of an electron and a hole leads to formation of a hydrogen atom-like quantum state called exciton. The exciton has a discrete energy level structure similar to that of a hydrogen atom, and thus has well-defined energy, and the annihilation of the exciton generates a narrow-band thermal radiation reflecting the exciton energy. To theoretically investigate light emission due to thermal excitons, we used fluctuational electromagnetics to derive a simple and practical formula for emissivity $e(\omega)$ that appropriately incorporates the structure of SWCNTs and exciton effect

$$e(\omega) = \frac{\omega d}{3c}\mathrm{Im}[\varepsilon(\omega)],$$

where d is the diameter, c is the speed of light, and $\varepsilon(\omega)$ is the dielectric function. With this formula, the emissivity can be easily obtained given the diameter and dielectric function of the SWCNTs, allowing us to study the thermal radiation due to thermal excitons at various diameters.

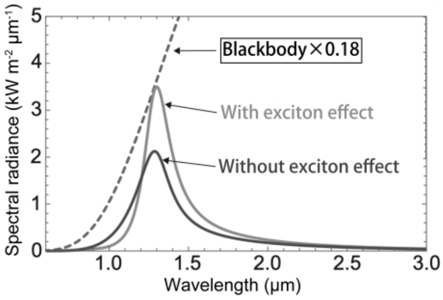


Fig. 2 Theoretically calculated thermal radiation spectra of an SWCNT at 1300 K with and without considering the excitonic effect. Dashed curve indicates 0.18-multiplied black body radiation spectrum at 1300 K.

Figure 2 shows the calculated thermal radiation spectra of an SWCNT with a diameter of 1.1 nm at 1300 K with and without exciton effect (the dotted line is the blackbody radiation spectrum at 1300 K). It is clearly shown that the exciton effect increases the thermal radiation intensity and narrows the line width. Also, compared to the blackbody thermal radiation spectrum, the thermal radiation from an SWCNT has a very narrow line width. This result is in good agreement with the experimental result shown in Figure 1b and proves the correctness of the thermal radiation theory of thermal excitons obtained in this study [2].

2. Complex refractive index measurement of carbon nanotube membranes - Toward wavelength selective radiation and absorption applications

In order to design thermo-optic devices such as wavelength-selective emitters that require precise control of spectral emissivity, information on the complex refractive index spectrum, which defines the macroscopic optical properties of the material, is necessary. In particular, the complex refractive index spectra of SWCNT membranes with a well-defined chiral structure are required because there exist variety of nanotube species with different chiral structures reflecting the degree of freedom in the wrapping of graphene, and the exciton energy is determined by the structure of the SWCNTs. However, broadband complex refractive index spectra of single chiral structure SWCNT membranes have not been reported so far, which has hindered the development of SWCNT-based optical devices, including wavelength selective emitters.

Response functions, such as optical susceptibility describing the response of a material to light, are generally complex numbers. Therefore, physical properties such as the refractive index obtained from the susceptibility are also generally expressed in terms of complex numbers that depend on the frequency. In this study, we determined the complex refractive index spectra of membranes of five different chiral structures. The results are summarized in Figure 3, which shows similar spectral shapes except for the difference in the resonance energy of the exciton peak sensitive to the nanotube chiral structure (chirality) indicated by two integers. From this similarity, we further examined whether the complex refractive index spectra can be reproduced simply by using only the average values of the parameters obtained from the five types of SWCNT membranes. The gray shaded area in Figure 3b shows the reproduced values, and it is found that most of the experimental data can be covered by taking into account an error of ±20%. This result implies that the complex refractive index spectra of SWCNT membranes other than these five types of chirality could also be predicted to some extent by extrapolation. Using the empirical formula for the complex refractive index spectrum, now one can design various optical and thermo-optical devices such as wavelength-selective emitters matching the band gap of photovoltaic cells, wavelength-selective absorber films, and dielectric multilayers combining SWCNTs and other materials [3].

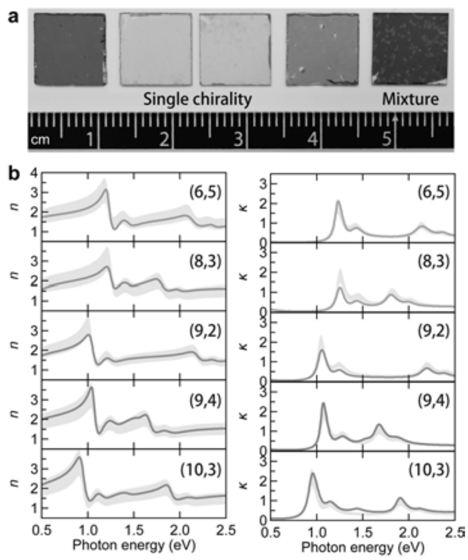


Fig. 3 (a) Photograph of single chirality (left four samples) and mixed chirality SWCNT membrane (right). (b) Real (left) and imaginary (right) parts of the complex refractive index spectra of five different SWCNT membranes.

Acknowledgement

These researches were partly supported by JST CREST (Grant No. JPMJCR18I5), JSPS KAKENHI (JP19K15384, JP20H02605, JP20H05664), and ZE Research Program, IAE (ZE2020B-33, ZE2021B-02).

References

[1] T. Nishihara, A. Takakura, Y. Miyauchi, K. Itami, Nat. Commun., **2018**, 9, 3144.

[2] S. Konabe, T. Nishihara, Y. Miyauchi, Opt. Lett., **2021**, 46, 3021.

[3] T. Nishihara *et al.*, Nanophotonics **2022**, 11, 1011.

Financial Support

1. Grant-in-Aid for Scientific Research
宮内雄平，基盤研究(B)，量子物質を用いた非従来型赤外光電変換学理の開拓

西原大志，若手研究，低次元量子非平衡系における非従来型高温発光物理の解明

2. Others

宮内雄平，科学技術振興機構，原子層ヘテロ構造の光物性・機能開拓

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

Publications

K. Kato, K. Takaba, S. Maki-Yonekura, N. Mitoma, Y. Nakanishi, T. Nishihara, T. Hatakeyama, T. Kawada, Y. Hijikata, J. Pirillo, L.T. Scott, K. Yonekura, Y. Segawa, K. Itami, Double-Helix Supramolecular Nanofibers Assembled from Negatively Curved Nanographenes, Journal of the American Chemical Society, 143, 14, 5465-5469, 2021

S. Konabe, T. Nishihara, Y. Miyauchi, Theory of exciton thermal radiation in semiconducting single-walled carbon nanotubes, Optics Letters, 46, 13, 3021-3024, 2021

J. Pu, W. Zhang, H. Matsuoka, Y. Kobayashi, Y. Takaguchi, Y. Miyata, K. Matsuda, Y. Miyauchi, T. Takenobu, Room-Temperature Chiral Light-Emitting Diode Based on Strained Monolayer Semiconductors, Advanced Materials, 2021, 2100601, 2021

T. Nishihara, A. Takakura, M. Shimasaki, K. Matsuda, T. Tanaka, H. Kataura, Y. Miyauchi, Empirical formulation of broadband complex refractive index spectra of single-chirality carbon nanotube assembly, Nanophotonics, 2022, 11, 1011-1020, 2022

Presentations

西原大志，髙倉章，島﨑雅史，松田一成，田中丈士，片浦弘道，宮内雄平，単一構造カーボンナノチューブ薄膜の複素屈折率スペクトル，第 58 回日本伝熱シンポジウム，オンライン開催, 2021.5.25

T. Nishihara, A. Takakura, K. Matsuda, T. Tanaka, H. Kataura, Y. Miyauchi, Empirical Modeling of Broadband Complex Optical Spectra of Single-Chirality-Enriched Carbon Nanotube Films for Optical Desiign, 239th ECS Meeting, Online, 2021.6.3

Y. Miyauchi, Carbon nanotubes as high temperature quantum functional materials, Materials Science Colloquia, Online, 2021.7.21

西原大志，髙倉章，小鍋悟，田中丈士，片浦弘道，宮内雄平，カーボンナノチューブ薄膜の偏光·角度分解分光測定"，ふく射勉強会，オンライン開催，2021.8.27

Yina Du, Tatsuya Hinoki, Effect of Er2O3 interphase on SiC fiber reinforced W composites，日本原子力学会秋の大会，オンライン開催, 2021.9.8

T. Nishihara, A. Takakura, M. Shimasaki, K. Matsuda, T. Tanaka, H. Kataura, Y. Miyauchi, Empirical modeling of broadband complex refractive index spectra of single-chirality-enriched carbon nanotube membranes，第 82 回応用物理学会秋季学術講演会，オンライン開催，2021.9.11

M. Shimasaki, T. Nishihara, K. Matsuda, T. Endo, Y. Miyata, Y. Miyauchi, Optical properties of lateral heteromonolayer WSe2-MoSe2，第 82 回応用物理学会秋季学術講演会，オンライン開催, 2021.9.11

宮内雄平，カーボンナノチューブの光物性とエネルギー工学への展開, 2021 年秋季大会，オンライン開催, 2021.9.21

Y. Miyauchi, Toward applications of excitonic properties in carbon nanotubes and atomically thin semiconductors, The 11th Asian Nanomaterials Symposium on Emerging Materials, Online, 2021.12.4

J. Lee, T. Hinoki, Development of Pressureless Liquid Phase Sintered SiC ceramics and SiCf/SiC Composites, 46th International Conference and Expo on Advanced Ceramics and Composites (ICACC2022), Online, 2022.1.24

西原大志，金属型カーボンナノチューブの特異なジュール熱発光，ふく射勉強会，オンライン開催，2022.1.27

宮内雄平, ナノスケール物質科学と未来のエネルギー, 第 17 回京都大学附置研究所・センターシンポジウム, 松山市民会館, 2022.3.5

Y. Miyauchi, Exciton properties in one- and two-dimensional semiconducting nanomaterials and their applications, 14th International Symposium on Advanced Plasma Science and its Applications for Nitrides and Nanomaterials (ISPlasma2022) / 15th International Conference on Plasma-Nano Technology & Science (IC-PLANTS2022), Online, 2022.3.9

B. Wang, Y. Zhong, Y. Du, B. Huang, K. Kawasaki, F. Shinoda, Y. Hayashi, T. Hinoki, Effect of Ion Irradiation on Mechanical Properties of Silicon Carbide, 2022 Annual Meeting of Atomic Energy Society of Japan, Online, 2022.3.18

Y. Zhong, B. wang, Y. Du, B. Huang, K. Kawasaki, F. Shinoda, T. Hinoki, Ion-irradiation Effect on Swelling and Microstructure of C/BN Particle Dispersed SiC, 2022 Annual Meeting of Atomic Energy Society of Japan, Online, 2022.3.18

Advanced Laser Science Research Section

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

1. Introduction

Laser is a very powerful tool to probe physical or chemical processes and fabricate/modify the target materials. This year we have developed a few different techniques to probe the electrochemical processes, fabricate the functional metal surfaces, and modify the size and shape of nanoparticles.

2. Probing the electrochemical process through optical detection of laser-assisted bubbles during electrolysis

In recent years hydrogen evolution reaction (HER) through electrolysis of water is considered to be one of the promising methods to store renewable energy. While water electrolysis is a well-known process, realization of highly efficient HER still remains very challenging, since, first of all, nucleation of hydrogen gas bubble formation itself is not yet very well-understood, and this is particularly true for the case of macroscopic commercial electrodes which do not provide ideally flat and smooth surfaces. Recall that nucleation dynamics crucially depends on the surface roughness. Not only the nucleation dynamics but also the detachment of the bubbles also critically depends on the surface structures with a roughness of sub-μm.

Last year we have developed a new technique to probe the concentration profile of dissolved gas by optically monitoring the ascending bubbles in vicinity to the electrode, and extrapolated the concentration profile toward the electrode surface, because the direct probe of bubbles on the electrode was technically difficult. This year we have developed a new technique to directly probe bubbles on the electrode. The electrolysis condition where our optical technique is applicable is also extended to the lower current density where no bubbles are formed. The key technique is to introduce a laser pulse to form laser-assisted bubbles on the electrode even under very low current densities. The experimental setup is shown in Fig. 1. Representative photos of the bubbles formed on the electrode upon irradiation of a laser pulse from the bottom is shown in Fig. 1(a) and (b). Obviously the higher the current density the more the laser-assisted bubbles are formed underneath the electrode.

Using a diffusion model we can estimate the dissolved H_2 gas concentration from the growth rates of

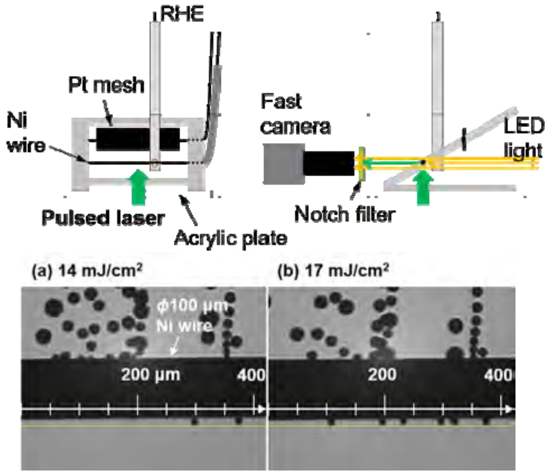


Fig. 1 (top) Experimental setup to detect laser induced bubbles during electrolysis and the measured bubbles underneath the Ni wire electrode at 20 ms after the laser pulse at the laser fluences of (a) 14 and (b) 17 mJ/cm^2.

the bubbles which varies in time after the laser pulse. Employing the two methods we have developed last year and this year, we estimate the dissolved H_2 gas concentration as a function of current density, and the results are compared in Fig. 2. We notice that the H_2 gas concentrations at the electrode obtained by the two methods, i.e., optical monitoring of ascending bubbles in vicinity to the electrode and laser-assisted bubbles on the electrode, are in reasonable agreement, and the latter shows the nicer linearity in current density, indicating the superiority of the method uti-

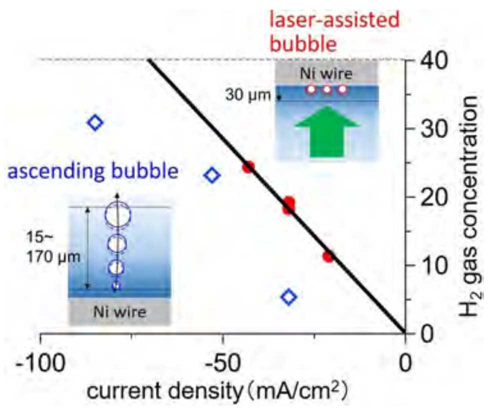


Fig. 2 Comparison of dissolved H_2 gas concentration at the Ni wire electrode by the two different methods we have developed, i.e., detection of ascending and laser-assisted bubbles.

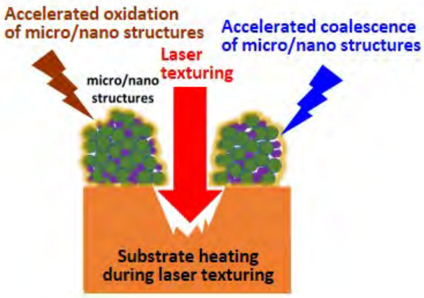


Fig. 3 Enhanced light absorption of metal surfaces by heat-assisted laser texturing.

lizing laser-assisted bubbles on the electrode.

3. Broadband light absorption of metal surfaces by heat-assisted laser texturing

Metal surfaces with high absorbance draw a lot of attention in recent years. In this work we have developed a new technique, heat-assisted laser texturing, to fabricate metal surfaces with broadband light absorption. In Fig. 3 we illustrate the underlying mechanism of enhanced light absorption by laser textured metal surfaces. Briefly, it comes from the geometric light trapping by micro/nano structures produced by laser texturing. The essence of heat-assisted laser texturing is to elevate the substrate temperature (by a few hundred °C) during laser texturing so that the texturing efficiency and oxidation speed are significantly promoted.

In Fig. 4 we summarize the reflectance of the Cu surfaces textured by the three different methods, i.e., laser texturing at room temperature, laser texturing at room temperature followed by thermal annealing at 300 °C for 1 hour, and heat-assisted laser texturing at 300 °C. It is clear that heat-assisted laser texturing is most effective.

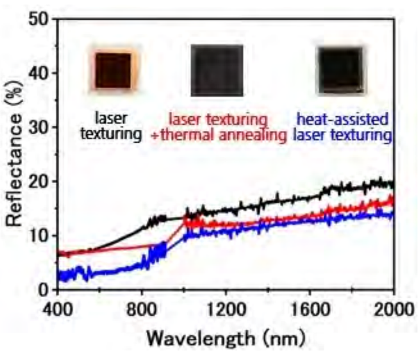


Fig. 4 Reflectance of Cu surfaces fabricated by the three different laser texturing methods.

4. Enhancing laser-nanoparticle interactions using a diffused laser beam

A laser beam with a good (flat-top or Gaussian) spatial profile is usually believed to be a prerequisite to maximize laser-matter interactions. What we have found in this work is that this is not necessarily true. As an example we demonstrate the efficient size-reduction of colloidal nanoparticles by a diffused laser beam. Representative results are summarized in Fig. 5, where colloidal silver nanoparticles with an initial diameter of 100 nm are irradiated by the pulsed laser beam at 532 nm with two different spatial profiles, normal and diffused beams. The normal beam directly coming from the laser output is converted to the diffused beam simply by placing a commercial holographic diffuser with transmission of 85 % and divergence angle of ~0.5°. From Fig. 5 we notice that the diffused beam significantly outperforms the normal beam in terms of the size reduction efficiency of nanoparticles, and the eminent peak appeared at ~400 nm by the diffused beam implies the very rapid size reduction of 100 nm Ag nanoparticles. To find the physical origin of this counterintuitive results we measure the beam profile to find that there are many bright speckles in the diffused beam as shown in the middle of Fig. 5. The XY-cuts of the normal and diffused beam profiles shown in the bottom of Fig. 5 clearly shows that the height of the speckles are by a few time higher than that of the normal beam with a nearly flat-top shape. Therefore, we can conclude that the physical origin of the counter-intuitively efficient laser-nanoparticle interactions by the diffused beam arises from the redistribution of laser energy by the formation of speckles where the local laser fluence exceeds the threshold of laser-induced size reduction.

Clearly, the demonstrated technique should be applicable to any kinds of nanoparticles and nanorods for size-reduction, reshaping, welding, etc., where a certain laser fluence threshold for the process exists.

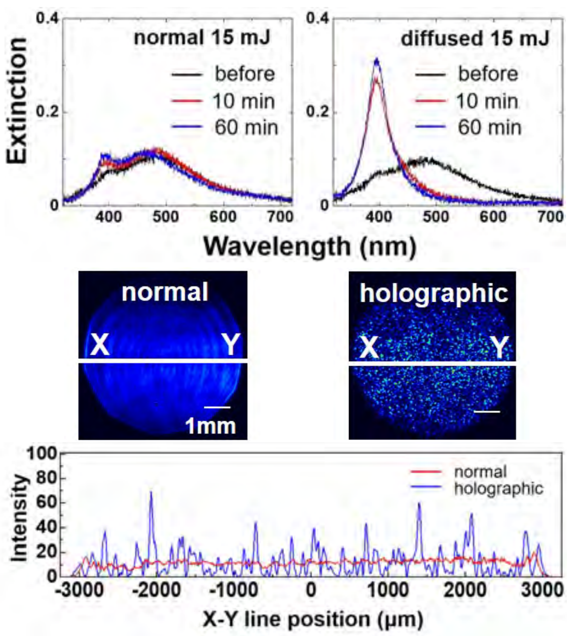


Fig. 5 Laser-induced size-reduction of Ag nanoparticles by the normal and diffused beams through a holographic diffuser.

Financial Support

中嶋隆，新エネルギー・産業技術総合開発機構，水素利用等先導研究開発事業/水電解水素製造技術高度化のための基盤技術研究開発/アルカリ水電解及び固体高分子形水電解の高度化

Publications

K. Ando, Y. Uchimoto, T. Nakajima, Probing the Dissolved Gas Concentration on the Electrode through Laser-Assisted Bubbles, Journal of Physical Chemistry C, 125, 38, 20952-20957, 2021

Presentations

中嶋隆，溶存濃度/レーザー駆動バブルの光学計測法の開発，京都大学 微細気泡研究会ワークショップ，京都大学宇治キャンパス, 2021.12.7-8

Advanced Energy Structural Materials Research Section

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

1. Introduction

In order to achieve the safety and efficient operations of advanced nuclear energy systems, the development and use of robust materials and the establishment of reliable system maintenance management are essential. This section addresses the mission of establishing the maintenance management methodology as well as material R & D for advanced nuclear energy systems such as fusion and fission reactors. Current main researches are as follows:

(1) Materials modeling and data-driven science & technology

Radiation damage processes in nuclear materials occur at a wide variety of time and length scales. To understand this process, so-called multiscale viewpoint and statistical arguments are required. In this section, efforts are made to model material behavior during irradiation complementarily using several computational techniques such as molecular dynamics, ab-initio quantum calculations, kinetic Monte-Carlo, rate-equation theory analysis, FEM and CFD. Recently, additional efforts have also been devoted to this research using machine learning, AI (artificial intelligence) and data-driven techniques.

(2) Plant integrity analysis

The structural integrity of the reactor pressure vessel (RPV) is critical to the reactor safety. Here, this is evaluated using three-dimensional computational fluid dynamics (3D-CFD) and the finite element method (FEM). Pressurized thermal shock (PTS) events during emergency water cooling, the most severe situation, are focused in this study. Through this evaluation, the risk of the RPV function loss is quantified and it is proposed as an indicator available for optimizing maintenance strategy.

(3) Effects of irradiation on the microstructure and mechanical property changes of materials

High energy particle irradiation leads to the formation of oversaturated interstitials and vacancies. The behavior of point defects is responsible for the evolution of the microstructure, which may cause degradation, (or development), of the mechanical properties of the material. The elucidation of the behavior of point defects is essential for understanding the mechanisms responsible for the changes in mechanical properties. In our study, the microstructure evolution under high energy particle irradiation has been investigated experimentally and computationally.

2. Statistical arguments on non-equilibrium point defect production in materials under irradiation

In fusion reactor structural materials, displacement cascade process is initiated by collisions of incident high energy neutrons with target atoms, resulting in the production of a large number of athermal point defects, which significantly affects the microscopic composition and microstructure of the materials and changes their mechanical properties; hence, it is of great importance to investigate this process in depth. However, since the displacement cascade process occurs on a time scale of several tens of picoseconds, it is very difficult to observe by experiments, and computer simulation techniques are needed instead. Molecular dynamics (MD) is one of the most powerful tools to investigate the defect production process in materials due to displacement cascades. In this study, molecular dynamics simulations are performed to investigate displacement cascades in Fe as a function of primary knock-on atom (PKA) energy. The statistics of defect production due to displacement cascades is focused, where 1000 cases are simulated for individual PKA energies. It is found in our simulations that the simulated probability density function of the number of athermal point defects produced by displacement cascade exhibits approximately a normal distribution as shown in Fig. 1. For PKA energies below

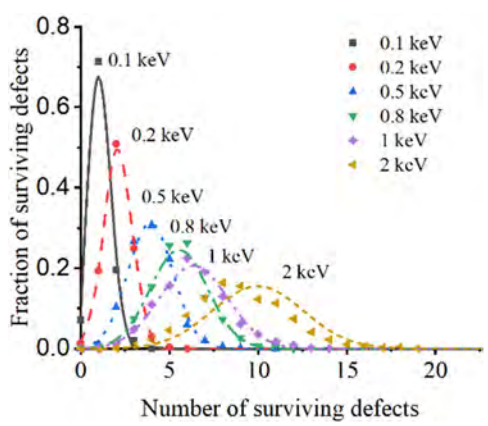


Fig. 1: PKA energy dependence of the number of point defects produced by displacement cascades.

100 eV, the average number of surviving point defects is in proportion to PKA energy with a constant standard deviation. For higher energies, on the other hand, the average and the standard deviation individually show power dependence on PKA energy. These PKA energy dependences of the average number of surviving point defects are consistent with those of the NRT and Bacon models for lower and higher PKA energies, respectively. Statistical characteristics of displacement cascades will help to describe the changes in the microstructure and mechanical properties of materials under irradiation.

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

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

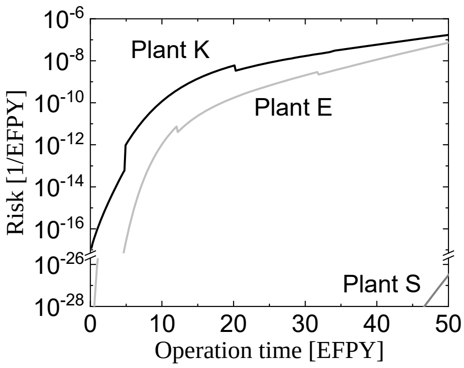


Fig. 2: The time evolutions of the predicted and corrected DBTT values and embrittlement risks for the three plants.

4. Effects of irradiation on microstructural evolution in materials and corresponding mechanical properties

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

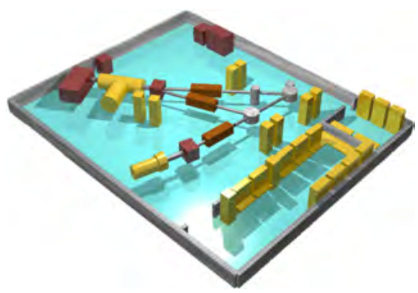


Fig. 3: Ion-accelerator (DuET)

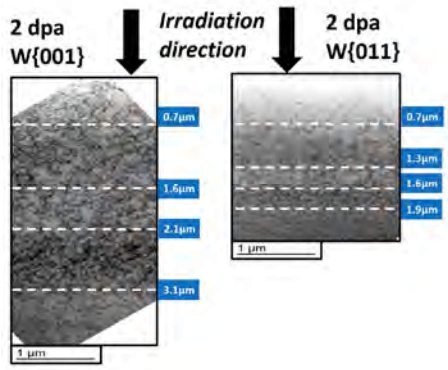


Fig. 4: TEM micrographs of W single crystals after irradiation

5. Application of AI technology to the image analysis for nuclear materials development

TEM image analysis of post-irradiation metals has often been conducted in the field of nuclear material development research, where an interpretation of imges is different unfortunately from person to person. To avoid this gap, a new attempt is being made to apply the state-of-the art AL technology to the image analysis. If this attempt progresses successfully, it should be possible to bridge the gap between the skill levels of skilled and novice users.

Financial Support

1. Grant-in-Aid for Scientific Research

森下和功，基盤研究(C)，ミクロからマクロまで総動員して老朽化設備の破損リスクを管理する方法

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

木村晃彦，基盤研究(B)，低放射化 ODS 鋼における耐照射脆性のナノ・メゾ組織定量化モデルの構築（繰越し）

2. Others

森下和功，量子科学技術研究開発機構，核融合中性子照射場の理論的定量化に関する研究

藪内聖皓，長瀬産業（株），インフラ鋼構造物に生成するさびの構造解明

藪内聖皓，（株）原子力安全システム研究所，原子炉容器鋼の照射ミクロ組織変化へのＮｉ影響の検討

Publications

H. Yuya, R. Kobayashi, K. Otomo, K. Yabuuchi, A. Kimura, Microstructure and mechanical properties of HAZ of RPVS clad with duplex stainless steel, Journal of Nuclear Materials, 545, 152756, 2021

X. Yi, Y. Du, D. Geng, Z. Li, W. Han, P. Liu, J. Chen, K. Yabuuchi, K. Yoshida, S. Ohnuki, Q. Zhan, F. Wan, Y. Nagai, Heavy-ion irradiation and post-irradiation annealing effects in explosion-welded CuCrZr/316LN joints for ITER application, Materials Characterization, 178, 111252, 2021

K. Fukumoto, T. Mabuchi, K. Yabuuchi, K. Fukui, Irradiation hardening of stainless steel model alloy after Fe-ion irradiation and post-irradiation annealing treatment, Journal of Nuclear Materials, 557, 153296, 2021

H. Yuya, K. Yabuuchi, A. Kimura, Radiation embrittlement of clad-HAZ of RPV of a decommissioned BWR plant, Journal of Nuclear Materials, 557, 153300, 2021

L. Zhang, Y.F. Du, W.T. Han, P.P. Liu, X.O. Yi, K. Yabuuchi, S. Ohnuki, F.R. Wan, An approximate in-situ method for investigating irradiation damage of grain boundary, Nuclear Materials and Energy, 29, 101056, 2021

K. Yabuuchi, S. Kondo, T. Hinoki, R. Kasada, 複合ビーム材料照射装置 DuET を用いた核融合炉材料研究と関連材料研究の展開, Journal of Plasma and Fusion Research, 97, 7, 403, 418, 2021

Y. Chen, K. Morishita, Molecular dynamics simulation of defect production in Fe due to irradiation, Nuclear Materials and Energy, 30, 101150, 2022

Presentations

森下和功, 福島第一原発事故で顕在化した課題，日本保全学会第 17 回学術講演会, オンライン開催, 2021.7.6-8

阮小勇， 森下和功，RPV 保全最適化のための３D-CFD＆FEM による PTS 時の構造健全性評価：非対称原子炉冷却の効果, 日本保全学会第 17 回学術講演会, オンライン開催, 2021.7.6-8

陳昱婷，豊田達也，祝梁帆，森下和功，渡辺淑之，野澤貴史，核融合中性子照射場の理論的定量化に関する研究，量子科学研究開発機構六ケ所研究所 BA 共同研究令和 3 年度キックオフ会合，オンライン開催, 2021.7.30

阮小勇，渡辺淑之，安堂正巳，野澤貴史，森下和功, 核融合中性子照射場の理論的定量化に関する研究, 量子科学研究開発機構六ケ所研究所 BA 共同研究令和 3 年度キックオフ会合，オンライン開催, 2021.7.30

陳昱婷，豊田達也，祝梁帆，森下和功，渡辺淑之，野澤貴史, PKA energy dependence of defect production in collision cascades, Institute of Advanced Energy, Kyoto University, 12th International Symposium of Advanced Energy Science, オンライン開催, 2021.9.7

祝梁帆，森下和功，渡辺淑之，藪内聖皓, 中性子照射下における材料損傷過程の反応速度論解析，日本原子力学会 2021 年秋の大会，オンライン開催, 2021.9.10

豊田達也，森下和功，藪内聖皓, 破壊き裂進展における照射効果の分子動力学評価，日本原子力学会 2021 年秋の大会，オンライン開催, 2021.9.10

國分悠輔，藪内聖皓，森下和功, Deep Learning を用いた透過型電子顕微鏡画像解析技術の開発，日本原子力学会 2021 年秋の大会，オンライン開催, 2021.9.14

Y. Chen, K. Morishita, Y. Watanabe, T. Nozawa, Molecular Dynamics Simulation of Defect Production in Fe due to Irradiation, ICFRM-20 組織委員会 20th International Conference on Fusion Reactor Materials (ICFRM-20), オンライン開催, 2021.10.24-29

X. Ruan, Y. Watanabe, K. Morishita, M. Ando, T. Nozawa, Relaxation volume of irradiation-induced defects in pure iron: Molecular-statics calculation with linear elasticity theory, ICFRM-20 組織委員会 20th International Conference on Fusion Reactor Materials (ICFRM-20), オンライン開催, 2021.10.24-29

岡本研正，岡本賢一郎，森下和功, 光電変換型トランジスタ「ダイスター」を用いた電力制御, 電気学会半導体電力変換／モータドライブ合同研究会, 立命館大学びわこ・くさつキャンパス＆WEB（ハイブリッド）, 2022.1.27

Yuting Chen，豊田達也，祝梁帆，森下和功, 核融合中性子照射場の理論的定量化に関する研究，量子科学研究開発機構六ケ所研究所令和３年度原型炉研究開発共同研究成果報告会，オンライン開催, 2022.2.7

祝梁帆，森下和功，渡辺淑之，藪内聖皓, 軽水炉圧力容器鋼における溶質原子クラスター形成のシミュレーション（ポスター），日本原子力学会春の年会，オンライン開催, 2022.3.16

祝梁帆，森下和功，渡辺淑之，藪内聖皓, 軽水炉圧力容器鋼における溶質原子クラスター形成のシミュレーション（口頭），日本原子力学会春の年会，オンライン開催, 2022.3.17

Yuting Chen，森下和功, 照射カスケード損傷による鉄の欠陥クラスター生成に関する統計的な研究 分子動力学シミュレーション，日本原子力学会春の年会，オンライン開催, 2022.3.17

岡本賢一郎，岡本研正，森下和功, バイポーラトランジスタの動作に関する新仮説－トランジスタ光動説－，応用物理学会春季学術講演会，青山学院大学相模原キャンパス, 2022.3.22-26

岡本賢一郎，岡本研正，森下和功, パワーダイスター―を用いたEV制御とDC/AC変換，電気学会全国大会，オンライン開催, 2022.3.23

Nano Optical Science Research Section

K. Matsuda, Professor
K. Shinokita, Assistant Professor

1. Introduction

We are working on basic and applied research of nano-materials from a viewpoint of optics and material science. Our research aims at exploring new physical and chemical phenomena leading to applications of novel nano-materials including carbon nanotubes, layered transition metal dichalcogenides, perovskite for efficient utilization of light energy and development of future optoelectronic devices with ultra-low energy consumption. Followings are main research achievements in the year of 2021.

1. Moiré exciton-phonon coupling in a $WSe_2/MoSe_2$ heterobilayer

The interference of two similar patterns is a universal concept in physics that plays a pivotal role in modern science and technology such as in gravitational wave detection, optical frequency combs, superconducting quantum interference devices (SQUIDs), and cold atoms in optical lattices. The moiré patterns of van der Waals heterostructures arising from interference of angular- or lattice-mismatched atomically thin materials with honeycomb structures, such as graphene and semiconducting transition metal dichalcogenides (TMDs), have attracted increasing attention because of the potential for engineering a range of emergent quantum phenomena. Examples include superconductivity, ferromagnetism near ¾ filling, and correlated insulator phases in twisted bilayer graphene. In a two-dimensional (2D) semiconducting TMD heterostructure, the stacking of two different monolayer TMDs usually results in staggered type II band alignment, which causes separation of electrons and holes in different layers, or interlayer excitons (Coulomb-bound electron-hole pairs). The nature of the interlayer excitons is modulated by the moiré pattern because of the spatially varying atomic registry. The moiré pattern works as a periodic trap potential to confine the interlayer exciton in zero dimensions (0D) (moiré exciton, Fig. 1) and spatially organize the moiré-trapped excitons, which results in an array of quantum-dot-like 0D systems composed of a moiré exciton ensemble. In addition, the moiré period and interaction between the moiré excitons can be tailored by the stacking angle. Therefore, moiré exciton ensembles in periodic moiré potentials have potential for dense coherent quantum emitters and quantum simulation of many-body physics, which could result in a number of applications in quantum optics, including quantum dot lasers, entangled photon lasers, and Dicke superradiance.

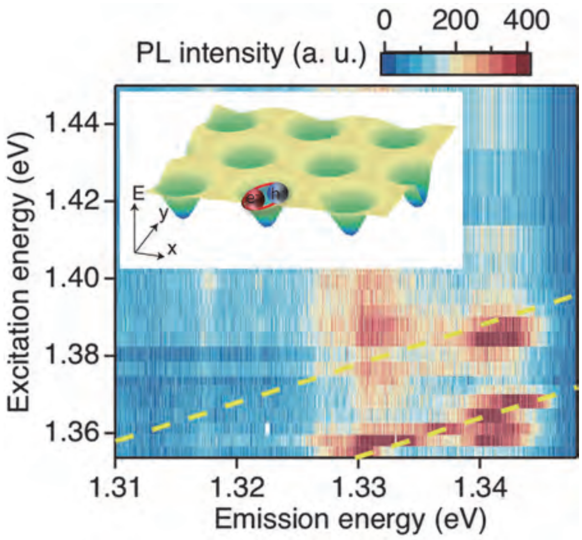


Fig. 1 2D PLE map of $WSe_2/MoSe_2$ heterobilayer, measured at low temperature. Dotted lines correspond to phonon resonances. Inset shows schematic of moiré exciton.

The electronic, optical, and transport properties of solids are frequently dominated by electron-phonon or exciton-phonon interactions. Extensive works on exciton and phonon interactions in 2D materials and their van der Waals heterostructures have been performed. For instance, emergent interlayer exciton-phonon coupling was observed in a WSe_2/*h*-BN heterostructure system, which provides important information for the generation and control of intriguing physical properties of 2D materials. The exciton-phonon interaction of the heterostructure can also be modified by the periodic moiré potential, which would pave a new way for control of diverse fascinating physical behaviours of 0D-like moiré excitons towards coherent quantum emitters and quantum simulation of many-body physics. To date, the signatures of moiré excitons have been optically studied by absorption and photoluminescence (PL) measurements, where the moiré exciton was confirmed by the appearance of sharp peaks in low-temperature PL spectra under low excitation power conditions, reflecting the trapping of excitons in the moiré potential. However, the interaction between the moiré exciton and phonon have yet to be studied experimentally. To explore novel quantum phenomena in moiré superlattices, it is important to understand the moiré exciton-phonon interaction, which play a dominant role in the intriguing properties of moiré exciton ensembles and quantum applications.

Here, we study the moiré exciton and phonon interaction in a twisted $WSe_2/MoSe_2$ heterobilayer based on near-resonant photoluminescence excitation (PLE) spectroscopy, taking advantage of extraction of coupling of specific moiré exciton to phonon. The experimentally observed PL spectrum strongly depending on the excitation energy shows highly selective excitation of the ground state of the moiré exciton at phonon resonances. On the other hand, the negligibly small off-resonant PLE signal in the interlayer region suggests δ-function discrete energy levels, which reflects density of states of a 0D-like system for the interlayer moiré exciton. In addition, the excitation power dependence of the PL spectra reveals the moiré exciton dynamics between different potential minima with discrete energy levels via the resonant phonon scattering process.

Our results shed light on new aspects of moiré exciton and phonon coupling and lay the groundwork to explore quantum phenomena in moiré superlattices for quantum emitters with extremely low threshold lasing and so on.

2. Experimental Evidence of Magonon-Moiré Trion Complex in Monolayer Semiconductor and Antiferromagnet vdW Heterostructures

Since the discovery of 2D layered ferromagnetic and antiferromagnetic materials, the intriguing magnetic properties of 2D materials have attracted considerable interest in the research field of material science. Among 2D layered magnetic materials, transition metal phosphorous dichalcogenides ($TMPX_3$; TM = Mn, Ni, Fe, Co; X = S, Se) have been extensively studied as a model system of layered magnetic materials. For instance, free excitons coupled to magnons were reported in both bulk antiferromagnetic $MnPS_3$ and heterostructures composed of semiconducting $MoSe_2$ and antiferromagnetic $MnPSe_3$. Moreover, novel excitons with an ultra-narrow PL peak were found in bulk $NiPS_3$; these excitons arise from the many-body states of Zhang–Rice singlets and reach a coherent state assisted by the antiferromagnetic order. However, the interaction between moiré excitonic states (excitons and trions) and magnetic elementary excitations in magnetic materials has yet to be experimentally studied. To explore novel quantum phenomena in moiré superlattices, it is important to prove the existence of moiré excitonic states (excitons and trions) coupled with magnetic elementary excitations, which would give rise to the intriguing properties of moiré excitonic systems with magnetic functionalities.

Here, we report the emergence of intralayer trions

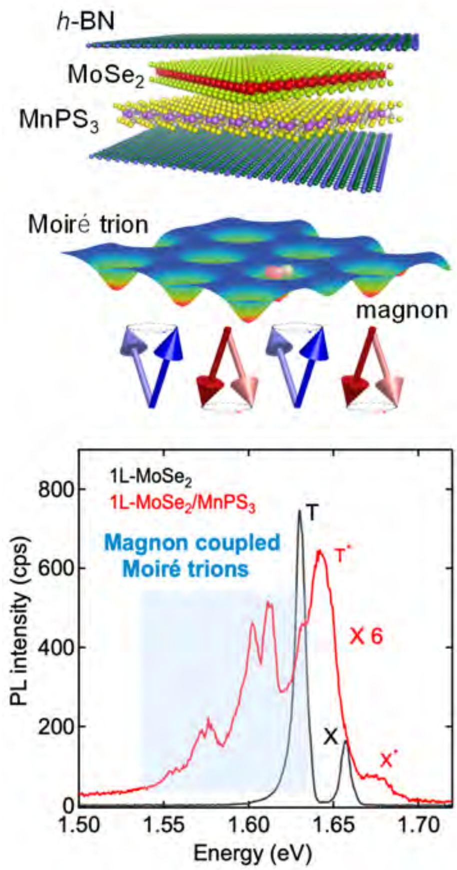


Fig. 2 Schematic of $MoSe_2/MnPS_3$ vdW heterostructure. Schematic of magnon-moiré charged exciton (trion) complex. Low temperature photoluminescence spectra of reference monolayer $MoSe_2$ and $MoSe_2/MnPS_3$ vdW heterostructure. Exciton and trion related peaks are denoted as X and T, respectively.

localized in the moiré potentials formed by twisted monolayer $MoSe_2$ and antiferromagnetic $MnPS_3$ vdW heterostructure. We carefully investigated the low-temperature PL spectra of the vdW heterostructure and found additional fine spectral structures on the low-energy side of the coupled magnon–trion peaks below the Néel temperature (78 K) of $MnPS_3$ (Figure 2). The fine spectral structures with long lifetime and coherence time are assigned to localized intralayer trion–magnon complexes in the moiré potentials (moiré trion–magnon complexes), which makes the moiré excitons different from those frequently observed in bilayer semiconducting TMD heterostructures, implying the appearance of magnetic moiré excitonic states.

We envisage that novel vdW heterostructures characterized by a combination of monolayer semiconductor TMDs and antiferromagnetic $TMPX_3$ will reveal the existence of magnetic moiré excitonic states. The precise energies and light emission intensities of these magnetic moiré-excitonic states can be tuned and controlled by applying external magnetic fields. Therefore, these states also provide a good platform toward for future application of quantum emitters with magnetic functionalities.

Collaboration Works

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

Financial Support

Grant-in-Aid for Scientific Research

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

松田一成，学術変革領域研究(A)，２.５次元構造の分析技術開発

松田一成，学術変革領域研究(A)，２.５次元物質科学の総括（分担金）

松田一成，挑戦的研究（萌芽），高次データー科学による原子層物質のバレースピン制御

篠北啓介，基盤研究(B)，モアレ超構造における協力的量子光学現象の開拓

田中絢也，特別研究員奨励費，室温動作超広帯域光検出器の実現に向けた量子物質赤外応答の解明

Publications

Y. Yamada, Y. Zhang, H. Ikeno, K. Shinokita, T. Yoshimura, A. Ashida, N. Fujimura, K. Matsuda, D. Kiriya, Ultralarge Photoluminescence Enhancement of Monolayer Molybdenum Disulfide by Spontaneous Superacid Nanolayer Formation, ACS Applied Materials & Interfaces, 13, 21, 25280-25289, 2021

K. Shinokita, Y. Miyauchi, K. Watanabe, T. Taniguchi, K. Matsuda, Resonant Coupling of a Moiré Exciton to a Phonon in a WSe2/MoSe2 Heterobilayer, Nano Letters, 2021

J. Pu, W. Zhang, H. Matsuoka, Y. Kobayashi, Y. Takaguchi, Y. Miyata, K. Matsuda, Y. Miyauchi, T. Takenobu, Room-Temperature Chiral Light-Emitting Diode Based on Strained Monolayer Semiconductors, Advanced Materials, 2021, 2100601, 2021

Y. Sato, T. Nishimura, D. Duanfei, K. Ueno, K. Shinokita, K. Matsuda, K. Nagashio, Intrinsic Electronic Transport Properties and Carrier Densities in PtS2 and SnSe2: Exploration of n+-Source for 2D Tunnel FETs, Advanced Electronic Materials, 2021, 2100292, 2021

X. Wang, K. Shinokita, K. Matsuda, Radiative lifetime and dynamics of trions in few-layered ReS2, Applied Physics Letters, 2021, 113103, 2021

T. Nishihara, A. Takakura, M. Shimasaki, K. Matsuda, T. Tanaka, H. Kataura, Y. Miyauchi, Empirical formulation of broadband complex refractive index spectra of single-chirality carbon nanotube assembly, Nanophotonics, 2022

Y. Yakiyama, M. Li, J.Y. Wu, K. Sambe, T. Akutagawa, T. Kajitani, T. Fukushima, K. Matsuda, H. Sakurai, Dielectric Response of Difluorinated Sumanene Caused by the Inplane Motion, Materials Chemistry, 2022

Y. Zhang, H. Kim, W. Zhang, K. Watanabe, T. Taniguchi, Y. Gao, M. Maruyama, S. Okada, K. Shinokita, K. Matsuda, Magnon-Coupled Intralayer Moiré Trion in Monolayer Semiconductor–Antiferromagnet Heterostructures, Advanced Materials, 2022

Presentations

K. Matsuda, Novel Optical Science in Monolayer Transition Metal Dichalcogenide and its Heterostructure, The 8th International Workshop on 2D Material, ハイブリッド開催(Fudan, China), 2021.6.29

M. Kobayashi, K. Shinokita, N. Wada, T. Endo, Y. Miyata, K. Matsuda, Optical properties of transition metal dichalcogenides with microshperical optical cavity, 第 61 回フラーレン・ナノチューブ・グラフェン総合シンポジウム，オンライン開催, 2021.9.1

K. Shinokita, Y. Miyauchi, K. Watanabe, T. Taniguchi, K. Matsuda, Novel excitonic features of moiré exciton in twisted van der Waals heterostructures, 第 61 回 フラーレン・ナノチューブ・グラフェン総合シンポジウム，オンライン開催, 2021.9.3

M. Shimasaki, T. Nishihara, K. Matsuda, T. Endo, Y. Miyata, Y. Miyauchi, Optical properties of lateral heteromonolayer WSe2–MoSe2, 2021 JSAP-OSA symposium, Online, 2021.9.10

H. Kim, K. Shinokita, W. Zhang, K. Watanabe, T. Taniguchi, K. Matsuda, Dynamics of Moiré Exciton in MoSe2-WSe2 Heterstrosucture, 2021 JSAP-OSA symposium, Online, 2021.9.10

K. Shinokita, Y. Miyauchi, K. Watanabe, T. Taniguchi, K. Matsuda, Moiré exciton-phonon resonance in WSe2/MoSe2 heterobilayer, 2021 JSAP-OSA symposium, Online, 2021.9.10

松田一成，原子層半導体・ヘテロ構造の光科学とその展開，日本物理学会 2021 秋季大会，オンライン開催, 2021.9.22

篠北啓介，宮内雄平，松田一成, WSe2/MoSe2 ヘテロ二層の発光スペクトルの強度依存性，日本物理学会 2021 秋季大会，オンライン開催, 2021.9.22

K. Matsuda, "Optical Physics of Moiré Excitonic Systems in Two-Dimensional (2D) Hetero-Structures ", The 11th A3 symposium on Emerging Materials，ハイブリッド開催(Wuhan, China), 2021.12.15

K. Matsuda, Optical probing of excitonic states in nano-carbon and anisotropic atomically thin two-dimensional materials, The 2021 International Chemical Congress of Pacific Basin Societies, Online, 2021.12.21

H. Wu, T. Nishihara, A. Takakura, K. Matsuda, T. Tanaka, H. Kataura, Y. Miyauchi, Tailoring optical characteristics of single-chirality carbon nanotube assemblies toward opto-thermal applications，第 62 回 フラーレン・ナノチューブ・グラフェン総合シンポジウム，オンライン開催, 2021.3.2

K. Shinokita, K. Aino, K. Watanabe, T. Taniguchi, K. Matsuda, Negative circularly polarization of moiré exciton luminescence in WSe2/MoSe2 heterobilayers, 第 62 回 フラーレン・ナノチューブ・グラフェン総合シンポジウム，オンライン開催, 2021.3.2

D. Dong, W. Zhang, K. Watanabe, T. Taniguchi, K. Shinokita, K. Matsuda, Electrically tunable moiré trions in twisted WSe2/MoSe2 heterobilayers，第 62 回 フラーレン・ナノチューブ・グラフェン総合シンポジウム，オンライン開催, 2021.3.3

Y. Okamura, K. Shinokita, K. Watanabe, T. Taniguchi, K. Matsuda, A small number of moiré exciton photoluminescence in nanofabricated MoSe2/WSe2 heterobilayers，第 62 回 フラーレン・ナノチューブ・グラフェン総合シンポジウム，オンライン開催, 2021.3.4

S. Asada, K. Shinokita, K. Watanabe, T. Taniguchi, K. Matsuda, Spontaneous photocurrent of WSe2/CrPS4 hetero-interface with in-plane polarization and highly air-stability，第 62 回 フラーレン・ナノチューブ・グラフェン総合シンポジウム，オンライン開催, 2021.3.4

篠北啓介，相野薫平，渡邊賢司，谷口尚，松田一成, WSe2/MoSe2ヘテロ二層におけるモアレ励起子の円偏光発光分光，日本物理学会第 77 回年次大会，オンライン開催, 2022.3.16

岡村勇輝，篠北啓介，渡邊賢司，谷口尚，松田一成, 微細加工した MoSe2/WSe2 ヘテロ二層の少数モアレ励起子による光学特性，第 69 回応用物理学会春季学術講演会，オンライン開催, 2022.3.22

Clean Energy Conversion Research Section
(Two-dimensional tunnel FET)

Kosuke Nagashio, Visiting Professor
(The University of Tokyo)

1. Introduction

For the 2D/2D interfacial properties in TFET, the defect-free clean heterointerface is critical for obtaining the BTBT dominant current under reverse bias at the diode. Although the BTBT current has been demonstrated at low temperatures [1], thermally activated behavior often appears at higher temperatures near RT. That is, the generation current governs the total current, resulting in degradation of the SS at RT. This suggests that interface states exist even for 2D/2D interfaces. In general, high-*k* top gate oxides have been used in most of 2D TFETs reported thus far to enhance the gate capacitance. However, how the quality of the 2D/2D interface is affected by the deposition of high-*k* oxides has not been revealed yet. Therefore, comparisons between high-*k* and *h*-BN gate insulators should be carried out systematically in the same 2D TFET system because the use of *h*-BN in TFETs has been quite limited.

In this work, we systematically studied all 2D heterostructure TFETs produced by combining the type III n-MoS_2/p^+-MoS_2 heterostructure with the *h*-BN top gate in order to achieve SS values less than 60 $mVdec^{-1}$ at RT.

2. Strategy in 2D/2D TFET structure

There are three strategies to further reduce the SS values: (i) Recently, we have discovered that the deposition of Al_2O_3 top gate oxide on the MoS_2 channel increases the interface states density due to the introduction of strain in the MoS_2 channel on the *h*-BN substrate, as shown in Fig. 1.[2] Therefore, an *h*-BN top gate insulator was adopted to benefit from the electrically inert interface in 2D heterostructure TFETs. (ii) The p^+-MoS_2 source was used because the E_F of p^+-MoS_2 cannot be modulated due to the degenerately high doping of the p^+-MoS_2. (iii) According to the transmission probability calculated for carrier transport through the BTBT barrier,[3] the E_G for the channel should be larger than that for the source to keep the off current low but E_G also should be as small as possible to increase the transmission probability. Therefore, the 1L and 3L MoS_2 channels were compared. Based on these three considerations, all 2D heterostructure TFETs were fabricated to achieve SS values lower than 60 $mVdec^{-1}$.

3. Results & Discussion

Fig. 2 shows a schematic (a) and an optical micrograph (b) of a typical *h*-BN/n-MoS_2/p^+-MoS_2/*h*-BN all 2D heterostructure TFET. The heterostructure

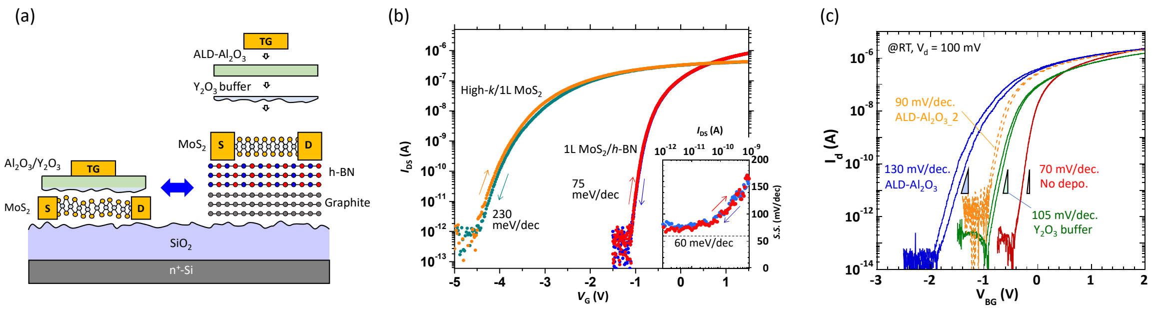


Fig. 1 a) Schematic illustration of two kinds of 1L-MoS_2 FET. One is FET with high-k top gate insulator, the other is heterostructure FET with h-BN and graphite. b) Transfer characteristics of two kinds of 1L-MoS_2 FET. The heterostructure MoS_2 FET shows better SS value. c) Transfer characteristics of 1L-MoS_2/h-BN FET before top-gate deposition (red), after Y_2O_3 buffer layer deposition (green), and after ALD-Al_2O_3 deposition (blue). Initially, back gate heterostructure 1L-MoS_2 FET was prepared and then top gate was deposited. The transfer characteristics were measured through the back gate. The back side MoS_2/h-BN interface was degraded by the top gate deposition, suggesting that top gate deposition may degrade

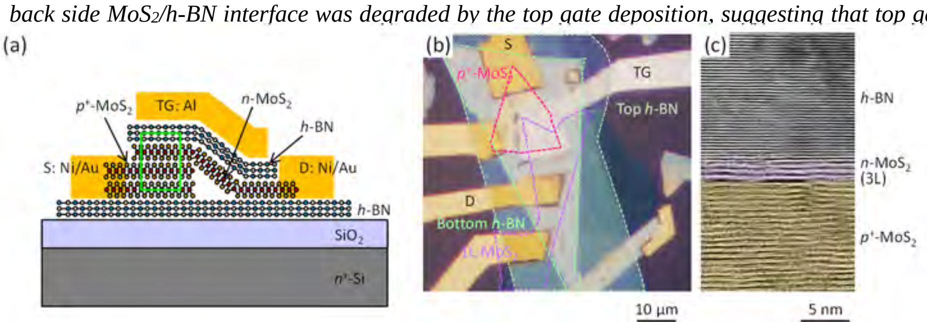


Fig. 2 a) Schematic illustration and b) optical micrograph of all 2D heterostructure TFET. c) Cross sectional TEM image of all 2D heterostructure at the solid rectangular in a). The number of MoS_2 layers is 3.

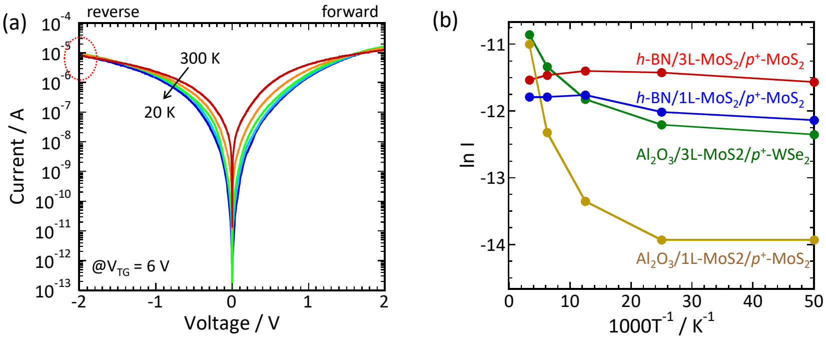


Fig. 3 a) Diode properties in the 3L-n-MoS_2/p^+-WSe_2 heterostructure at V_{TG} = 6 V and different temperatures (20, 40, 80, 160, and 300 K). b) Arrhenius plot of the current at the reverse bias of -2 V for different heterostructures.

device was prepared by pinpoint pickup and bubble free assembly technique.[4] The typical thickness for the top gate *h*-BN insulator and the p^+-MoS_2 source are ~15 nm and ~30 nm, respectively. The atomically sharp gate stack interfaces are clearly seen in the cross-sectional TEM image of Fig. 2c since all of the 2D materials are stable in air. As was expected, the diode properties of the all 2D heterostructure TFET with the 3L-*n*-MoS_2 channel in Fig. 3a shows the type III band alignment at V_{TG} = 6 V. The negative differential resistance (NDR) trend at the forward side is not visible. This could be explained by the suppression of the diffusion current due to the larger barrier between the conduction band minimum for p^+-MoS_2 and the valence band maximum for the *n*-MoS_2 channel because the E_G of bulk MoS_2 (~1.4 eV) is larger than the E_G of bulk WSe_2 (~1.2 eV). An Arrhenius plot of the current at the reverse bias of -2 V is compared with other heterostructures in Fig. 3b. It should be noted that all four heterostructure TFETs exhibit type III band alignment. For the *h*-BN top gate heterostructure devices with the 1L and 3L MoS_2 channels, temperature-independent behavior is evident over the entire temperature range, indicating that BTBT is dominant even at RT. This is quite promising for TFET operation with low SS values at RT. On the other hand, when Al_2O_3 was used as the top gate insulator, thermally activated behavior at high temperatures was clearly observed regardless of the source crystal. These comparisons indicate that the trap-related generation-recombination current [5] and/or the trap-assisted tunneling current under reverse bias are drastically suppressed by the successful integration of the electrically inert interface in the 2D heterostructure TFET.

Finally, the transfer characteristics of the 2D heterostructure TFETs at the reverse bias of -2 V at RT are shown in Fig. 4a. The estimated SS values are shown as a function of ID in Fig. 4b. For the 3L-*n*-MoS_2 channel, low *SS* value comparable with 60 $mVdec^{-1}$ of the Boltzmann limit was achieved at RT. Since the *SS* value for the 1L-*n*-MoS_2 channel was over 100 mV/dec, the smaller E_G of the 3L-*n*-MoS_2 channel was preferable. However, leakage current contributions should be considered carefully since artificially low SS values are often reported. We have confirmed that I_D overlaps with I_S for the 3L-*n*-MoS_2 channel because there is no gate leakage, which supports that the *SS* value is low comparable to 60 $mVdec^{-1}$ at RT.

4. Summary

The key finding regarding the quality of the heterointerface is that producing the defect-free clean heterointerface via integration of the *h*-BN top gate provides the BTBT dominant current even at RT. All 2D heterostructure TFETs produced by combining the type III *n*-MoS_2/p^+-MoS_2 heterostructure with the *h*-BN top gate insulator resulted in low SS values at RT.

References

[1] J. He, *et al.*, Adv. Electronic Mater. 2018, 4, 1800207.
[2] N. Fang, *et al.*, Adv. Func. Mater. 2019, 29, 1904465.
[3] A. M. Ionescu, H. Riel, Nature 2011, 479, 329-337.
[4] S. Toyoda, et *al.*, APEX 2019, 12, 055008.
[5] T. Gotow, *et al.*, J. Appl. Phys. 2019, 126, 214502.

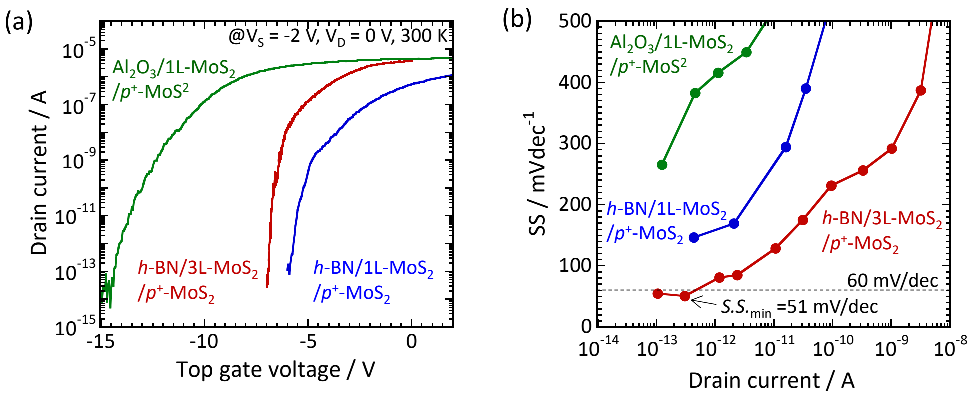


Fig. 4 a) Transfer characteristics for the three different heterostructure TFETs. b) SS as a function of I_D for the three different heterostructure TFETs.

Clean Energy Conversion Research Section

Hisayoshi Matsushima, Visiting Associate Professor
(Hokkaido University)

1. Introduction

Fusion reactor is one of the key technologies to achieve the zero-emission energy [1]. Hydrogen isotopes (hydrogen: H, deuterium: D, and tritium: T) are used as fuels in the reactor, but the present production process requires high energy consumption. For solving this problem, we have proposed the unique separation method, combined electrolysis and fuel cell (CEFC) [2]. Hydrogen and oxygen gases generated by water electrolysis are used for fuel cell as the power generation, while the hydrogen isotope separation is conducted. In fuel cell, the heavy isotopes are concentrated in the produced water, which can be returned to the electrolyte during the electrolysis [3].

The D separation by the aqueous solution and polymer electrolyte electrolysis has been reported [4]. It is suggested that the separation efficiency depends on the electrochemical kinetic factors, *ex.* hydrogen evolution reaction (HER). However, there are few papers about the fundamental study.

In molten salt, the HER occurs through the oxidation reactions of hydride ions (H^-) and deuteride ions (D^-), which is different from that in aqueous solution systems. That is, due to the difference in the HER mechanism, the high isotope separation can be expected. In addition, the electrochemical reaction rate can be increased due to the high temperature. The low overvoltage reduces the energy consumption of the separation system. Therefore, in the present project, a novel method using molten salt electrolysis is focused and the D separation is studied.

2. Electrochemical Measurement

In this study, experiments were conducted in the three electrodes system (Fig. 1). The chemicals were dried in vacuum environment at 723 K for 24 hours. They were mixed with the ratio of LiCl:KCl = 58.5:41.5 mol% and melted at 673 K. Three different electrode materials (Mo, Pt, Zn) were used for the working electrode, and a glassy carbon rod or an Al wire was used for the counter electrode. The reference electrode was an Al-Li alloy in an electrochemically formed (α + β) two-phase coexisting state. The potential was calibrated against the Li^+/Li electrode. The LiH and LiD were added to the molten salt at 1.0 mol% and 0.2-1.0 mol%, respectively.

Cyclic voltammograms (CV) with a several of potential scanning speeds was measured. Figure 2 shows the CV of the Mo electrode when LiD (0.4 mol%) was added in the LiCl-KCl molten salt. When the potential was scanned in the anodic direction, the oxidation peak associated with the deuterium evolution reaction (DER) was observed at 0.7-0.8 V *vs.* Li^+/Li. As the scanning speed was increased in the range of 0.2~5.0 V s^{-1}, the peak current increased and the peak shape was clearer. When the potential reached at 1.0 V, the scan direction was reversed to examine the reduction reaction. Interestingly unlike HER, the reduction current was hardly measured in DER. This may be explained by the low solubility of D_2 gas in the molten salt.

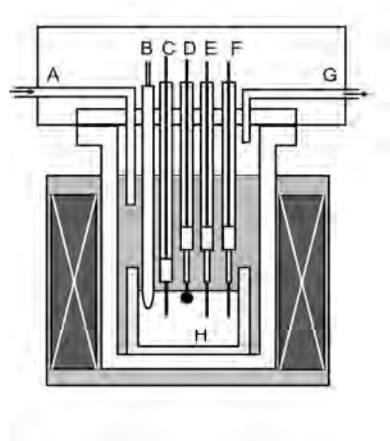


Fig. 1 Schematic illustration of experimental setup; (A) Ar gas inlet, (B) thermocouple, (C) counter electrode, (D) working electrode, (E) Al-Li wire reference electrode, (F) Al wire counter electrode, (G) gas outlet, (H) electrolyte.

3. D Separation

The hydrogen gas during the potentiostatic electrolysis was discharged from the outlet with Ar

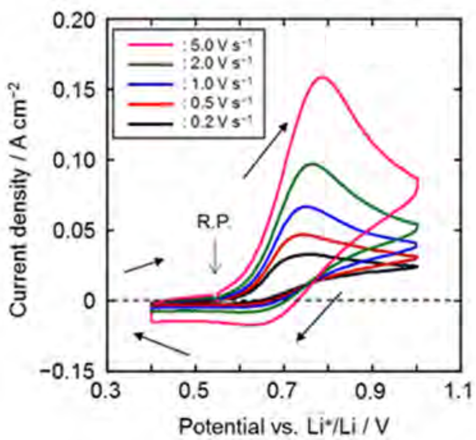


Fig. 2 Cyclic voltammograms of Mo electrode in LiCl-KCl-LiD (0.4 mol%) at various scanning rate.

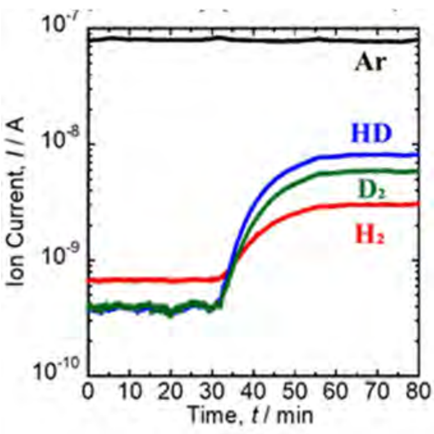


Fig. 3 QMS results of the hydrogen gas evolved from Mo electrode.

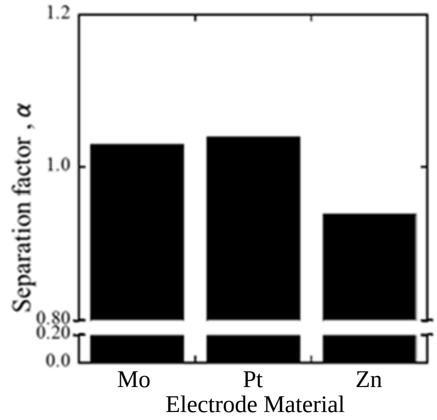


Fig. 4 Bar graph of separation factor at several electrode materials; Mo, Pt, and Zn.

carrier gas. It was introduced into a quadrupole mass spectrometer (QMS) for the gas analysis. Figure 3 shows the result of the QMS analysis, when the electrolysis was conducted at 0.7 V. The concentration of LiH and LiD was 1.0 mol%. The gas components were consisted of mass number $m = 2$ (H_2), $m = 3$ (HD), and $m = 4$ (D_2). Among the three gas mixtures, the ratio of HD gas was the largest, as seen in the water electrolysis in 10 at% D [4].

To quantitatively evaluate the separation, the separation factor, α, was defined in Eq. (1),

$$\alpha = \{[H]/[D]\}_g / \{[H]/[D]\}_m \qquad (1)$$

where [L] is atomic concentration of the hydrogen isotopes (H and D), subscript of "g" is gas and "m" is molten salt. The atomic concentration in the hydrogen gas was calculated from the ion current of QMS by following equation,

$$[H]/[D]=[(i_{H2}\times 2+i_{HD}) / (i_{D2}\times 2+i_{HD})] \qquad (2)$$

where i_x is the ion current of gas x.

The α value of the electrode materials are summarized in Fig. 4. For Mo and Pt electrodes, α was slightly larger than 1.0. This suggested that D was enriched in the electrolyte, as done by water electrolysis. On the other hand, for Zn electrode, the α value less than 1.0. That is, D was enriched in the generated hydrogen gas. This phenomenon was inverse against the well-known electrolysis process.

5. Summary

The hydrogen isotope separation by the molten salt electrolysis showed different behavior form the water electrolysis. This suggests that not only kinetic factors related to electrode reactions, but also the state of the dissolved gas differs among the isotopes. In the future, we will investigate the reduction reaction of the hydrogen isotopes on several electrode materials.

References

[1] E.S. Hanley, J.P. Deane, B.P.O. Gallachoir, *Renew. Sustain. Energy Rev.*, **82** (2018) 3027.

[2] R. Ogawa, R. Tanii, R. Dawson, H. Matsushima, M. Ueda, *Energy*, **149** (2018) 98.

[3] S. Shibuya, H. Matsushima, M. Ueda, *J. Electrochem. Soc.*, **163** (2016) F704.

[4] H. Matsushima, H. Sato, M. Ueda, H. Ito, *J. Electrochem. Soc.*, **166** (2019) F566.

Chemical Reaction Complex Processes Research Section

T. Nohira, Professor
T. Kodaki, Associate Professor
K. Kawaguchi, Program-Specific Associate Professor
T. Yamamoto, Assistant Professor

1. Introduction

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

In this fiscal year, we have researched an electrodeposition process of tungsten, sodium and potassium secondary batteries using ionic liquids, and an efficient bioethanol production process using ionic liquids.

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

Tungsten is a metal with excellent properties such as high heat resistance, high strength, and low thermal expansion. Therefore, it is used in a variety of applications, including carbide tools, heat sinks, and divertors in nuclear fusion reactors. However, due to its hardness and brittleness, tungsten is difficult to process into complex shapes and thin films. If tungsten can be plated on substrates with good processability, the range of applications will be greatly expanded. Thus, electrodeposition of tungsten in high-temperature molten salts has been investigated as one of the promising plating methods [1–3].

We have already reported the electrodeposition of α-W films in molten KF–KCl–WO_3 at 923 K and mixed phase films of α-W and β-W in molten CsF–CsCl–WO_3 at 873 K [4]. We also reported that β-W films with mirror-like surface were electrodeposited in molten CsF–CsCl–WO_3 at 773 K [5]. As continuing research, in this fiscal year, we investigated the effect of bath temperature on the smoothness and crystal structure of W films electrodeposited from molten CsF–CsCl–WO_3.

Fig. 1 shows the samples obtained at 6–25 mA cm^{-2} and 773–923 K. At 25 mA cm^{-2} and 773 K, no W deposits were obtained due to co-deposition of Cs metal fog because the potential during electrolysis was close to 0 V with respect to Cs^+/Cs potential. Under other conditions, gray or silver-colored deposits were obtained. The results of XRD analysis showed that all electrodeposits were metallic W. Interestingly, only β-W was detected below 823 K, both α-W and β-W were detected at 873 K, and only α-W was detected at 923 K. This indicates that the crystal structure of W electrodeposited varies with bath temperature. At 6 mA cm^{-2} and 773 K, a mirror-like surface was obtained, indicating that the surface of the electrodeposited W film was highly smooth. The reason for the smoother surface at lower bath temperatures is speculated to be due to the crystal structure of β-W and the suppression of crystal growth.

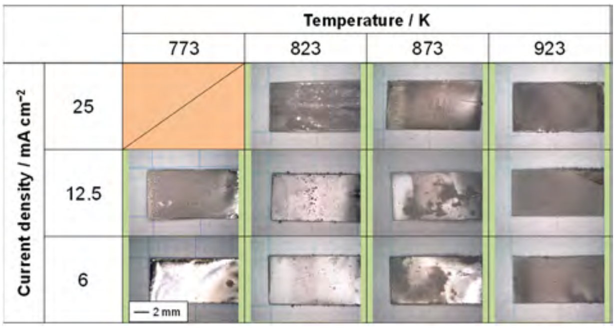


Fig. 1. Optical images of the samples obtained by galvanostatic electrolysis of Cu plate electrodes at various current densities and temperatures in molten CsF–CsCl–WO_3 (1.0 mol%). Charge density: 90 C cm^{-2}.

3. Development of Sodium and Potassium Secondary Batteries Using Ionic Liquid Electrolytes

The establishment of zero-carbon society requires the popularization of renewable energy and large-scaled energy storage devices. Although current lithium-ion batteries (LIBs) have been considered to the candidates because of their high energy densities, scarce lithium resources and flammable organic solvents are used, possibly leading to a major barrier to further distribution as large-scaled batteries. Our group has focused on sodium and potassium secondary batteries using ionic liquid electrolytes because sodium and potassium resources are abundant in the earth's crust and ionic liquids possess high safety such as negligible volatility and non-flammability [6,7].

In this fiscal year, we investigated charge–discharge performance of Hard carbon/$NaCrO_2$ full cell using Na[FSA]–[C_3C_1pyrr][FSA] ionic liquid electrolytes (FSA = bis(fluorosulfonyl)amide, C_3C_1pyrr = *N*-methyl-*N*-propylpyrrolidinium) with various Na^+ concentrations (C(Na^+) = 1.0–2.2 mol dm^{-3}). As reported in our previous study [6], the highly concentrated electrolytes conferred the superior rate capability. Then, *in-situ* Raman spectroscopy was attempted, revealing that the Na^+ ion shortage hardly occurred at the electrode/electrolyte interface for the highly concentrated electrolytes. We also tried to improve the performance of graphite negative electrode in K[FTA]–[C_4C_1pyrr][FTA] ionic liquid (FTA = (fluorosulfonyl)(trifluoromethylsulfonyl)amide, C_4C_1pyrr = *N*-butyl-*N*-methylpyrrolidinium). By changing the binder material from PVdF to CMC (PVdF = Polyvinylidene difluoride, CMC = Sodium carboxymethyl cellulose), initial reversible capacity and coulombic efficiency increased from 227 to 267 mAh g^{-1} and 55 to 85%, respectively. As shown in Fig. 2, stable cycle performance was obtained for 30 cycles with negligible capacity decline.

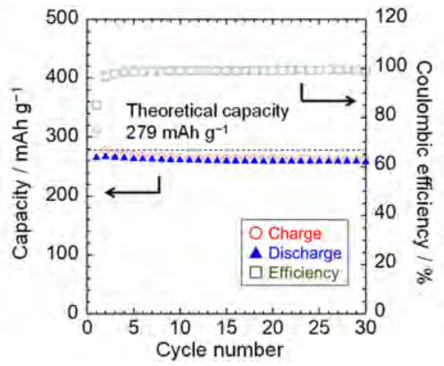


Fig. 2. Cycling properties of a K/graphite cell using K[FTA]–[C_4C_1pyrr][FTA] electrolyte and 313 K. Current rate: 0.1C rate (= 27.9 mA g^{-1}). Binder: CMC.

4. Efficient Bioethanol Production from Lignocellulosic Biomass Using Ionic Liquid

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

We have recently isolated several mutant strains of yeast with enhanced tolerance to an ionic liquid, 1-butyl-3-methylimidazolium chloride ([Bmim]Cl) in order to improve fermentation efficiency in the presence of ionic liquid by means of “adaptive laboratory evolution” [8] and conventional UV irradiation.

In this fiscal year, we first performed whole genome analysis of mutant strains obtained by conventional UV irradiation to identify genetic mutations. ATP synthase genes (*ATP1* and *ATP2*) were identified as candidates for mutations to improve ionic liquid tolerance, in addition to genes already known to confer ionic liquid tolerance, *PTK2* and *SKY1*. *ATP1* and *SKY1* or *ATP2* and *PTK2* mutations were introduced into the recombinant xylose fermenting yeast (SK-N1). These strains showed ionic liquid tolerance to growth (Fig. 3) and ethanol fermentation (Fig.4), conforming that *ATP1* or *ATP2* mutations, along with *SKY1* or *PTK2* mutations, emphasized ionic liquid tolerance.

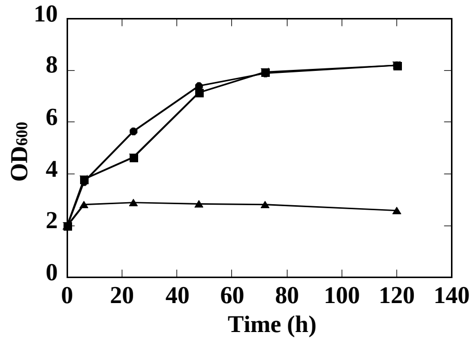


Fig. 3. Growth in the presence of 300 mM [Bmim]Cl. *ATP1* and *SKY1* mutated strain: square, *ATP2* and *PTK2* mutated strain: circle, SK-N1: triangle.

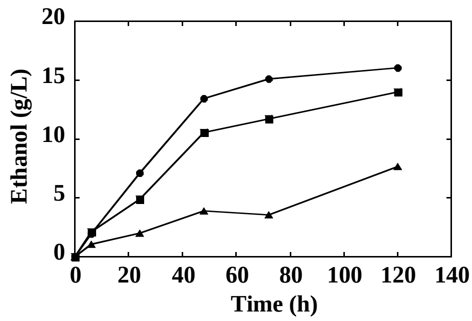


Fig. 4. Ethanol fermentation from glucose and xylose containing medium in the presence of 300 mM [Bmim]Cl. *ATP1* and *SKY1* mutated strain: square, *ATP2* and *PTK2* mutated strain: circle, SK-N1: triangle.

Acknowledgement

These researches were partly supported by grants to T. K. from JST SICORP (JPMJSC18E1) and to T. Y. from JSPS KAKENHI (21K14718) and Research Foundation for the Electrotechnology of Chubu.

References

[1] S. Senderoff and G. W. Mellors, *Science*, **153**, 3743 (1966).

[2] A. Katagiri, M. Suzuki, and Z. Takehara, *J. Electrochem. Soc*., **138**, 767 (1991).

[3] Y. Liu, Y. Zhang, F. Jiang, B. Fu, and N. Sun, *J. Nucl. Mater*., **442**, S585 (2013).

[4] T. Nohira, T. Ide, X. Meng, Y. Norikawa, and K. Yasuda, *J. Electrochem. Soc*., **168**, 046505 (2021).

[5] X. Meng, Y. Norikawa, and T. Nohira, *Electrochem. Commun*., **132**, 107139 (2021).

[6] T. Yamamoto, K. Mitsuhashi, K. Matsumoto, R. Hagiwara, A. Fukunaga, S. Sakai, K. Nitta, T. Nohira, *Electrochemistry*, **87**, 175 (2019).

[7] T. Yamamoto, S. Nishijima, T. Nohira, *J. Phys. Chem. B*, **124**, 8380 (2020).

[8] T. Kodaki, T. Kishiro, Y. Sugie, T. Nohira, *J. Jpn. Inst. Energy* **101**, 83 (2022)

Collaboration Works

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

Financial Support

1. Grant-in-Aid for Scientific Research

野平俊之，基盤研究(A)，液体亜鉛陰極を利用した太陽電池用シリコンの新製造法

野平俊之，挑戦的研究（萌芽），二酸化炭素を原料とした革新的常圧ダイヤモンド電解合成法の開発

山本貴之，若手研究，反応電位に立脚したデュアルカーボン電池の構築

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

2. Others

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

野平俊之，国際協力機構，JICA 研修員受入

小瀧努，科学技術振興機構，サトウキビ収穫廃棄物の統合バイオリファイナリー

山本貴之，（公財）高橋産業経済研究財団，汎用元素を用いた高安全性を有する大容量二次電池の開発

Publications

Y. Ma, K. Yasuda, A. Ido, T. Shimao, M. Zhong, R. Hagiwara, T. Nohira, Silicon Refining by Solidification from Liquid Si–Zn Alloy and Floating Zone Method, Materials Transactions, 62, 3, 403, 411, 2021

H. Hua, K. Yasuda, H. Konishi, T. Nohira, Electrochemical Formation of Nd–Ni Alloys in Molten $CaCl_2$–$NdCl_3$, Journal of The Electrochemical Society, 168, 3, 032506, 2021

T. Nohira, T. Ide, X. Meng, Y. Norikawa, K. Yasuda, Electrodeposition of Tungsten from Molten KF–KCl–WO_3 and CsF–CsCl–WO_3, Journal of The Electrochemical Society, 168, 4, 046505, 2021

Y. Ma, T. Yamamoto, K. Yasuda, T. Nohira, Raman Analysis and Electrochemical Reduction of Silicate Ions in Molten NaCl–$CaCl_2$, Journal of The Electrochemical Society, 168, 4, 046515, 2021

T. Yamamoto, K. Matsumoto, R. Hagiwara, T. Nohira, Charge–Discharge Performance of Copper Metal Positive Electrodes in Fluorohydrogenate Ionic Liquids for Fluoride-Shuttle Batteries, Journal of The Electrochemical Society, 168, 4, 040530, 2021

K. Kawaguchi, T. Nohira, Electrochemical Formation of Nd-Fe Alloys in Molten LiF-CaF_2-NdF_3, Journal of The Electrochemical Society, 168, 8, 082503, 2021

K. Yasuda, T. Oishi, T. Kagotani, K. Kawaguchi, M. Yaguchi, T. Enomoto, T. Nohira, Electrochemical Dy-Alloy Behaviors of Ni-Based Alloys in Molten LiF–CaF_2–DyF_3 and LiCl–KCl: Effects of Temperature and Electrolysis Potential, Journal of Alloys and Compounds, 889, 161605, 2022

X. Meng, Y. Norikawa, T. Nohira, Electrodeposition of mirror surface β-W films in molten CsF–CsCl–WO_3, Electrochemistry Communications, 132, 107139, 2021

H. Hua, K. Yasuda, T. Nohira, Thermodynamic Properties of Ni-Dy Intermetallic Compounds Measured Electrochemically in Molten $CaCl_2$-$DyCl_3$, Journal of The Electrochemical Society, 168, 10, 102501, 2021

K. Yasuda, T. Kato, Y. Norikawa, T. Nohira, Silicon Electrodeposition in a Water-Soluble KF–KCl Molten Salt: Properties of Si Films on Graphite Substrates, Journal of The Electrochemical Society, 168, 112502, 2021

T. Oishi, M. Yaguchi, Y. Katasho, T. Nohira, Selective Permeation of Neodymium through an Alloy Diaphragm in Molten Chloride Systems, Journal of the Electrochemical Society, 168, 10, 103504, 2021

H. Hua, K. Yasuda, T. Nohira, Thermodynamic properties of Ni–Nd intermetallic compounds measured electrochemically in molten $CaCl_2$–$NdCl_3$, Journal of the Electrochemical Society, 168, 11, 112506, 2021

Presentations

Y. Norikawa, A. Kondo, K. Yasuda, T. Nohira, Electrodeposition of Si in CsF–CsCl Eutectic Melt, 239th ECS meeting, Online, 2021.5.30-6.3

A. Yadav, T. Yamamoto, T. Nohira, Comparative studies on graphite negative electrode for alkali metal-ion batteries using FSA-based ionic liquid, 第 89 回マテリアルズ・テーラリング研究会，オンライン開催, 2021.8.6-7

眞鍋光毅，山本貴之，野平俊之，高ナトリウムイオン濃度の FSA 系イオン液体電解質を用いたナトリウム二次電池, 第 89 回マテリアルズ・テーラリング研究会，オンライン開催, 2021.8.6-7

茂木渉，法川勇太郎，野平俊之, KF–KCl 溶融塩中における液体 Zn 電極を用いた結晶性シリコン電析, 第 89 回マテリアルズ・テーラリング研究会，オンライン開催, 2021.8.6-7

杉江祐紀，小瀧努，野平俊之，イオン液体存在下でキシロース発酵可能な遺伝子組み換え酵母の開発, 第 89 回マテリアルズ・テーラリング研究会，オンライン開催, 2021.8.6-7

小林大展，山本貴之，野平俊之, FTA 系イオン液体電解質を用いたカリウム二次電池におけるグラファイト負極の電気化学挙動, 第 89 回マテリアルズ・テーラリング研究会，オンライン開催, 2021.8.6-7

二階堂貴文，山本貴之，野平俊之, FSA 系イオン液体中におけるグラファイト正極へのアニオン挿入挙動, 第 89 回マテリアルズ・テーラリング研究会，オンライン開催, 2021.8.6-7

堀場由梨奈，法川勇太郎，野平俊之，溶融 LiCl–KCl–K_2CO_3–KOH 中でのダイヤモンド電析における再現性の向上, 第 89 回マテリアルズ・テーラリング研究会，オンライン開催, 2021.8.6-7

A. Yadav, T. Yamamoto, T. Nohira, Comparative Studies on Graphite as Negative Electrode for Alkali Metal-Ion Batteries Using FSA-Based Ionic Liquids, The 12th International Symposium of the Institute of Advanced Energy Science, Online, 2021.9.7

W. Moteki, Y. Norikawa, T. Nohira, Electrodeposition of Crystalline Silicon Using a Liquid Zn Electrode in KF–KCl Molten Salt, The 12th International Symposium of the Institute of Advanced Energy Science, Online, 2021.9.7

K. Yasuda, Y. Ma, T. Yamamoto, T. Nohira, Electrodeposition of Si in Molten Salts Containing Silicate Ions towards the Production of Solar-Grade Silicon, The 12th International Symposium of the Institute of Advanced Energy Science, Online, 2021.9.7

T. Nago, Y. Norikawa, H. Matsushima, T. Nohira, Study of Hydrogen Isotope Separation Technology by Molten Salt, The 12th International Symposium of the Institute of Advanced Energy Science, Online, 2021.9.7

H. Usui, Y. Domi, Y. Itoda, T. Yamamoto, T. Nohira, K. Matsumoto, R. Hagiwara, H. Sakaguchi, Bi-Based Alloy Anode Materials for Na-Ion Batteries, The 12th International Symposium of the Institute of Advanced Energy Science, Online, 2021.9.7

K. Kuritani, Y. Domi, H. Usui, T. Yamamoto, T. Nohira, H. Sakaguchi, Potassiation–Depotassiation Properties of Various Antimony-Based Alloys as Novel Anode Materials of K-Ion Battery, The 12th International Symposium of the Institute of Advanced Energy Science, Online, 2021.9.7

T. Nohira, Electrolytic synthesis of diamond in molten salt under atmospheric pressure, The 12th International Symposium of Advanced Energy Science, Online, 2021.9.8

川口健次，野平俊之，廃ネオジム磁石からの希土類元素リサイクルを目的とした溶融 LiF-CaF2-NdF3 中における Nd-Fe 合金の電気化学的形成，溶融塩委員会第 206 回定例委員会，オンライン開催, 2021.9.28

T. Nohira, K. Kawaguchi, T. Kagotani, K. Yasuda, H. Konishi, T. Oishi, A Novel Electrochemical Recycling Method for Rare Earth Metals from Scrap Magnets Using Molten Salt Electrolysis and Alloy Diaphragms, 240th ECS Meeting, Online, 2021.10.10-14

A. Yadav, T. Yamamoto, T. Nohira, Graphite as negative electrode for potassium-ion batteries using FSA-based ionic liquid electrolytes, 第 11 回イオン液体討論会，オンライン開催, 2021.11.18-19

眞鍋光毅，山本貴之，野平俊之, Probing the mechanism of improved performance for sodium secondary batteries utilizing ionic liquid electrolytes with high Na+ ion concentrations, 第 11 回イオン液体討論会，オンライン開催, 2021.11.18-19

小林大展，Alisha Yadav，山本貴之，野平俊之, Electrochemical behavior of graphite negative electrode for potassium secondary battery using FTA-based ionic liquid electrolyte, 第 11 回イオン液体討論会, オンライン開催, 2021.11.18-19

二階堂貴文，山本貴之，野平俊之, Charge–discharge behavior of graphite positive electrodes in FTA-based ionic liquids, 第 11 回イオン液体討論会, オンライン開催, 2021.11.18-19

杉江祐紀，小瀧努，野平俊之, Development of Ionic Liquid Tolerant Yeast Capable Xylose Fermentation, 第 11 回イオン液体討論会, オンライン開催, 2021.11.18-19

川口健次，野平俊之, 溶融 $LiF-CaF_2-DyF_3$ 中における Dy-Fe 合金の電気化学的形成, 第 53 回溶融塩化学討論会, 東京大学生産技術研究所/Online (Hybrid), 2021.11.18-19

堀場由梨奈，法川勇太郎，野平俊之, 溶融 LiCl-KCl-K_2CO_3-KOH 系におけるダイヤモンドの電解合成に与える KOH 濃度の影響, 第 5 回溶融塩化学討論会, 東京大学生産技術研究所/Online (Hybrid), 2021.11.18-19

茂木渉，法川勇太郎，野平俊之，溶融 KF–KCl–K_2SiF_6 中における液体 Zn 電極を用いた結晶性 Si 電析に与える電流密度の影響, 第 53 回溶融塩化学討論会, 東京大学生産技術研究所/Online (Hybrid), 2021.11.18-19

華航，安田幸司，野平俊之, 溶融塩を用いた廃ネオジム磁石からの希土類元素の抽出および電解分離プロセス, 第 53 回溶融塩化学討論会, 東京大学生産技術研究所/Online (Hybrid), 2021.11.18-19

T. Nohira, X. Meng, Y. Norikawa, K. Yasuda, Electrodeposition of Bright Tungsten Coatings from Molten CsF–CsCl–WO_3, 7th Asian Conference on Molten Salt Chemistry and Technology, Institute of Industrial Science, The University of Tokyo, Japan/University of Science and Technology Beijing, China/Online (Hybrid), 2021.11.20

山本貴之，松本一彦，萩原理加，野平俊之，フッ化物シャトル電池用 Ag 正極の充放電メカニズムの解析，第 62 回電池討論会，パシフィコ横浜ノース/Online (Hybrid), 2021.11.30-12.2

眞鍋光毅，山本貴之，野平俊之，高 Na+濃度イオン液体電解質を用いたナトリウム二次電池におけるレート特性向上要因の検討, 2021 年度第 3 回関西電気化学研究会，オンライン開催, 2021.12.4

茂木渉，法川勇太郎，野平俊之, KF–KCl 溶融塩中における液体 Zn 電極を用いた結晶性 Si 電析, 2021 年度第 3 回関西電気化学研究会，オンライン開催, 2021.12.4

川口健次，野平俊之，溶融 $LiF-CaF_2-REF_3$ (RE = Nd or Dy)中における RE-Fe 合金の電気化学的形成，第 45 回電解技術討論会，オンライン開催, 2021.12.9-10

杉江祐紀，小瀧努，野平俊之, 木質バイオマスからキシロース発酵可能なイオン液体耐性強化酵母の開発，第 17 回バイオマス科学会議，オンライン開催, 2022.1.19-20

山本貴之，イオン液体および種々の電荷担体を用いた次世代型蓄電池に関する研究，電気化学会第 89 回大会，オンライン開催, 2022.3.15-17

山本貴之，松本一彦，萩原理加，野平俊之，柔粘性イオン結晶電解質を用いたフッ化物シャトル電池用正極材料の充放電挙動，電気化学会第 89 回大会, オンライン開催, 2022.3.15-17

Alisha Yadav，山本貴之，野平俊之, Potassium storage behavior of graphite negative electrode in FSA-based ionic liquid electrolyte, 電気化学会第 89 回大会，オンライン開催, 2022.3.15-17

二階堂貴文, 山本貴之, 野平俊之, FSA 系および FTA 系イオン液体中におけるグラファイト正極挙動の比較検討，電気化学会第 89 回大会，オンライン開催, 2022.3.15-17

小林大展，Alisha Yadav，山本貴之，野平俊之, K[FTA]–[C_4C1pyrr][FTA]イオン液体中におけるグラファイト負極の充放電挙動，電気化学会第 89 回大会，オンライン開催, 2022.3.15-17

石尾吉史，眞鍋光毅，山本貴之，野平俊之，イオン液体電解質を用いたナトリウム二次電池におけるレート特性の Na+濃度依存性，電気化学会第 89 回大会，オンライン開催, 2022.3.15-17

Molecular Nanotechnology Research Section

H. Sakaguchi, Professor
T. Kojima, Assistant Professor
S. Nobusue, Assistant Professor

1. Introduction

Nanotechnology is essential for highly efficient energy use. Our group studies the basics of assembling small molecules into the advanced materials and devices in energy sector with high efficiency. We have already developed several unique techniques which are totally new molecular assembling methodology such as 'electro-chemical Epitaxial Polymerization' and 'Two-Zone Chemical Vapor Deposition (2Z-CVD)' which enable to produce molecular wires on metal surface from small molecules. By using these techniques, organic electronic devices such as field-effect transistors and organic solar cells will be developed.

Main research achievements in Molecular Nanotechnology Research Section in 2021 are described below.

2. Bottom-Up On-Surface Synthesis of Edge-functionalized Graphene Nanoribbon

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

We have developed 2Z-CVD to produce densely packed, parallelly aligned self-assembled GNRs on Au(111) under low vacuum condition of 1 Torr from halogenated polycyclic aromatic hydrocarbon (PAH) precursors. This technique successfully produced a series of armchair-edged GNRs in high yield. Attractive features of this method originate from an independent temperature-control of radical-generation process (zone 1) and the growth process (zone 2), which afforded GNRs in high yield without using UHV conditions. The precursor was sublimated to the Au(111) substrate in zone 2 by passing through zone 1 in a quartz tube. The mechanism is supposed to involve radical generation in zone 1, polymerization of the radicals on the Au(111) substrate in zone 2, and subsequent dehydrogenation to form GNRs.[1] Additionally, we demonstrate a new concept of 'conformation-controlled surface catalysis'; the 2Z-CVD of the 'Z-bar-linkage' precursor, which represents two terphenyl units are linked like a 'Z', exhibiting flexible geometry that allows it to adopt chiral conformations with height-asymmetry on a Au(111) surface, results in the efficient formation of acene-type GNRs with a width of 1.45 nm through optimized cascade reactions. These cascade reactions on surface include the production of self-assembled homochiral polymers in a chain with a planar conformation, followed by efficient stepwise dehydrogenation via a conformation-controlled mechanism. Our proposed concept analogous to the biological catalyst, enzyme, is useful for the fabrication of new nanocarbon materials. [2]

Recently, GNRs having asymmetrically functional substitution at each edge have attracted much attention due to realization of ferroelectric or ferromagnetic property predicted by theory. However, it has been difficult to produce them because of decomposition of functional substitution at high temperature process during dehydrogenation reaction. To overcome the problem, we have developed low temperature GNR growth method with hydrogen acceptor.

After producing precursor polymers using 2Z-CVD method with Z-bar-linkage having different substitution at each edge as precursor, hydrogen acceptor was fed into the reactor (evacuated quartz tube), which promote dehydrogenation reaction resulting in giving asymmetrical GNRs without decomposition of functional substitution at lower temperature. Then, we have succeeded in direct observation of asymmetric GNRs produced on Au(111) with low-temperature scanning tunneling microscope.

3. Solution Synthesis of Asymmetrically Function-

alized Graphene Nanoribbon toward the Application for Functional Materials

Solution-phase synthesis is one of the most promising strategies to obtain well-defined graphene nanoribbon (GNR) with tunable electronic and optical properties. Asymmetrically edge-functionalized GNR have attracted a great deal of interest in view of the relationship between the unique structure and properties. Several theoretical predictions have been made to change the properties of these systems through edge modifications. Introduction of different functional groups to the edges of GNR backbone would offer a promising strategy to exhibit new properties. Although the solution-phase syntheses of GNRs having symmetric substitutions have already reported, our approach, however, has remained unexplored.

We previously reported the on-surface synthesis of acene-type GNR from the Z-shaped precursor which consists of two terphenyl units. Inspired by this work, we envisioned that the asymmetrically substituted GNRs would be obtained from asymmetrically Z-shaped precursor in the solution synthesis. However, the desired product was not obtained probably due to the skeletal rearrangement in the oxidative dehydrogenation reaction. To develop the synthetic method for asymmetrically edge-functionalized GNR, we have synthesized nanographenes as a model compound and GNRs from Z-shaped precursor by Pd-catalyzed cyclization followed by oxidative dehydrogenation reactions.

Based on this method, we investigated the synthesis of GNR having symmetric substitutions. As a result, we have developed the synthetic method via head-to-tale polymerization followed by cyclization with Pd-catalyzed bond formations and oxidative dehydrogenation reactions. This method is applicable to the preparation of asymmetric GNR having different functional groups at opposite side of the edges. We developed this method for the asymmetric GNR. The relationship between the functionalization of edge structures and their properties was identified by absorption spectra.

As an additional step, we designed asymmetric functional GNR. Asymmetrically functionalized and sterically hindered GNRs adopt twisted conformation and have dipolar moment along long axis by asymmetrically modifying both edges. We hypothesized that the orientation of the twisted direction would be controlled by applying an electric field. We succeeded in the preparation of helically twisted GNR with modified synthetic methods. As a result, when the positive and negative electric fields were applied to asymmetrically-functionalized GNR-doped liquid crystal, inversions of the CD signal were observed. These results indicated that the helical switching take place by applying electric field.

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

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

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

References

1. *Adv. Mater.*, **2014**, *26*, 4134-4138.
2. *Nat. Chem.*, **2017**, *9*, 57-63.
3. *Chem. Sci.*, **2021**, *12*, 11659-11667.

Financial Support

1. Grant-in-Aid for Scientific Research

(代表)
坂口浩司，挑戦的研究（萌芽），電子的異方性を有するグラフェンナノリボンの開発と巨大強誘電性

信末俊平，若手研究，機能性材料への応用を志向した非対称グラフェンナノリボンの創出

2. Others

坂口浩司，(株)KRI，1 ナノ構造炭素材料の構造解析

Publications

S. Song, .L. Wang, J. Su, Z. Xu, C-H. Hsu, C. Hua, P. Lyu, J. Li, X. Peng, T. Kojima, S. Nobusue, M. Telychko, Y. Zheng, F-C. Chuang, H. Sakaguchi, M.W. Wong, J. Lu, Manifold dynamic non-covalent interactions for steering molecular assembly and cyclization., *Chem. Sci.*, **2021**, *12*, 11659-11667.

R. Kotani, S. Yokoyama, S. Nobusue, S. Yamaguchi, A. Osuka, H. Yabu, S. Saito, Bridging pico-to-nanonewtons with a ratiometric force probe for monitoring nanoscale polymer physics before damage., *Nat. Commun.*, **2021**, *13*, 303.

小島崇寛， 大西臣禎， 中江隆博， 坂口浩司， トポロジカルエンジニアリングによるグラフェンナノリボンの合成とデバイス応用，炭素，2021，*298*， 95-104.

信末俊平， 中江隆博， 坂口浩司， 生物原理を用いる新ナノ炭素の気相表面合成，高分子，2021，70， 367-368.

Biofunctional Chemistry Research Section

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

1. Introduction

A transition to renewable energy technologies requires new chemistry to learn from nature. Nature has developed fantastic solutions to convert the solar energy to the chemical energy and to utilize them in the exceptionally efficient manners for almost 3 billion years. It is our challenge to understand the efficient bioenergetic processes of nature and to construct bio-inspired energy utilization systems. The research interests in our group focus on the design of biomacromolecules and their assemblies for molecular recognition, catalysis and signal transduction in water, the solvent of life. We take synthetic, organic chemical, biochemical and biophysical approaches to understand the biological molecular recognition and chemical reactions. Proteins and protein/nucleic acids assemblies are explored to realize biomimetic function of biological systems, such as visualization of cellular signals by fluorescent biosensors, directed self-assembly of peptides and proteins to build up nanobiomaterials, tailoring artificial receptors and enzymes based on the complex of RNA and a peptide or a protein, and reconstitution of the functional assemblies of receptors and enzymes on the nanoarchitectures. Followings are main research achievements in fiscal year 2021.

2. Dynamic shape transformation of a DNA scaffold applied for an enzyme nanocarrier

In this study, a three-dimensional DNA scaffold was designed to enable a dynamic shape transition from an open plate-like structure to its closed state of a hexagonal prism structure. A dimeric enzyme xylitol dehydrogenase (XDH) was assembled on the DNA scaffold in its open state in a high loading yield. The enzyme loaded scaffold was subsequently transformed to its closed state by the addition of short DNA closing keys. The enzyme encapsulated in the closed state displayed comparable activity to that in the open state, ensuring that the catalytic activity of enzyme was well maintained in the DNA nanocarrier (Fig. 1).

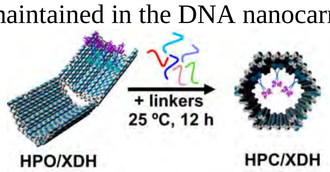


Fig. 1 Schemes representing transformation of XDH-loaded 3D DNA scaffold.

3. Conditional dependence of enzyme cascade reaction efficiency on the inter-enzyme distance

Cascade enzymes in cellular metabolic reactions often suffer from unfavorable kinetics of upstream and downstream enzymes. The kinetic parameters of such sequential enzymes are suggested to be critical in considering the inter-enzyme distance dependence of the cascade efficiencies. In this work, this issue is addressed by evaluating the reaction kinetics of imbalanced cascade enzymes.

An enzyme cascade of XDH and xylulose kinase (XK), derived from the xylose metabolic pathway, was constructed on a 3D DNA scaffold with a dynamic shape transition ability as described above. Evaluation of the cascade reaction efficiencies in the open and closed states revealed little or no inter-enzyme distance dependence, presumably due to the far larger catalytic constant of the downstream enzyme (Fig. 2). The inter-enzyme distance was not the dominant factor for cascade efficiency when the kinetic parameters of the cascade enzymes were imbalanced with the highly efficient downstream enzyme.

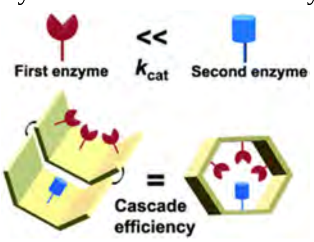


Fig. 2 Schematic representations of the cascade reaction of XDH and XK from a part of xylose metabolic pathway was loaded on 3D DNA scaffold.

4. Tuning the reactivity of a substrate for SNAP-Tag expands its application for recognition driven DNA-protein conjugation

Recognition-driven modification has been emerging as a novel approach to modifying biomolecular targets of interest site-specifically and efficiently. Protein modular adaptors (MAs) are the ideal reaction model for recognition-driven modification of DNA as they consist of both a sequence-specific DNA-binding domain and a self-ligating protein-tag. Coupling a DNA recognition by DNA-binding domain and a chemoselective reaction of protein tag could provide a highly efficient sequence-specific reaction. However, a MA consisting of a reactive protein-tag and its substrate, for example, SNAP-tag and benzyl guanine, revealed rather nonselective reaction with DNA. Therefore, new substrates of SNAP-tag have been designed to realize sequence-selective rapid crosslinking reactions of MA with SNAP-tag (Fig. 3). The reactions of substrates with SNAP-tag were verified by kinetic analyses to enable the sequence selective crosslinking reaction of MA.

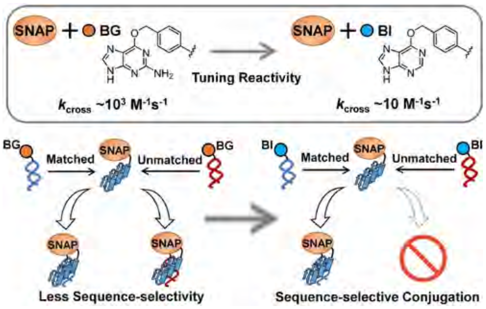


Fig. 3 An illustration of newly designed substrate of SNAP-tag to realize sequence-selective rapid crosslinking by MAs with SNAP-tag.

5. A facile combinatorial approach to construct a ratiometric fluorescent sensor: application for the real-time sensing of cellular pH changes

Realtime monitoring of the cellular environment, such as the intracellular pH, in a defined cellular space provides a comprehensive understanding of the dynamics processes in a living cell. Considering the limitation of spatial resolution in conventional microscopy measurements, multiple types of fluorophores assembled within that space would behave as a single fluorescent probe molecule. Such a character of microscopic measurements enables a much more flexible combinatorial design strategy in developing fluorescent probes for given targets. Nanomaterials with sizes smaller than the microscopy spatial resolution provide a scaffold to assemble several types of fluorophores with a variety of optical characteristics, therefore enablinging a convenient strategy for designing fluorescent pH sensors. In this study, fluorescein (CF) and tetramethylrhodamine (CR) were assembled on a DNA nanostructure with controlling the number of each type of fluorophore. By taking advantage of the different responses of CF and CR emissions to the pH environment, an appropriate assembly of both CF and CR on DNA origami enabled a controlled intensity of fluorescence emission and ratiometric pH monitoring within the space defined by DNA origami. The CF and CR-assembled DNA origami was successfully applied for monitoring the intracellular pH changes (Fig. 4).

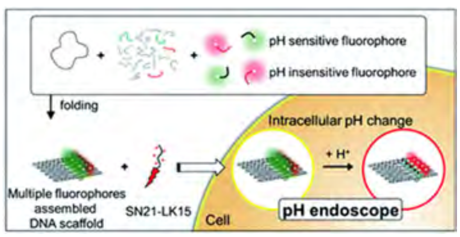


Fig. 4 a DNA origami scaffold assembled with multiple fluorophores to study intracellular pH change.

6. Stabilization and structural changes of 2D DNA origami by enzymatic ligation

The low thermal stability of DNA nanostructures is the major drawback in their practical applications. Detailed analyses of the conditions for the enzymatic ligation of the staple strands in 2D square lattice DNA origami provided optimized conditions to enhance the thermal stability of DNA nanostructures (Fig. 5).

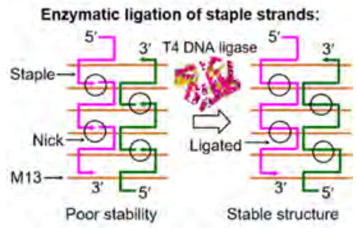


Fig. 5 Enzymatic ligation of staple strands in DNA origami scaffold.

7. Topologically-Interlocked Minicircles as Probes of DNA Topology and DNA-Protein Interactions

The topologically-interlocked minicircle rotaxane and catenane inside a frame-shaped DNA origami were synthesized. To probe the DNA-protein interactions, restriction reactions were carried out on the prepared interlocked structures and other DNAs with different topologies (Fig. 6).

This collaboration work with Prof. Y. Kwon (Ewha Womans University, Korea) was started when she was appointed as a visiting professor of IAE (FY 2013).

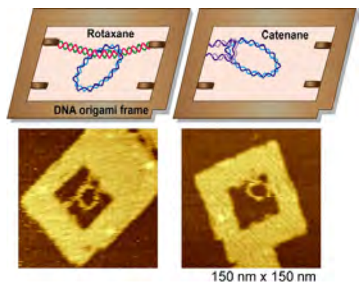


Fig. 6 An illustration of topologically-interlocked minicircles in DNA origami scaffold.

The presented works were supported in part by the Grants-in-Aid for Scientific Research (KAKENHI) from the Ministry of Education, Culture, Sports, Science and Technology (MEXT), Japan to T.M. (No.17H01213), E.N. (No.19H04653 and 20H02860) and S.N. (No.18K14335). And these works were also supported by JST CREST Grant Number JPMJCR18H5 to T.M.

Collaboration Works

森井孝，Ghent University（ベルギー），選択的 DNA 修飾

森井孝，中田栄司，Rajendran Arivazhagan，Ewha Womans University（韓国），トポイソメラーゼ反応の１分子計測

森井孝，仲野瞬，POSTECH（韓国），分子ライブラリーによる蛍光 RNP センサーの開発

森井孝，仲野瞬，POSTECH（韓国），生理活性物質を高感度で検出するセンサーの開発

森井孝，Rajendran Arivazhagan，Vanderbilt University School of Medicine（アメリカ），トポイソメラーゼ作用の分子機構

森井孝, 中田栄司, Seoul National University（韓国）, 細胞内酵素組織体の構築

大垣英明，森井孝，片平正人，野平俊之，モンゴル国立大学，インドネシア大学，フィリピン大学ディリマン校，ベトナム国家大学ハノイ校，ラオス国立大学，王立プノンペン大学，研究拠点形成事業 B. アジア・アフリカ学術基盤形成型

Financial Support

1. Grant-in-Aid for Scientific Research

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

2. Others

森井孝，科学技術振興機構，細胞内環境測定多元同時センサーの開発

Publications

L. Marongiu, F. Mingozzi, C. Cigni, R. Marzi, M.D. Gioia, M. Garrè, D. Parazzoli, L. Sironi, M. Collini, R. Sakaguchi, T. Morii, M. Crosti, M. Moro, S. Schurmans, T. Catelani, R. Rotem, M. Colombo, S. Shears, D. Prosperi, I. Zanoni, Inositol 1,4,5-trisphosphate 3-kinase B promotes Ca2+ mobilization and the inflammatory activity of dendritic cells, Science Signaling, 14, 676, eaaz2120, 2021

N. Yoshikawa, S, Yamazaki, Y. Kakimoto, S. Eguchi, R. Yokoyama, N. Kanehisa, N. Tohnai, E. Nakata, H. Takashima, Emission Properties of 1,10-phenanthroline Derivatives Induced by Protonation of a Nitrogen Atom, Journal of Molecular Structure, 1242, 130728, 2021

E. Nakata, H. Hirose, K. Gerelbaatar, J.V.V. Arafiles, Z. Zhang, S. Futaki, T. Morii, A facile combinatorial approach to construct a ratiometric fluorescent sensor: application for the real-time sensing of cellular pH changes, Chemical Science, 12, 23, 8231-8240, 2021

P. Lin, H. Dinh, E. Nakata, T. Morii, Dynamic Shape Transformation of a DNA Scaffold Applied for an Enzyme Nanocarrier, Frontiers in Chemistry, 9, 697857, 2021

A. Rajendran, K. Krishnamurthy, A. Giridasappa, E. Nakata, T. Morii, Stabilization and structural changes of 2D DNA origami by enzymatic ligation, Nucleic Acids Research, 49, 14, 7884-7900, 2021

M. Sawai, S. Matsumoto, Y. Mimura, Y. Imai, S. Yamazaki, N. Kanehisa, N. Tohnai, E. Nakata, H. Takashima, Circularly polarized luminescence (CPL) characteristics of hydrophobic pyrene derivatives/γ-cyclodextrin (γ-CD) complexes in aqueous solution dissolved by grinding, Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2021

P. Lin, H. Dinh, E. Nakata, T. Morii, Conditional dependence of enzyme cascade reaction efficiency on the inter-enzyme distance, Chemical Communications, 57, 85, 11197-11200, 2021

N. Yoshikawa, S. Yamazaki, A. Nishiyama, Y. Yamashita, N. Kanehisa, N. Tohnai, E. Nakata, H. Takashima, Structures, atomic charges, emission properties and DFT studies of biquinoline derivatives induced by protonation of a nitrogen atom, Journal of Molecular Structure, 131990, 2021

Z. Zhang, E. Nakata, H. Dinh, M. Saimura, A. Rajendran, K. Matsuda, T. Morii, Tuning the Reactivity of a Substrate for SNAP-Tag Expands Its Application for Recognition-Driven DNA-Protein Conjugation, Chemistry-A European Journal, 27, 18118-18128, 2021

H. Kimura, N. Nagasato, N. Kato, M. Kojima, C. Enomoto, E. Nakata, H. Takashima, Photophysical and elecron-transfer reaction properties of tris(2,2’-bipyridine)ruthenium(II)-based inhibitors that covalently bound to the active site of chymotrypsin, Photochemistry and Photobiology, 6, 100027, 2021

T. Hara, Y. Takatsuka, E. Nakata, T. Morii, Augmentation of an Engineered Bacterial Strain Potentially Improves the Cleanup of PCB Water Pollution, Microbiology Spectrum, 9, 3, e01926-21, 2021

Presentations

中田栄司，森井孝, 酵素を1分子ずつ並べる技術―カスタム装置開発の紹介も併せて―, 第38回京都大学宇治キャンパス産学交流会，オンライン開催, 2021.7.1

T. Morii, Spatially organized assembly of enzymes on DNA nanostructures, Pacifichem2021, Online, 2021.12.19.

K. Krishnamurthy, A. Rajendran, E. Nakata, T. Morii, Development of stable DNA nanomaterials for bioenergetic applications (Poster), 第12回エネルギー理工学研究所国際シンポジウム，オンライン開催, 2021.9.7-8

P. Lin, H. Dinh, E. Nakata, T. Morii, Enzyme cascade reactions on a dynamic DNA scaffold, The 15th Symposium on Biorelevant Chemistry, Online, 2021.9.8-10

K. Krishnamurthy, A. Rajendran, E. Nakata, T. Morii, Enhanced stability and structural changes of DNA origami by enzymatic ligation (Poster), The 15th Symposium on Biorelevant Chemistry, Online, 2021.9.8-10

S. Zhang, E. Nakata, T. Morii, DNA Origami as scaffolds to assemble quantifiable channel proteins on artifical organelles (Poster), The 15th Symposium on Biorelevant Chemistry, Online, 2021.9.8-10

H. Konish, H. Dinh, E. Nakata, H. Atomi, T. Morii, Folding of the multimer RuBisCO on the DNA nanostructure scaffold (Poster), The 15th Symposium on Biorelevant Chemistry, Online, 2021.9.8-10

S. Tajima, E. Nakata R. Sakaguchi, M. Saimura, Y. Mori, T. Morii, The construction strategy of AFP-based biosensors using the putative structural change (Poster), The 15th Symposium on Biorelevant Chemistry, Online, 2021.9.8-10

P. Lin, H. Dinh, E. Nakata, T. Morii, Enzyme cascade reactions on a DNA scaffold with shape transformation, The 48th International Symposium on Nucleic Acids Chemistry, Online, 2021.11.10-12

K. Krishnamurthy, A. Rajendaran, E. Nakata, T. Morii, Synthesis enhancing the stability of 2D DNA origami by enzymatic ligation (Poster), The 48th International Symposium on Nucleic Acids Chemistry, Online, 2021.11.10-12

Z. Zhang, E. Nakata, H. Dinh, M. Saimura, K. Matsuda, T. Morii, Design of DNA sequence-specific modular adaptors by tuning the reactivity of protein-tag substrate (Poster), The 48th International Symposium on Nucleic Acids Chemistry, Online, 2021.11.10-12

K. Gerelbaatar, E. Nakata, H. Hirose, S. Futaki, T. Morii, DNA nanostructure-based fluorescent pH sensor for cellular pH change (Poster), The 48th International Symposium on Nucleic Acids Chemistry, Online, 2021.11.10-12

H. Konishi, H. Dinh, E. Nakata, H. Atomi, T. Morii, Construction of a RubisCO assembly on 3D DNA scaffold(Poster), The 48th International Symposium on Nucleic Acids Chemistry, Online, 2021.11.10-12

A. Rajendran, S. Park, E. Nakata, Y. Kwon, T. Morii, Probing DNA topology and DNA-protein interactions by using topologically-interlocked DNA structures (Poster), The 48th International Symposium on Nucleic Acids Chemistry, Online, 2021.11.10-12

S. Zhang, E. Nakata, T. Morii, DNA origami as a scaffold to assemble membrane proteins on an artificial compartment (Poster), The 48th International Symposium on Nucleic Acids Chemistry, Online, 2021.11.10-12

K. Krishnamurthy, A. Rajendran, E. Nakata, T. Morii, Ligation of DNA Origami Nanostructures by Enzymatic and Chemical Approach (Poster), The International Chemical Congress of Pacific Basin Societies 2021, Online, 2021.12.16-21

K. Gerelbaatar, E. Nakata, Z. Zhang, T. Morii, Development of DNA nanostructure-based ratiometric fluorescent pH sensor (Poster), The International Chemical Congress of Pacific Basin Societies 2022, Oline, 2021.12.16-21

A. Rajendran, K. Krishnamurthy, E. Nakata, T. Morii, Cosolvent improves the enzymatic ligation of DNA origami, 日本化学会第102春季年会，オンライン開催, 2022.3.23-26

田嶋竣介，中田栄司，坂口怜子，才村正幸，森泰生，森井孝，蛍光タンパク質を用いた一酸化窒素バイオセンサーにおける蛍光応答増幅，日本化学会第102春季年会，オンライン開催, 2022.3.23-26

P. Lin, H. Dinh, E. Nakata, T. Morii, Effect of the ordered hydration layer for the enzymatic reactions on DNA scaffold, 日本化学会第 102 春季年会，オンライン開催, 2022.3.23-26

Z. Zhang, E. Nakata, H. Hirose, S. Futaki, T. Morii, Orthogonal FRET reporters on dextran for the real-time sensing of lysosomal proteases, 日本化学会第 102 春季年会，オンライン開催, 2022.3.23-26

小西宏明，H. Dinh，中田栄司，森井孝，跡見晴幸，3 次元 DNA ナノ構造体を用いた CO2 固定化酵素の集積化，日本化学会第 102 春季年会，オンライン開催, 2022.3.23-26

S. Zhang, E. Nakata, T. Morii, DNA origami as a scaffold to assemble membrane proteins on an artificial compartment, 日本化学会第 102 春季年会，オンライン開催, 2022.3.23-26

K. Krishnamurthy, A. Rajendaran, E. Nakata, T. Morii, Stabilization of DNA origami nanostructures by chemical ligation, 日本化学会第 102 春季年会，オンライン開催, 2022.3.23-26

馬場大芽，田嶋竣介，P. Lin，小西宏明，中田栄司，森井孝，補酵素受容体の近傍配置による酵素逐次反応の制御，日本化学会第 102 春季年会，オンライン開催, 2022.3.23-26

ちゃん やち，中田栄司，森井 孝, DNA-タンパク質の集合体に内包された酵素の活性評価，日本化学会第 102 春季年会，オンライン開催, 2022.3.23-26

W. Hou, S. Nakano, S. Tajima, M. Shimizu, M. Saimura, E. Nakata, T. Morii, Direct observation of the r(CUG) repeats in DM1 and MBNL1 aggregation complexes, 日本化学会第 102 春季年会，オンライン開催, 2022.3.23-26

K. Gerelbaatar, E. Nakata, H. Hirose, S. Futaki, T. Morii, Expanding the detectable pH range of DNA nanostructure-based fluorescent pH sensors, 日本化学会第 102 春季年会，オンライン開催, 2022.3.23-26

Structural Energy Bioscience Research Section

M. Katahira, Professor
T. Nagata, Associate Professor
Y. Yamaoki, Assistant Professor

1. Introduction

We explore the way how biomolecules such as proteins (involving enzymes) and functional nucleic acids (DNA and RNA) work at atomic resolution based on structural biology with NMR and X-ray. We determine both static and dynamical structures with the aid of our own development of the new methodology and elucidate the underlying mechanism of functions of these biomolecules. Structural biological approach is also applied to analyze enzymes involved in degradation of wood biomass at atomic resolution. The analysis is useful to develop the way to extract energy and valuable materials that can be used as starting materials of various products from the wood biomass. Thus, we pursue to contribute to the paradigm shift from oil refinery to biorefinery. Followings are main research achievements in the year of 2021.

2. Synergistic effect of a lytic polysaccharide monooxygenase and commercial cellulase cocktail

Cellulose is the most abundant organic polymer on earth. The second-generation biofuels are produced from cellulose by saccharification and following fermentation processes. However, the high cost of the saccharification process remains an issue. Cellulose-active lytic polysaccharide monooxygenases (LPMOs) catalyze the cleavage of cellulose chain on the crystalline cellulose surface by utilizing electron and oxygen source. Since this cleavage produces new accessible chain-ends for cellulases, LPMOs accelerate the saccharification of cellulose. Previously we solved the crystal structure of an LPMO of a white-rot fungus, *Ceriporiopsis subvermispora* (*Cs*LPMO). Then, a high synergistic effect of *Cs*LPMO and commercial cellulase cocktail was demonstrated. This year, we varied the ratio of *Cs*LPMO to cellulase cocktail, and optimized the conditions of saccharification reaction. By treatment of 5 mg/mL microcrystalline cellulose (MCC) with 37.5 µg/mL *Cs*LPMO and 12.5 µg/mL cellulase cocktail, the yield of reducing sugar reached 8.5-fold of the sum of the yields obtaind by the treatment with the individual enzymes (Figure 1). The degree of synergy turned out to be the highst among the reported ones for other LPMOs.

We also investigated the role of Tyr residues on the substrate-binding surface of *Cs*LPMO for substrate binding and synergistic effect. The two of the three Tyr residues, Y27 and Y74, were not conserved among LPMOs and unique for *Cs*LPMO. Site-direct mutagenesis and pull-down assay with MCC revealed that Y27 and Y74 are involved in substrate binding. Unexpectedly but interestingly, the synergistic effect of *Cs*LPMO increased by substituting Y27 and Y74 to Ala. It is known that unbound LPMOs produce H_2O_2, which is an efficient oxygen source for LPMO activity. We assume that the decrease in substrate affinity by the Y27 and Y74 to Ala substitution led to an increase of the substrate-unbound *Cs*LPMO, by which H_2O_2 was produced and provided to the substrate-bound *Cs*LPMO. The synergistic effect of *Cs*LPMO with the commercial cellulase cocktail may be applicable to the improvement of the process for cellulosic biomass utilization.

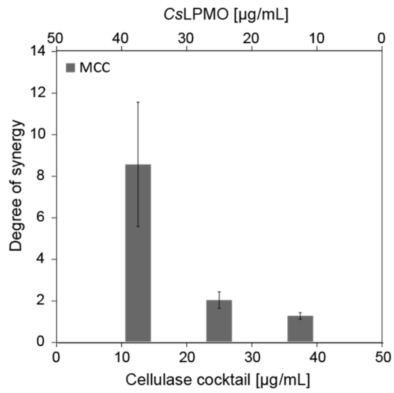


Figure 1. Degree of synergy (DS) at various ratios of *Cs*LPMO and cellulase cocktail on the degradation of 5 mg/mL MCC. DS was calculated using the following equition; $DS = Y_{CL}/(Y_C + Y_L)$, where Y_C, Y_L, and Y_{CL} are the yields of reducing sugars of the treatment with cellulase cocktail, *Cs*LPMO, and both, respectively.

3. Improving the degradation of lignin in beech wood by manganese peroxidase using a bioreactor system

Lignin, one of the major components of woody biomass, is a valuable aromatic polymer. For the utilization of lignin, efficient fragmentation of the lignin structure is required. Although ligninolytic enzymes such as manganese peroxidase (MnP) catalyzes lignin degradation, the degradation is reportedly competed by undesirable repolymerization. To prevent repolymerization, we deployed a semi-continuous bioreactor system to separate the fragmented lignin compounds from the reaction solution. By using this system, the overall net lignin degradation of beech wood catalyzed by MnP was successfully improved.

4. Determination of the crystal structure of *a* feruloyl esterase

Ferulic acids decorate hemicellulose via ester-linkage, and bridge hemicellulose and lignin in herbaceous biomass. Feruloyl esterases (FAEs) hydrolyze the ester-linkage between hemicellulose and ferulic acid and enhance the efficiency of hemicellulose degradation. Here, we determined the crystal structure of an FAE, which is phylogenetically related to acetyl xylan esterase (AXE), at 1.5 Å resolution. Additionally, the binding pocket for a substrate, methyl ferulate (MFA), was predicted by molecular docking analysis. Cys39, Glu49, Pro158, and Val163, were close to MFA (< 4 Å) in the docking model and thereby suggested to be involved in direct binding. This is the first structural characterizaion carried out for AXE-related FAE.

5. Finding of inhibitory effect of Vif on cytidine deamination of DNA by APOBEC3 proteins as revealed by biochemical and real-time NMR methods –new implication on the strategy for developing anti-HIV compounds-

APOBEC3 proteins (A3s), such as APOBEC3G (A3G) and APOBEC3F (A3F), convert cytidine residues to uracil residues through deamination of cytidine residues of minus strand DNA of HIV and thus destroy the genetic information of HIV. Thus, A3s function as guards against HIV. Vif protein of HIV forms a five-membered complex (VβBCC) which comprises a transcription factor, CBFβ, and the components of human E3 ubiquitin ligase, Elongin B, Elongin C, and Culin5 in infected cells. VβBCC ubiquitinates A3s and causes proteasomal degradation of A3s. Thus, Vif neutralizes A3s. In order to avoid the neutralization, compounds which interfere with the A3s-VβBCC interaction is being developed. Here, by means of biochemical and real-time NMR methods we found that VβBCC directly inhibits deamination by A3s independent of ubiquitination and resultant degradation. It was noted surprisingly that the inhibition is caused by the interaction between VβBCC and the C-terminal domain of A3G, which had been regarded not to interact directly with Vif. This finding implies that to develop anti-HIV-1 drugs that can avoid neutralization of A3G by Vif, it is necessary to consider the interference of the interaction of VβBCC with the C-terminal domain of A3G, in addition to the interference of the interaction of VβBCC with the N-terminal domain of A3G targeted for ubiquitination.

6. Proving the formation of parallel and antiparallel DNA triplex structures in living human cells

The parallel and antiparallel triplex structures comprise Watson-Crick duplex and an additional third strand that is oriented parallel and antiparallel with respect to the polypurine strand of the duplex. These triplex structures formed in human genomic DNA are believed to be involved in known diseases. However, there had been no direct evidence of the actual formation of these triplex structures in living human cells. To prove the formation of the triplx structures in living human cells, we used an advanced in-cell NMR technique incorporating bioreactor system that can supply fresh media to the living cells in NMR tube during spectral acquisition (Figure 2). The oligo DNAs, PT-ODN and APT-ODN, that form parallel and antiparallel triplex, respectively, in *in vitro* were introduced in living HeLa cells. The in-cell NMR spectra were acquired and compared with the *in vitro* NMR spectra. We identified the signals of all the imino protons belonging to the parallel and antiparallel triplex structures in in-cell NMR spectra. This is the first direct evidence of the formation of the parallel and antiparallel DNA triplex structures in living human cells. Additionaly, the imino proton signals derived from the duplex structures were also identified in in-cell NMR spectra. These duplexes were resultant of the triplex degradation. In-cell NMR spectra were also used to quantify the population of the triplex and duplex structures. Our in-cell NMR technique should be applicable for investigating the proteins and small compounds targeting the disease-related triplex structures in living human cells.

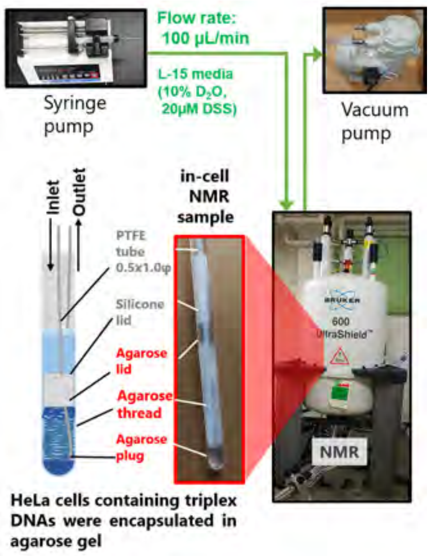


Figure 2. The bioreactor system for in-cell NMR experiment.

Collaboration Works

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

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

片平正人，山置佑大，Nanyang Technological University（シンガポール），University of Bordeaux（フランス），テロメアの i-モチーフ DNA と薬剤の相互作用の解析

片平正人，永田崇，BIOTEC，NSTDA （タイ），LIPI（インドネシア），NUOL （ラオス），e-ASIA

大垣英明，森井孝，片平正人，野平俊之，モンゴル国立大学，インドネシア大学，フィリピン大学ディリマン校，ベトナム国家大学ハノイ校，ラオス国立大学，王立プノンペン大学，研究拠点形成事業 B. アジア・アフリカ学術基盤形成型

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

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

Financial Support

1. Grant-in-Aid for Scientific Research

片平正人，学術変革領域研究(A)，ヒト生細胞中における核酸の構造と相互作用を解析するインセル NMR 法の開発と応用

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

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

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

永田崇，基盤研究(C)，データサイエンスを導入した原子間力顕微鏡による四重鎖 DNA 検出法の開発（分担金）

山置佑大，若手研究，In-cell NMR 法を用いたヒト生細胞内核酸の構造安定性および相互作用の評価

近藤敬子，基盤研究(C)，リグニンと多糖を分離する酵素の実バイオスに対する活性および構造機能相関の解析

2. Others

片平正人，日本医療研究開発機構，HIV 複製と創薬研究を推進する革新的な構造生物学研究基盤の創成

片平正人，科学技術振興機構，サトウキビ収穫廃棄物の統合バイオリファイナリー

片平正人，（株）ダイセル，木材や農水産廃棄物などのバイオマスの温和な変換

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

山置佑大，（公財）京都大学教育研究振興財団，生細胞内環境下の蛍光ＲＮＡアプタマーの構造機能相関解析

Publications

K. Kawata, A. Kitada, N. Tsuchida, M. Saimura, T. Nagata, M. Katahira, K. Fukami, K. Murase, Proton conduction in hydronium solvate ionic liquids affected by ligand shape, Physical Chemistry Chemical Physics, 23, 1, 449-456, 2021

A. Kitada, K. Kawata, M. Shimizu, M. Saimura, T. Nagata, M. Katahira, K. Fukami, K. Murase, Ligand Exchange Conduction of Lithium Ion in a Pentaglyme-Lithium Bis(trifluoromethylsulfonyl)amide Super-Concentrated Electrolyte, Journal of the Electrochemical Society, 168, 016506, 2021

K. Kawata, A. Kitada, K. Fukami, M. Saimura, T. Nagata, M. Katahira, K. Murase, An Ammonium Solvate Ionic Liquid, Journal of the Electrochemical Society, 168, 026515, 2021

A. Eladl, Y. Yamaoki, S. Hoshina, H. Horinouchi, K. Kondo, S. Waga, T. Nagata, M. Katahira, Investigation of the Interaction of Human Origin Recognition Complex Subunit 1 with G-Quadruplex DNAs of Human c-myc Promoter and Telomere Regions, International Journal of Molecular Sciences, 22, 7, 3481, 2021

N. Hamad, R. Yoneda, M. So, R. Kurokawa, T. Nagata, M. Katahira, Non-coding RNA suppresses FUS aggregation caused by mechanistic shear stress on pipetting in a sequence-dependent manner, Scientific Reports, 11, 1, 9523, 2021

D. Kashiwabara, K. Kondo, R. Usami, D. Kan, I. Kawamura, Y. Kawasaki, M. Sato, T. Nittami, I. Suzuki, M. Katahira, M. Takeda, Structural determination of the sheath-forming polysaccharide of Sphaerotilus montanus using thiopeptidoglycan lyase which recognizes the 1,4 linkage between α-d-GalN and β-d-GlcA, International Journal of Biological Macromolecules, 183, 992-1001, 2021

T. Sakamoto, Y. Yamaoki, T. Nagata, M. Katahira, Detection of parallel and antiparallel DNA triplex structures in living human cells using in-cell NMR, Chemical Communications, 57, 6364-6367, 2021

A. Kitada, Y. Koujin, M. Shimizu, K. Kawata, C. Yoshinaka, M. Saimura, T. Nagata, M. Katahira, K. Fukami, K. Murase, Glyme-Lithium Bis(trifluoromethylsulfonyl)amide Super-concentrated Electrolytes: Salt Addition to Solvate Ionic Liquids Lowers Ionicity but Liberates Lithium Ions, Journal of The Electrochemical Society, 168, 9, 090521, 2021

F. He, K. Kanako, M. Takizawa, M. Takahashi, K. Tsuda, T. Nagata, S. Watanabe, A. Tanaka, N. Kobayashi, T. Kigawa, P. Güntert, M. Shirouzu, S. Yokoyama, Y. Muto, 1H, 13C and 15N resonance assignments and solution structures of the two RRM domains of Matrin-3, Biomolecular NMR Assignments, 2021

K. Mikame, Y. Ohashi, Y. Naito, H. Nishimura, M. Katahira, S. Sugawara, K. Koike, T. Watanabe, Natural Organic Ultraviolet Absorbers from Lignin, ACS Sustainable Chemistry & Engineering, 9, 49, 16651-16658, 2021

H. Nguyen, K. Kondo, Y. Yagi, Y. Iseki, N. Okuoka, T. Watanabe, B. Mikami, T. Nagata, M. Katahira, Functional and structural characterization of a lytic polysaccharide monooxygenase, which cooperates synergistically with cellulases, from Ceriporiopsis subvermispora, ACS Sustainable Chemistry & Engineering, 10, 2, 923-934, 2022

山置佑大，永田崇，片平正人，「生命金属ダイナミクス～生体内における金属の挙動と制御～」（分担）、第 4 章 維持 —分子—"金属原子による RNA 立体構造形成とその生理活性のスイッチングへの応用"，エヌ・ティー・エス，198，204，2021

Presentations

中山千尋，山置佑大，永田崇，片平正人，NMR を用いた DNA:RNA ハイブリッドグアニン四重鎖とタンパク質の相互作用解析，蛋白質科学会若手の会第 1 回研究交流会，オンライン開催, 2021.6.14

M. Katahira, Structural Energy Bioscience Research Section, KU Chemistry Talent-Spot 2021 Manila, Online, 2021.7.3

T. Sakamoto, Y. Yamaoki, T. Nagata, M. Katahira, First observation of DNA triplex structures in living human cells using in-cell NMR, FIBER 日本核酸化学会若手フォーラム，オンライン開催, 2021.8.5-6

T. Nagata, Y. Yamaoki, T. Sakamoto, K. Kondo, S. Takami, M. Katahira, Analysis of structure and dynamics od oligonucleotides in intracellular conditions, ISMAR-APNMR-NMRSJ-SEST 2021, Online, 2021.8.22-27

Y. Yamaoki, T. Nagata, K. Kondo, T. Sakamoto, S. Takami, M. Katahira, In-cell NMR Analyses of the Structure and Dynamics of Hairpin and G-quadruplex Structures in the Living Human Cells, ISMAR-APNMR-NMRSJ-SEST 2021, Online, 2021.8.22-27

A. Eladl, Y. Yamaoki, S. Hoshina, H. Horinouchi, K. Kondo, T. Nagata, S. Waga, M. Katahira, Study of the interaction between human origin recognition complex subunit 1 and G-quadruplex forming nucleic acids, ISMAR-APNMR-NMRSJ-SEST 2021, Online, 2021.8.22-27

K. Kamba, L. Wan, S. Unzai, R. Morishita, T. Nagata, M. Katahira, Catalytic analysis of A3G demonstrates that the inhibition of deamination reaction of A3G by Vif complex can be independent of A3G’s ubiquitination, ISMAR-APNMR-NMRSJ-SEST 2021, Online, 2021.8.22-27

W. H. Tu, K. Kamba, T. Nagata, M. Katahira, Structural basis for Musashi-1-RNA complex formation, ISMAR-APNMR-NMRSJ-SEST 2021, Online, 2021.8.22-27

K. Kondo, Y. Sakai, Y. Yonezawa, M. I. Lin, T. Nagata, M. Katahira, NMR spectroscopic analysis of enzyme cleavage of lignin-carbohydrate linkage in woody biomass by fungal glucuronoyl esterase, ISMAR-APNMR-NMRSJ-SEST 2021, Online, 2021.8.22-27

T. Sakamoto, Y. Yamaoki, T. Nagata, M. Katahira, In-cell NMR analysis of the DNA triplex structures inside the living human cells, ISMAR-APNMR-NMRSJ-SEST 2021, Online, 2021.8.22-27

片平正人, FUS の凝集/インセル NMR, RNA/LLPS 等勉強会, Online, 2021.9.2

片平 正人, NMR で迫るヒト生細胞内の核酸分子の挙動と木質バイオマスの超微細胞構造，キンカ京都化学者クラブ第 375 回例会，楽友会館, 2021.9.4

R. Kurokawa, N. Hamad, R. Yoneda, M. So, K. Kondo, Y. Yamaoki, T. Nagata, M. Katahira, Analysis of fused in sarcoma aggregation caused by shear stress and suppression of aggregation by non-coding RNA, 12th International Symposium of Advanced Energy Science, Online, 2021.9.7-8

M. Katahira, Function and structure of a lytic polysaccharide monooxygenase which cooperates synergistically with cellulases toward zero-emission energy, 12th International Symposium of Advanced Energy Science, Online, 2021.9.7-8

A. Kitada, Y. Koujin, M. Shimizu, K. Fukami, Z. Zhang, M. Saimura, T. Nagata, M. Katahira, K. Murase, Elucidation of hopping conduction in lithium excess solvate ionic liquids, 12th International Symposium of Advanced Energy Science, Online, 2021.9.7-8

H. Morita, K. Kondo, S. Chida, M. Katahira, M. Takeda, Functionalization of amino sugar-containing polysaccharides using environmental microbes, 12th International Symposium of Advanced Energy Science, Online, 2021.9.7-8

T. Watanabe, Y. Tokunaga, T. Nagata, K. Kondo, M. Katahira, Interaction analysis between cellulase carbohydrate-binding module and lignin by ultra-high sensitivity NMR for biorefinery, 12th International Symposium of Advanced Energy Science, Online, 2021.9.7-8

M. Horiuchi, S. Kuninaga, I. Saito, M. Katahira, T. Nagata, Development of the crystalline cellulose degradation system consisting of the psychrophilic fungus-type hybrid enzymes, 12th International Symposium of Advanced Energy Science, Online, 2021.9.7-8

K. Matsumoto, H. Iyama, R. Hagiwara, M. Saimura, Y. Yamaoki, T. Nagata, M. Katahira, Strucutral analysis of fluorine-containing compounds by NMR spectroscopy, 12th International Symposium of Advanced Energy Science, Online, 2021.9.7-8

S. Waga, Y. Yamaoki, A. Eladl, S. Hoshina, H. Horinouchi, K. Kondo, T. Nagata, M. Katahira, Human origin recognition complex subunit 1 bound to DNAs that form G-quadruplex structures, 12th International Symposium of Advanced Energy Science, Online, 2021.9.7-8

O. Eladl, Y. Yamaoki, K. Kondo, T. Nagata, M. Katahira, Monitoring a structure of functional RNA in living human cell by in cell NMR, 12th International Symposium of Advanced Energy Science, Online, 2021.9.7-8

A. Eladl, A. Elganiny, M. Katahira, Estimation of different antibiotic formulations′ potency after resistance genes assignment using standard strains, 12th International Symposium of Advanced Energy Science, Online, 2021.9.7-8

K. Ali, A. Eladl, Y. Ogino, T. Sakamoto, C. Meas, T. Sakabe, O. Eladl, J. Cravioto, K. Mukai, C. Qu, K. Ueda, S. Konishi, H. Ohgaki, Carbon-neutral transitions: An evaluation of industrial strategies to advance renewable energy supply in some sectors of the Japanese manufacturing, 12th International Symposium of Advanced Energy Science, Online, 2021.9.7-8

山置佑大，In-cell NMR 法によるヒト生細胞内環境下の核酸の構造およびダイナミクスの解析，第 21 回 若手 NMR 研究会，オンライン開催, 2021.9.21-22

宮内滉平，山置佑大，今村比呂志，加藤稔，c-MYC 遺伝子のグアニン四重鎖構造の安定性に及ぼす圧力効果の FTIR 研究，第 62 回高圧討論会，アクリエひめじ, 2021.10.18-20

片平正人，抗プリオン病・抗アルツハイマー病効果が期待される RNA 分子の構造・機能研究と in-cell NMR，日本分光学会 NMR 分光部会集中講義，オンライン開催, 2021.10.22

奥岡奈宜，徳永有希，井関優侑，橋爪知弘，近藤敬子，永田崇，片平正人，渡辺隆司，選択的白色腐朽菌の溶解性多糖モノオキシゲナーゼによる人口リグニンとセルロースの共役反応系の解析，第 66 回リグニン討論会，オンライン開催, 2021.11.4-5

井関優侑，奥岡奈宜，橋爪知弘，近藤敬子，永田崇，片平正人，渡辺隆司，広葉樹リグニンとセルロース共存下における溶解性多糖モノオキシゲナーゼの反応性解析，第 66 回リグニン討論会，オンライン開催, 2021.11.4-5

片平正人，ヒト生細胞内におえる核酸の構造と相互作用を解析するインセル NMR 法の開発と応用，学術変革「物質共生」の領域会議，オンライン開催, 2021.11.4-5

Y. Yamaoki, T. Sakamoto, K. Kondo, S. Takami, T. Nagata, M. Katahira, Structures and dynamics of oligonucleotides in living human cells evaluated by in-cell NMR, The 48th International Symposium on Nucleic Acids Chemistry 2021, Online, 2021.11.10-12

T. Sakamoto, Y. Yamaoki, T. Nagata, M. Katahira, Detection of DNA triplex structures in living human cells by in-cell NMR, The 48th International Symposium on Nucleic Acids Chemistry 2021, Online, 2021.11.10-12

A. Eladl, O. Eladl, A. Elganiny, Susceptibility of Pseudomonas aeruginosa to different antimicrobials and studies on multidrug resistant isolates, 2021 Ajou – Kyoto – Zhejiang Joint Symposium on Energy Science, Online, 2021.11.29

T. Sakamoto, Y. Yamaoki, T. Nagata, M. Katahira, Observation of DNA triplex structures in living human cells using in-cell NMR technique, 2021 Ajou – Kyoto – Zhejiang Joint Symposium on Energy Science, Online, 2021.11.29

O. Eladl, Y. Yamaoki, K. Kondo, A. Eladl, T. Nagata, M. Katahira, Detection of interaction between functional RNA and its target compound in living human cell using 2D in-cell NMR, 2021 Ajou – Kyoto – Zhejiang Joint Symposium on Energy Science, Online, 2021.11.29

Y. Yamaoki, T. Sakamoto, K. Kondo, S. Takami, T. Nagata, M. Katahira, In-cell NMR study on the base pair dynamics of nucleic acid in the living human cells, The 59th Annual Meeting of the Biophysical Society of Japan, Online, 2021.11.25-27

C. Nakayama, Y. Yamaoki, K. Kondo, T. Nagata, M. Katahira, Simultaneous monitoring of DNA, RNA, and DNA:RNA hybrid G-quadruplexes, and their interaction with arginine-glycine-rich peptide by NMR, The 59th Annual Meeting of the Biophysical Society of Japan, Online, 2021.11.25-27

K. Miyauchi, Y. Yamaoki, H. Imamura, M. Kato, FTIR study of pressure-induced denaturation of the guanine quadruplex of the c-MYC gene, The 59th Annual Meeting of the Biophysical Society of Japan, Online, 2021.11.25-27

山置佑大，ヒト生細胞内における核酸の構造およびダイナミクスの評価，京都大学エネルギー理工学研究所 附属エネルギー複合機構研究センター 令和 3 年(2021 年)度第 3 回センター談話会，京都大学エネルギー理工学研究所, 2021.11.30

M. Katahira, Non-coding RNA suppresses FUS aggregation caused by mechanistic shear stress on pipetting in a sequence-dependent manner, The 44th Annual Meeting of the Molecular Biology Society of Japan, Pacifico Yokohama, 2021.12.1-3

K. Kamba, Li Wan, S. Unzai, R. Morishita, T. Nagata, M. Katahira, Effect of the charged residues on inhibition of APOBEC3G by HIV-1 Vif, The 44th Annual Meeting of the Molecular Biology Society of Japan, Pacifico Yokohama, 2021.12.1-3

W. H. Tu, K. Kamba, T. Imai, N. Kobayashi, P. Guntert, T. Nagata, M. Katahira, Structural basis for Musashi-1-RNA complex formation, The 44th Annual Meeting of the Molecular Biology Society of Japan, Pacifico Yokohama, 2021.12.1-3

阪本知樹，山置佑大，永田崇，片平正人，ヒト生細胞内における平行型及び逆平行 DNA 三重鎖構造の in-cell NMR 法を用いた初観測，第 44 回日本分子生物学会年会，パシフィコ横浜, 2021.12.1-3

中山千尋，山置佑大，近藤敬子，永田崇，片平正人，NMR 法による DNA-RNA ハイブリッドグアニン四重鎖とアルギニンーグリシンリッチペプチドの相互作用解析，第 44 回日本分子生物学会年会，パシフィコ横浜, 2021.12.1-3

Y. Yamaoki, T. Nagata, T. Sakamoto, S. Takami, M. Katahira, The structure and dynamics of DNA and RNA in living human cells studied by in-cell NMR, The 2021 International Chemical Congress of Pacific Basin Societies, Online, 2021.12.16-21

M. Katahira, Quadruplex RNA aptamers with anti-disease activities and in-cell NMR of nucleic acids, The 2021 International Chemical Congress of Pacific Basin Societies, Online, 2021.12.16-21

M. Katahira, Behavior of APOBEC3 proteins as revealed by real-time monitoring of deamination with NMR, The 2021 International Chemical Congress of Pacific Basin Societies, Online, 2021.12.16-21

T. Nagata, M. Katahira, Structural and physical basis for anti-prion activity and destruction of the Alzheimer's disease-related complex of an RNA-aptamer, The 2021 International Chemical Congress of Pacific Basin Societies, Online, 2021.12.16-21

K. Kondo, M. Katahira, Analysis of enzymatic cleavage of lignin-carbohydrate linkage in woody biomass by fungal glucuronoyl esterase, The 2021 International Chemical Congress of Pacific Basin Societies, Online, 2021.12.16-21

K. Kamba, M. Katahira, Deamination reaction of APOBEC3G is inhibited by Vif five-membered complex including human protein Culin5, The 2021 International Chemical Congress of Pacific Basin Societies, Online, 2021.12.16-21

片平正人, ヒト生細胞内におえる核酸の構造と相互作用を解析するインセル NMR 法の開発と応用, 学術変革「物質共生」の班会議, オンライン開催, 2022.1.22

宮内滉平, 山置佑大, 今村比呂志, 加藤稔, 小角 X 線散乱法による c-MYC 遺伝子プロモーターのグアニン四重鎖構造とコイル構造の観測, 2021 年度量子ビームサイエンスフェスタ, オンライン開催, 2022.3.7

A. Phienluphon, Cell surface display of fungal feruloyl esterase in Pichia pastoris, The 72nd Annual Meeting of Japan Wood Research Society, Online, 2022.3.15-17

K.Teo, Boost in beech wood's lignin degradation by heterogeneously expressed manganese peroxidase by using a semi-continuous bioreactor system, The 72nd Annual Meeting of Japan Wood Research Society, Online, 2022.3.15-17

片平正人, ＲＮＡアプタマーの構造・抗プリオン活性・抗アミロイドβ活性及びヒト細胞中における核酸の in-cell NMR, 日本農芸化学会 2022 京都年度大会, オンライン開催, 2022.3.15-18

A. Phienluphon, Effect of site-directed mutagenesis of Aspergillus sydowii feruloyl esterase on substrate preference, The 2022 Annual Meeting of the Japan Society for Bioscience, Buitechnology and Agrochemistry, Online, 2022.3.15-18

八木勇成, 木材腐朽菌 Ceriporiopsis subvermispora 由来 LPMO9 がセルロース分解に及ぼすシナジー効果, 日本農芸化学会 2022 京都年度大会, オンライン開催, 2022.3.15-18

Self-Assembly Science Research Section

A. Rajendran, Junior Associate Professor

1. Introduction

Nucleic acids and their nanostructures, such as scaffolded DNA origami,[1] have been used for organizing enzyme cascades and shown to enhance the efficiency and rate of sequential reactions.[2] Besides some proof-of-concept experiments, the use of DNA origami for templating the biomass-related enzymes is hampered by their unsatisfactory stability to withstand the folded structure under application-specific conditions. For example, the origami structures are only stable below the melting temperature of around 50 °C.[3] Also, the origami materials poorly withstand the mechanical forces and break even under the mild forces applied during the structural analysis by force-based methods such as atomic force microscopy (AFM).[4] Further, it requires a significantly high ionic strength of typically 5-20 mM of $MgCl_2$.[5] Ionic strengths in physiological conditions where enzymes are often handled are much lower than needed to ensure origami stability. The typical Mg^{2+} concentration in cell culture media is 0.04 to 0.8 mM, and that of Na^+ and K^+ are about 150 and 5.5 mM, respectively, making these environments significantly destabilizing toward DNA origami materials.[6] Moreover, the solutions containing enzymes often undergo desalting and buffer exchanging processes and may also be stored in pure water to adapt the optimum conditions suitable for the enzymatic reactions. However, in pure water or low ionic strength buffers, the DNA origami immediately unfolds, and it is not very convenient to store the templated enzymes under these conditions and carry out multienzyme reactions. Biomass often undergoes chemical pretreatments using strong acids or bases to break down the lignin. Also, the biomass product contains several carboxylic acids with a pH of 2 to 2.5. Though the DNA origami materials were shown to be stable up to a pH of 11, the low pH values below 4 were found to denature the DNA origami.[5] Thus, it is necessary to develop methods to stabilize the DNA origami nanomaterials for various applications, particularly for handling the enzymes related to biomass energy conversion.

2. Methods to improve the stability of DNA origami

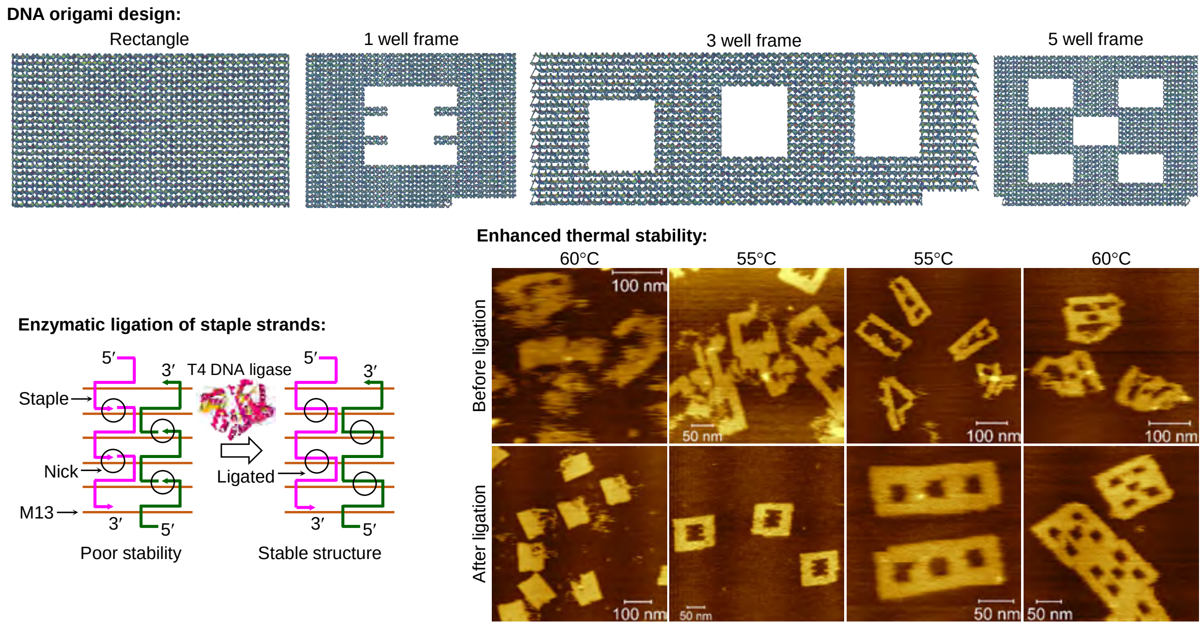


Figure 1. Top: Structures of the 2D DNA origami used in this study. Bottom left: Schematic illustration of enzymatic ligation of the nicks in DNA origami. Bottom right: AFM images evidencing the enhanced thermal stability of origami after enzymatic ligation.

One primary reason for the stability issues of the origami structures is the presence of breaks in the phosphate backbone, the so-called nicks of the staple strands. Increasing the staple length would improve the thermal stability but, at the same time, will lead to practical difficulties such as increased cost of synthesis, decreased product yield and purity, and limitations on the maximum length of synthetic oligo DNAs. We have previously reported a method to stabilize the DNA origami structures by photo-cross-linking of 8-methoxypsoralen.[3] Another method is the UV light-induced cyclobutane pyrimidine dimer formation by placing thymidines in close proximity within the DNA origami.[7] However, these methods are not suitable where native-like DNA is anticipated, as they introduce chemical cross-links to the DNA strands. Also, the irradiation of UV light for 1 to 2 h often leads to DNA damage. The alternative method is the enzymatic ligation of the nicks, which is routinely used in molecular biology. Enzymatic ligation was applied for a few small non-scaffolded and scaffolded DNA structures.[8-12] However, the conditions for enzymatic ligation of DNA origami were not optimized, and no evidence was provided to support the success of the ligation. Thus, to improve the stability of DNA origami, in this study, we aimed to perform the enzymatic ligation, cosolvent-assisted enhancement in enzymatic ligation, and chemical ligation of DNA origami. For this purpose, we have made a collaboration with Prof. Takashi Morii's group at the Biofunctional Chemistry Research Section of the Advanced Energy Utilization Division.

3. Enzymatic ligation of DNA origami nanomaterials

At first, we have carried out a detailed analysis and optimization of the conditions for the enzymatic ligation of the staple strands in four types of 2D square lattice DNA origami, namely rectangle (Rec),[1] 1 (1WF),[13] 3 (3WF),[14] and 5 well-frame (5WF,[15] Figure 1). Our results indicated that the ligation takes overnight, is efficient at 37 °C rather than the usual 16 °C or room temperature, and typically requires a much higher concentration of T4 DNA ligase.[16] Under the optimized conditions, up to 10 staples ligation with a maximum ligation efficiency of 55% was achieved. Also, the ligation is found to increase the thermal stability of the origami as low as 5 °C to as high as 20 °C, depending on the structure (Figure 1). Further, our studies indicated that the ligation of the staple strands influences the globular structure/planarity of the DNA origami, and the origami is more compact when the staples are ligated. The globular structure of the native and ligated origami was also found to be altered dynamically and progressively upon ethidium bromide intercalation in a concentration-dependent manner.[16] Moreover, our results shed light on the structural features and mechanistic insights on the DNA-ligase interaction and accessibility to the nick site in DNA origami.

4. Cosolvent-assisted enhanced enzymatic ligation of DNA origami

Besides our initial demonstration, due to the tightly-packed anti-parallelly oriented arrangement of multiple duplexes in the origami and the difficulties in the accessibility of the nicks by ligase, enzymatic ligation was only partly successful. To further enhance the enzymatic ligation of origami, we have carried out the effect of cosolvent and identified the best performing cosolvent. Our results indicated that the cosolvent enhances enzymatic ligation. Further, we have successfully carried out the chemical ligation of 2D and 3D DNA origami and enhanced the thermal stability of the DNA origami materials.

Overall, our results are useful to understand the optimized conditions for the enzymatic and chemical ligations of DNA origami structures, ligation-induced structural rigidity and compactness, the access of ligase enzyme in a tightly packed environment, and the nature of ethidium bromide binding and its influence on the conformational change in DNA origami materials.

5. References

1. P. W. K. Rothemund, *Nature* **2006,** *440*, 297-302.

2. A. Rajendran, E. Nakata, S. Nakano, T. Morii, *ChemBioChem* **2017,** *18*, 696-716.

3. Rajendran et al., *J. Am. Chem. Soc.* **2011,** *133*, 14488-14491.

4. A. Rajendran, M. Endo, H. Sugiyama, *Chem. Rev.*, **2014**, 114, 1493-1520.

5. S. Ramakrishnan, H. Ijas, V. Linko, A. Keller, *Compu. Struct. Biotechnol. J.* **2018,** *16*, 342-349.

6. H. Bila, E. E. Kurisinkal, M. M. C. Bastings, *Biomater. Sci.* **2019,** *7*, 532-541.

7. T. Gerling, M. Kube, B. Kick, H. Dietz, *Sci. Adv.* **2018,** *4*, eaau1157.

8. P. O'Neill, P. W. K. Rothemund, D. K. Fygenson, *Nano Lett.*, **2006**, *6*, 1379-1383.

9. M. Mousavi-Khattat, A. Rafati, P. Gill, *J. Nanostruct. Chem.*, **2015**, *5*, 177-183.

10. X. Yang, L. A. Wenzler, J. Qi, X. Li, N. C. Seeman, *J. Am. Chem. Soc.*, **1998**, *120*, 9779-9786.

11. M. L. Petrillo, C. J. Newton, R. P. Cunningham, R.-I. Ma, N. R. Kallenbach, N. C. Seeman, *Biopolymers*, **1988**, *27*, 1337-1352.

12. T. H. LaBean, H. Yan, J. Kopatsch, F. Liu, E. Winfree, J. H. Reif, N. C. Seeman, *J. Am. Chem. Soc.*, **2000**, *122*, 1848-1860.

13. M. Endo, Y. Katsuda, K. Hidaka, H. Sugiyama, *J. Am. Chem. Soc.*, **2010**, *132*, 1592-1597.

14. T. A. Ngo, E. Nakata, M. Saimura, T. Morii, *J. Am. Chem. Soc.*, **2016**, *138*, 3012-3021.

15. E. Nakata, F. F. Liew, C. Uwatoko, S. Kiyonaka, Y. Mori, Y. Katsuda, M. Endo, H. Sugiyama, T. Morii, *Angew. Chem. Int. Ed.*, **2012**, *51*, 2421-2424.

16. A. Rajendran, K. Krishnamurthy, A. Giridasappa, E. Nakata, T. Morii, *Nucleic Acids Res.* **2021,** *49*, 7884-7900.

Collaboration Works

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

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

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

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

Financial Support

Grant-in-Aid for Scientific Research
Rajendran Arivazhagan, Scientific Research (C), Retroviral integration into topologically-interlocked DNAs to probe the role of DNA structure and screen viral inhibitors, FY2021-FY2023

Publications

A. Rajendran, K. Krishnamurthy, A. Giridasappa, E. Nakata, T. Morii, Stabilization and structural changes of 2D DNA origami by enzymatic ligation, *Nucleic Acids Res.*, **2021**, *49*, 7884-7900.

Z. Zhang, E. Nakata, H. Dinh, M. Saimura, A. Rajendran, K. Matsuda, T. Morii, Tuning the Reactivity of a Substrate for SNAP-Tag Expands Its Application for Recognition-Driven DNA-Protein Conjugation, *Chem. Eur. J.*, **2021**, *27*, 18118-18128.

A. Joseph, A. Rajendran, A. Karithikeyan, B.G. Nair, Implantable Microfluidic Device: An Epoch of Technology, *Curr. Pharm. Des.*, **2022**, In press.

A. Rajendran, K. Krishnamurthy, S. Park, E. Nakata, Y. Kwon, T. Morii, Topologically-Interlocked Minicircles as Probes of DNA Topology and DNA-Protein Interactions, *Chem. Eur. J.*, **2022**, In press.

A. Rajendran, K. Krishnamurthy, S. Park, E. Nakata, Y. Kwon, T. Morii, Journal Front Cover, *Chem. Eur. J.*, **2022**, In press.

A. Rajendran, K. Krishnamurthy, S. Park, E. Nakata, Y. Kwon, T. Morii, Cover Profile, *Chem. Eur. J.*, **2022**, In press.

Presentations

K. Krishnamurthy, A. Rajendran, E. Nakata, T. Morii, Ligation of DNA Origami Nanostructures by Enzymatic and Chemical Approach, Zhejiang-Kyoto-Ajou Joint Symposium on Energy Science, Online, 2020.12.01

K. Krishnamurthy, A. Rajendran, E. Nakata, T. Morii, Development of Stable DNA Nanomaterials for Bioenergetic Applications, The 12th International Symposium of the Institute of Energy Science and Technology-Research Activities on Zero-Emission Energy Network, Online, 2021.09.07-08

K. Krishnamurthy, A. Rajendran, E. Nakata, T. Morii, Enhanced Stability and Structural Changes of DNA Origami by Enzymatic Ligation, The 15th Bio-related Chemistry Symposium, Online, 2021.09.08-10

A. Rajendran, S. Park, E. Nakata, Y. Kwon, T. Morii, Probing DNA Topology and DNA-Protein Interactions by Using Topologically-Interlocked DNA Structures, The 48th International Symposium on Nucleic Acids Chemistry, Online, 2021.11.10-12

K. Krishnamuthy, A. Rajendran, E. Nakata, T. Morii, Enhancing the Stability of 2D DNA Origami by Enzymatic Ligation, The 48th International Symposium on Nucleic Acids Chemistry, Online, 2021.11.10-12

K. Krishnamurthy, A. Rajendran, E. Nakata, T. Morii, Ligation of DNA Origami Nanostructures by Enzymatic and Chemical Approach, The 2021 International Chemical Congress of Pacific Basin Societies, Online, 2021.12.16-21

Broad Band Energy Science Research Section

T. Nohira, Professor
Y. Norikawa, Assistant Professor

1. Introduction

In recent years, renewable energy is attracting a great deal of attention as a means of achieving a sustainable society. Solar cells are one of the promising renewable energies. Thus, the annual installation of PV cells exceeded 117 GW $year^{-1}$ in 2019 [1]. Nowadays, crystalline Si solar cells account for 96.5% of total solar cell production due to its high efficiency and durability, with demand continuing to increase in 2020. However, the major disadvantages of the conventional Si substrate manufacturing method are the low productivity of the Siemens process and the considerable kerf loss in the Si slicing process. As the demand for crystalline Si solar cells continues to grow, there is a strong need to develop alternative manufacturing methods for Si solar cells.

In this research section, as the one of the new manufacturing methods for Si solar cells, electrodeposition process was developed.

2. Development of Si Plating Processes Using Molten Salt Electrolytes: Direct Plating of n- and p-type Si

Plating n-type and p-type Si directly on the substrates is one of the most promising methods for manufacturing solar cells with fewer steps. We have already proposed new electrodeposition process of Si utilizing KF–KCl as an electrolyte and $SiCl_4$ as a Si ion source [1]. We also reported electrodeposition of dense Si films with smooth surface in KF–KCl at 923–1073 K [2–5]. In this fiscal year, we investigated the semiconductor characteristics of Si films electrodeposited in KF–KCl–K_2SiF_6 and KF–KCl–K_2SiF_6–KBF_4 at 1023 K. Also, we measured the solar cell characteristics of p–n junction Si films formed by two-step electrodeposition.

Fig. 1 shows photoresponses during the linear sweep voltammetry of Si films electrodeposited in KF–KCl–K_2SiF_6, where the light was chopped at a frequency of 1 Hz. For Si films electrodeposited at lower current densities, anodic currents change with the light chopping, indicating that the obtained Si films are n-type semiconductors. Fig. 2 shows photoresponses of Si films electrodeposited in KF–KCl–K_2SiF_6–KBF_4. When the added amount of KBF_4 was 2 and 5 mol ppm, cathodic currents change with the light chopping. This indicates that the addition of boron, an acceptor element, causes the deposited

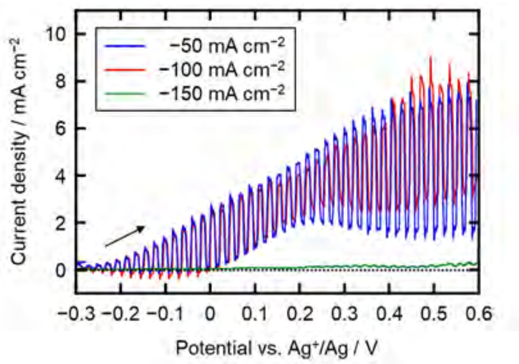


Fig. 1. Linear sweep voltammograms in acetonitrile containing 0.1 M $TBAPF_6$ and 0.05 M Fc at 298 K. Working electrodes were the Si films obtained by galvanostatic electrolysis of graphite plates at cathodic current densities of 50–150 mA cm^{-2} (charge density: −90 C cm^{-2}) in molten KF–KCl–K_2SiF_6 (KF:KCl = 60:40 mol%, K_2SiF_6: 3.5 mol%) at 1023 K. Xe light was chopped at a frequency of 1 Hz by a chopper. Scan rate: 10 mV s^{-1}.

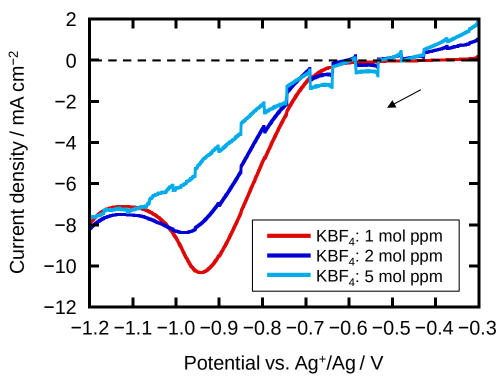


Fig. 2. Linear sweep voltammograms of Si films obtained by galvanostatic electrolysis at −100 mA cm^{-2} in molten KF–KCl–K_2SiF_6–KBF_4 (KF:KCl = 60:40 mol%, K_2SiF_6: 3.5 mol%, KBF_4: 1, 2, 5 ppma) at 1023 K. Xe light was chopped at a frequency of 1 Hz by a chopper. Scan rate: 50 mV s^{-1}.

Si films to become p-type.

Next, we conducted two steps electrodeposition; n-type Si was electrodeposited on graphite substrates in KF–KCl–K_2SiF_6, and then p-type Si was deposited in KF–KCl–K_2SiF_6–KBF_4(5 mol ppm). The characteristics of the solar cells was evaluated by the current-voltage curve as shown in Fig. 3. Power generation was confirmed and j_{sc} = 5.8×10^{-3} mA cm^{-2} and V_{oc} = 0.38 mV. These values were much smaller than the desired value, which might be caused by impurities in Si films and failure to accurately define the area of light exposure. Therefore, both the electrodeposition method and the measurement method need to be improved.

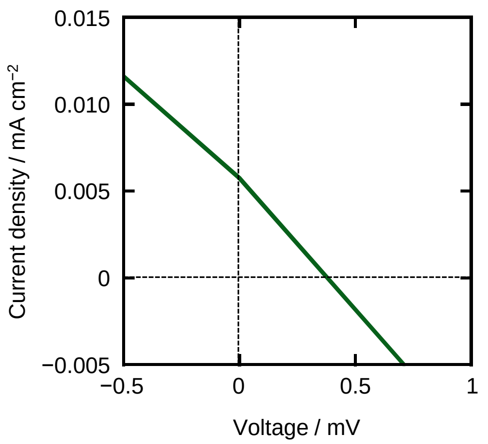


Fig. 3. Current-voltage characteristics of the p–n junction Si film on graphite plate under 1 sun, AM 1.5G illumination.

3. Development of Si Plating Processes Using Molten Salt Electrolytes: Deposition of Large Grain Si Utilizing Zn Liquid Electrode

We have investigated the Si electrodeposition in KF–KCl molten salt and confirmed that p–n junction Si films can be formed directly by electrodeposition. However, one of the issues was that the small crystal grains resulted in a large number of Si boundaries, which reduced the efficiency of solar cells. When Si was electrodeposited on solid substrates, the grain size was 50 nm at 923 K and 20 µm at 1073 K [5]. On the other hands, Maldonado *et al*. obtained crystalline Si by using a liquid metal electrode even at 373 K, where crystalline Si cannot be deposited on solid substrates [6]. They called this method "electrochemical liquid–liquid–solid (ec-LLS) process". With this background, we conceived the idea of applying the ec-LLS process to Si electrolysis at high temperatures to obtain large Si grains. In this fiscal year, fundamental study was conducted to verify the principle of ec-LLS process in high-temperature molten salt.

Fig. 4(a) shows a photo of the obtained Zn ingot after potentiostatic electrolysis at 0.75 V vs. K^+/K for 48 hours in molten KF–KCl–K_2SiF_6 (2.0 mol%) at 923 K. Si was present on the surface of the Zn ingot facing the BN crucible, not in the molten salt. This indicates that Si precipitation occurred inside the Zn electrode. The precipitation mechanism is thought to be as follows:

(1) Si(IV) ions are reduced on the surface of the Zn electrode to form a liquid Si–Zn alloy.
(2) Alloyed Si diffuses into the interior of the Zn electrode.
(3) Saturated Si precipitates as solid Si.

As shown in Fig. 4(b), grain size of the obtained Si was more than 1 mm, confirming that Si grows at high speed by the ec-LLS process.

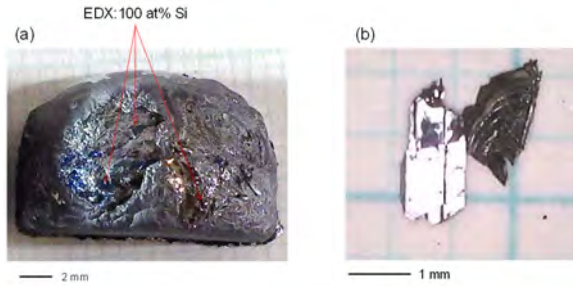


Fig. 4. (a) A photo of the sample obtained by potentiostatic electrolysis at 0.75 V for 48 hours in molten KF–KCl–K_2SiF_6 (2.0 mol%) at 923 K. (b) A photo of a separated large Si after HCl treatment.

Acknowledgement

These researches were partly supported by grants to T. N. from JSPS KAKENHI (21H04620).

References

[1] International Renewable Energy Agency (IRENA), (2019), Report "Future of Solar Photovoltaic" (https://irena.org/publications/2019/Nov/Future-of-Solar-Photovoltaic).
[2] K. Maeda, K. Yasuda, T. Nohira, R. Hagiwara and T. Homma, *J. Electrochem. Soc.*, **162**, D444 (2015).
[3] K. Yasuda, K. Maeda, T. Nohira, R. Hagiwara and T. Homma, *J. Electrochem. Soc.*, **163**, D95 (2016).
[4] K. Yasuda, K. Maeda, T. Nohira, R. Hagiwara and T. Homma, *J. Electrochem. Soc.*, **164**, D67 (2017).
[5] K. Yasuda, K. Saeki, T. Kato, R. Hagiwara and T. Nohira, *J. Electrochem. Soc.*, **165**, D825 (2018).
[6] J. Gu, E. Fahrenkrug, S. Maldonado, *J. Am. Chem. Soc.*, **135**, 1684 (2013).

Publications

T. Nohira, T. Ide, X. Meng, Y. Norikawa, K. Yasuda, Electrodeposition of Tungsten from Molten KF–KCl–WO_3 and CsF–CsCl–WO_3, Journal of The Electrochemical Society, 168, 4, 046505, 2021

X. Meng, Y. Norikawa, T. Nohira, Electrodeposition of mirror surface β-W films in molten CsF–CsCl–WO_3, Electrochemistry Communications, 132, 107139, 2021

K. Yasuda, T. Kato, Y. Norikawa, T. Nohira, Silicon Electrodeposition in a Water-Soluble KF–KCl Molten Salt: Properties of Si Films on Graphite Substrates, Journal of The Electrochemical Society, 168, 112502, 2021

Presentations

Y. Norikawa, A. Kondo, K. Yasuda, T. Nohira, Electrodeposition of Si in CsF–CsCl Eutectic Melt, 239th ECS meeting, Online, 2021.5.30-6.3

茂木涉，法川勇太郎，野平俊之, KF–KCl 溶融塩中における液体 Zn 電極を用いた結晶性シリコン電析, 第 89 回マテリアルズ・テーラリング研究会，オンライン開催, 2021.8.6-7

堀場由梨奈, 法川勇太郎, 野平俊之，溶融 LiCl–KCl–K_2CO_3–KOH 中でのダイヤモンド電析における再現性の向上, 第 89 回マテリアルズ・テーラリング研究会，オンライン開催, 2021.8.6-7

W. Moteki, Y. Norikawa, T. Nohira, Electrodeposition of Crystalline Silicon Using a Liquid Zn Electrode in KF–KCl Molten Salt, The 12th International Symposium of the Institute of Advanced Energy Science, Online, 2021.9.7

T. Nago, Y. Norikawa, H. Matsushima, T. Nohira, Study of Hydrogen Isotope Separation Technology by Molten Salt, The 12th International Symposium of the Institute of Advanced Energy Science, Online, 2021.9.7

堀場由梨奈, 法川勇太郎, 野平俊之，溶融 LiCl–KCl–K_2CO_3–KOH 系におけるダイヤモンドの電解合成に与える KOH 濃度の影響，第 5 回溶融塩化学討論会, 東京大学生産技術研究所/Online (Hybrid), 2021.11.18-19

茂木涉，法川勇太郎，野平俊之，溶融 KF–KCl–K_2SiF_6 中における液体 Zn 電極を用いた結晶性 Si 電析に与える電流密度の影響，第 53 回溶融塩化学討論会，東京大学生産技術研究所/Online (Hybrid), 2021.11.18-19

T. Nohira, X. Meng, Y. Norikawa, K. Yasuda, Electrodeposition of Bright Tungsten Coatings from Molten CsF–CsCl–WO_3, 7th Asian Conference on Molten Salt Chemistry and Technology, Institute of Industrial Science, The University of Tokyo, Japan/University of Science and Technology Beijing, China/Online (Hybrid), 2021.11.20

茂木涉，法川勇太郎，野平俊之, KF–KCl 溶融塩中における液体 Zn 電極を用いた結晶性 Si 電析, 2021 年度第 3 回関西電気化学研究会，オンライン開催, 2021.12.4

茂木涉, 法川勇太郎, 野平俊之，溶融 KF–KCl–K_2SiF_6 中における液体 Zn 電極を用いた結晶性 Si 電析に与える電気量の影響，電気化学会第 89 回大会，オンライン開催, 2022.3.15-17

堀場由梨奈，法川勇太郎，野平俊之，溶融 LiCl–KCl 中における CO_2 と H_2O を原料としたダイヤモンド電解合成の試み，電気化学会第 89 回大会，オンライン開催, 2022.3.15-17

Environmental Microbiology Research Section

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

1. Introduction

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

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

Polychlorinated biphenyls (PCBs) are well-known environmental pollutants broadened in all living environments. Biphenyl dioxygenase (BDO) plays a crucial role in the degradation of PCBs. BDO catalyzes the incorporation of two oxygen atoms into the aromatic ring of PCB, which induces the aromatic ring cleavage. Significantly, we developed the composite type of catalytic enzyme consisting of the two BDOs with different substrate specificities; moreover, we developed the bioreactor for generating oxygen microbubbles that enhance the enzymatic activities BDOs (Figure 1). As a result, we succeeded in constructing the practical system that degraded 99.3% of 40 mg L^{-1} of major commercial PCBs (Kenechrol KC-300 and KC-400) in 24 hours (Figure 2). Moreover, this result achieved the waste disposal standard defined by the Ministry of the Environment of Japan. These technical foci were reported in the international journal published this fiscal year.

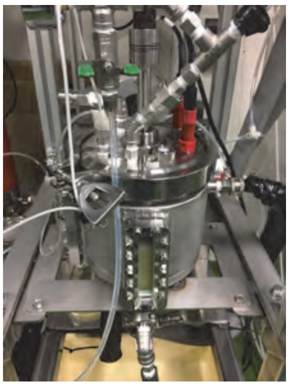


Figure 1. The composite BDOs-microbial catalyst was evaluated in the dedicated experimental bioreactor with the device of oxygen microbubble generation.

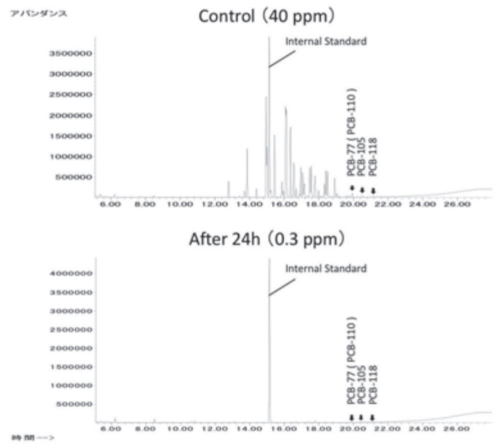


Figure 2. The data from the gas chromatography-quadrupole mass spectrometer showing the PCBs degradation by the composite BDOs-microbial catalyst.

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

To extend further the composite degrading reaction of PCBs, we have been trying to create a unique artificial enzyme that dechlorinates PCBs by two-electron reduction. Here, we collected fresh-water sediments from the contaminated site with PCBs in the Osaka area and investigated whether the bacteria associated with PCBs dechlorination exist. As a result, it was estimated that Dehalobacter sp. and *Desulfitobacterium* sp. by 16S rRNA gene phylogenetic analysis. Wang and He (Environ Sci Technol, 2013) reported that '*Deharobacter*' dechlorinates penta-/hexachlorinated biphenyls and '*Desulfitobacterium*' dechlorinates tetra-chlorinated biphenyls hydroxylated at the para position. We succeeded in preparing the media for growing these particular bacterial species and their cultivation method. Besides, we also observed that these two bacterial species reduce PCBs in the artificial model of the polluted environment. Even today, repeated long-term observation is being made to confirm whether the result is correct.

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

Many plant diseases are generally caused by either *Ascomycetes* or *Basidiomycetes* that belong to filamentous fungi. 'Filamentous fungi' are hyphae and proliferate to mycelia. The cell wall is a peculiar composite material that incorporates a mix of cross-linked fibers and matrix components. The fibrous components of the cell wall are glucan, chitin, and mannan, and these sugar chains contribute to forming a supple and solid filiform microfibril wall. Glycosidase is a hydrolase that catalyzes the hydrolysis of glycosidic bonds in complex sugars. We are developing a new bio-macromolecular type of fungicide utilizing the hydrolysis reactions of glycosidases against the fungal microfibril wall. So far, our composite type of bacterial catalyst composed of 5 strains from class *Bacilli*, which produce and secrete various glycosidases, controlled 99.3% of a tomato-Pestalotia disease with *Pestalotiopsis* sp. (Figure 3). Glycosidases are classified into approximately 130 families, and their catalytic reactions are roughly divided into anomeric inversion and/or anomer retention and exo-glycosidase or endo-glycosidase. Given that, the classification of glycosidase can be understood as diverse. We have considered it possible to efficiently digest fungi cell walls by compositely capably using these diversities of enzyme activities.

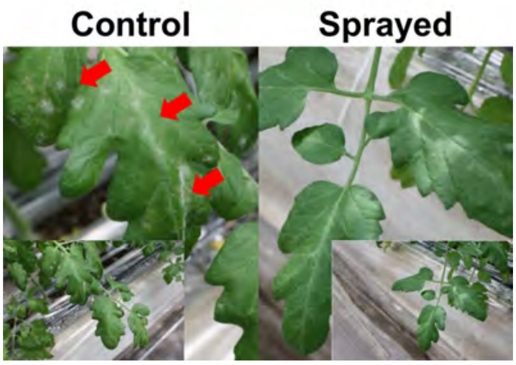


Figure 3. The glycosidase secreted type of the composite microbial catalyst inhibited tomato-*Pestalotia disease*.

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

We investigated the fungicidal properties of glycosidases produced by a phytopathogenic filamentous strain belonging to *Basidiomycetes*. When grown in a bran medium, this filamentous strain secretes enzymes and exhibits various glycosidase activities. This crude enzyme fraction showing composite glycosidase activities digested 3 out of 6 wet-rice-specific epidemically filamentous fungi (Figure 4). There are not almost enzymes showing high digesting activity against multiple strains of phytopathogenic filamentous fungi. In the case of single glycosidase activity, on the other hand, digested only 2 strains. These results suggested that the compositive glucosidase has a more fungicidal activity than the individual glycosidase. We try to purify the components of this crude enzyme. Soon, we may clarify the effectively fungicidal mechanism of this crude enzyme by definite the type of the enzyme(s), the amounts of the secretion, and the specific activities.

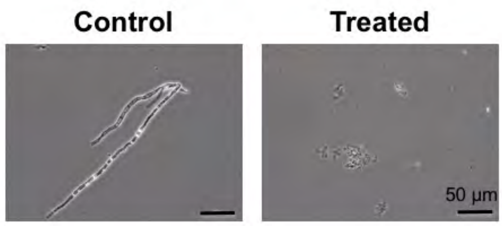


Figure 4. The crude enzyme fraction secreted from the phytopathogenic filamentous fungus digested a wet-rice specific epidemically filamentous fungal strain.

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

Our collaborative research with Vietnam National University revealed that two strains of *Bacillus* isolated from the intestinal tract of white-leg shrimp had excellent health-improving functions to the same class's shrimps. This *Bacillus* probiotic avoids using antibiotics and synthetic chemicals in feeding, enhances shrimp health and growth efficiency, and reduces the energy consumption in white-leg shrimp cultivation. This cultivated industry has been recently growing in Japan, but there is almost no appropriate feed. Therefore, we are collaborating with academic institutions specializing in crustaceans to verify their usefulness in detail.

Collaboration Works

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

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

Financial Support

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

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

原富次郎，東洋ガラス（株），環境微生物の探索と機能解明の研究のため

原富次郎，（株）竹中工務店，環境微生物の探索と機能解明の研究のため

原富次郎，（株）オーガニック・ソリューションズ・ジャパン，抗食品危害真菌物質の探索

Publications

Hara T, Takatsuka Y. Aerobic polychlorinated biphenyl-degrading bacteria isolated from the Tohoku region of Japan are not regionally endemic. Canadian Journal of Microbiology. 2022:1-12.

T. Hara, Y. Takatsuka, Y. Shiwa, K. Yokota, Draft Genome Sequence of the Polychlorinated Biphenyl Degrader *Comamonas testosteroni* Strain YAZ2 Isolated from a Natural Landscape in the Tohoku Region of Japan, Microbiol Resour Announcements, 11, 1, e00806-21, 2022

T. Hara, Y. Takatsuka, E. Nakata, T. Morii, Augmentation of an Engineered Bacterial Strain Potentially Improves the Cleanup of PCB Water Pollution, Microbiology Spectrum, 9, 3, e01926-21, 2021

T. Jamnongkan, A. Yosta, B. Thanesthakul, M. Sugimoto, T. Hara, Y. Takatsuka, R. Mongkholrattanasit, Effect of ZnO Nanoparticles on the Physical Properties of PLA/PBS Biocomposite Films, Materials Science Forum, 1033, 143-150, 2021

T. Hara, Y. Takatsuka, Y. Shiwa, K. Yokota, T. Shin-i, Manual recursive mapping method for the draft genome sequence of *Comamonas testosteroni* strain YAZ2., Figshare, 17132309, v7, 2021

Presentations

山岸純一, 髙塚由美子, 川端千翔, 上野 誠, 松本慎吾, 原富次郎, *Rhizoctonia solani* D138 株分泌酵素群による薬用ニンジン病害性糸状菌の成長阻害，第 73 回日本生物工学会大会，オンライン開催，2021.10.27-29

3-2. AWARD

Young Researcher Award of the Japanese Society of Infrared Science and Technology

Quantum Radiation Energy Research Section
Heishun Zen (Assistant Professor)

Assistant Professor Heishun Zen was awarded the Young Researcher Award of the Japanese Society of Infrared Science and Technology on June 4th, 2021. This award has been established to encourage young researchers in their research work and further enliven the community of infrared science and technology. He was awarded this award for his intensive research and development work of the mid-infrared free electron laser including his efforts in supporting the application experiments.

In his award lecture, which was held on July 4th, 2021 online, he presented his research work on the mid-infrared free electron laser and several application experiments performed in Kyoto University Free Electron Laser facility under the support of Joint Usage/Research Center for Zero-Emission Energy Research.


研究奨励賞

「中赤外自由電子レーザの高性能化とその利用推進」

全 炳俊 殿

貴殿の赤外線科学・技術に関する研究活動は顕著であり、その成果は優秀であるとともに赤外線科学・技術の発展に貢献するところ多大であります
よって、ここに第八回日本赤外線学会研究奨励賞を贈りその功を表彰いたします

令和三年六月四日

一般社団法人 日本赤外線学会
会長 長田 哲也

The 17th PASJ Award for Research Encouragement

Quantum Radiation Energy Research Section
Heishun Zen (Assistant Professor)

Assistant Professor Heishun Zen was awarded the 17th PASJ Award for Research Encouragement from the Particle Accelerator Society of Japan on June 10th, 2021. This award has been established to encourage young researchers in their research work and further enliven the community of particle accelerator. He was awarded this award for his research work on the improvement of the extraction efficiency of oscillator-type infrared free electron laser driven by a normal conducting linear accelerator. The research was performed under the support of MEXT Quantum Leap Flagship Program (MEXT Q-LEAP) Grant Number JPMXS0118070271.

In his award lecture, which was held on August 11th, 2021 online, he presented the recent achievement of the high extraction efficiency operation of the mid-infrared free electron laser. His talk included several efforts to achieve high extraction efficiency and prospects.


Particle Accelerator Society of Japan
presents
The 17th PASJ Award for
Research Encouragement
to
Dr. Heishun Zen
in recognition of valuable achievement on
"Research and development on improvement of extraction efficiency of free electron laser oscillator driven by a normal conducting accelerator"
June 10, 2021
Particle Accelerator Society of Japan (PASJ)
President
羽島良一

Student Poster Award, Atomic Energy Society of Japan

Advanced Atomic Energy Research Section
Yuto Murata (M2)

Yuto Murata (M2) was awarded Student Poster Award from Atomic Energy Society of Japan (AESJ) on 10th September 2021. This poster session was hosted by the AESJ Student Network and the AESJ Diversity Promotion Committee. In the poster session, there were diverse presentations by students (from undergraduate to doctoral course students).

In his work, the saturated solubility of Bi in liquid Li–Pb was measured in the temperature range from 508 to 623 K, in order to evaluate amount of Po production in a fusion reactor with liquid blanket. The measured results showed a positive temperature dependence where the solubility decreases as the temperature was lowered. The equation of the solubility curve of Bi in Li–Pb gave the dissolution enthalpy of Bi as –77 kJ/mol. By X-ray diffraction analysis of the precipitates, the formation of Li_3Bi phase was confirmed.

Student Poster Award, Atomic Energy Society of Japan

Advanced Atomic Energy Research Section
Yasuyuki Ogino (D3)

Yasuyuki Ogino (D3) was awarded Young Researcher Award from Atomic Energy Society of Japan (AESJ) Kansai branch. The young researcher workshop was held on 10th March 2022 virtually and hosted by the AESJ Kansai branch. In the workshop, young researchers in Kansai area had oral presentations.

In his work, the thermal and epi-thermal neutron fluxes in a blanket mock-up were measured by using metal foils and imaging plate. The metal foils were activated by deuterium–deuterium neutron irradiation with an average neutron production rate of 1.22 –1.31 x 10^7 n/sec. The radiations of β- and γ- rays emitted during each decay process were measured on an imaging plate of 2-dimensional radiation dosimeters. The detection range at measured positions was between 2 x 10^{-3} and 5 x 10^{-2} cm^2/n, and calculation to experimental values was 0.27–2.47.

Student Presentation Awared of the Physical Society of Japan

Complex Plasma Systems Research Section
Panith Adulsiriswad (D3)

2021 Autumn meeting of the Physical Society of Japan was held on September 20-23, 2021, on-line. This meeting has a long history since 1946 and it has covered almost all fields of physics.

Panith Adulsiriswad (D3) attended in the meeting and made a presentation titled “Study of the Interaction between Peripheral Energetic Particle Mode and Energetic Particles in Heliotron J with MEGA, a Hybrid MHD Simulation with Free Boundary Condition”.

He received the Student Presentation Award of the Physical Society of Japan (division 2, or plasma physics). This was the second time for him in this meeting; the first time being last year.


The Physical Society of Japan
日本物理学会学生優秀発表賞
領域2
Adulsiriswad Panith 殿
あなたの2021年日本物理学会秋季大会における講演
23aB2-3 Study of the Interaction between Peripheral Energetic Particle Mode and Energetic Particles in Heliotron J with MEGA a Hybrid MHD Simulation with Free Boundary Condition
は，当学会の学生優秀発表賞を受賞されましたことをここに証します
2021年10月9日
一般社団法人日本物理学会
会長 田島節子

JPS
CERTIFICATE
Student Presentation Award of the Physical Society of Japan
Division 2
To
Adulsiriswad Panith
Title of presentation
Study of the Interaction between Peripheral Energetic Particle Mode and Energetic Particles in Heliotron J with MEGA, a Hybrid MHD Simulation with Free Boundary Condition
At 2021 Autumn meeting of the Physical Society of Japan.
Presentation ID 23aB2-3.
October 9, 2021
President, The Physical Society of Japan
Setsuko Tajima
田島節子

Excellent Poster Presentation Award (The 34th Fall Meeting, The Ceramic Society of Japan)

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

The 34th Fall Meeting, the Ceramic Society of Japan, was held on 1st – 3rd of September, 2021. This event provides to promote the development of industry, science and technology related to the ceramics field.

Hiroyuki Sakai (M2) attended and made a poster presentation on the topic of “Effect of eutectic reaction on RE-silicate formation by surface modification of SiC”. He received the Excellent Poster Presentation Award from the Ceramic Society of Japan.

In this presentation, he presented about the effect of eutectic reaction on surface modification of liquid phase sintered SiC. This modification method works as an alternative technology to conventional environmental barrier coatings in particular for aerospace application.


表彰状
優秀賞
京都大学
堺　弘行 殿
あなたの研究発表は日本セラミックス協会第３４回秋季シンポジウムにおきまして、優秀ポスター発表賞と認められましたので表彰します。
令和３年９月１０日
日本セラミックス協会
第３４回秋季シンポジウム第09セ
「エンジニアリングセラミックスの
オーガナイザー代表 楠瀬

Osawa Award for Young Scientists (The Fullerenes, Nanotubes and Graphene (FNTG) Research Society)

Nano Optical Science Research Section
Keisuke Shinokita (Assistant Professor)

Assistant professor Keisuke Shinokita was awarded Osawa Award for Young Scientists from the Fullerenes, Nanotubes and Graphene (FNTG) Research Society. The Osawa Award for Young Scientists is given to researchers awarded to presentations on theory, experimentation, and application development of fullerene and its related substances. He was awarded this prize on the achievements of "Novel excitonic features of moiré exciton in twisted van der Waals heterostructures."

In his award lecture, which was held on 3rd September 2021, at the online meeting, he presented several emergent optical phenomena and the physical mechanism of the twisted $MoSe_2/WSe_2$

Young Scientist Poster Award (The Fullerenes, Nanotubes and Graphene Research Society) and Nanoscale Hrizon Presentation Prize (The Royal Society of Chemistry)

Nano Optical Science Research Section
Mikio Kobayashi (M2)

Mikio Kobayashi (M2) was awarded Young Scientist Poster Award (The Fullerenes, Nanotubes and Graphene Research Society) and Nanoscale Horizon Presentation Prize (The Royal Society of Chemistry) of The 62th Fullerenes-Nanotubes-Graphene General Symposium on March 2-4, 2022. The Young Scientist Poster Award is given to a few researchers who gave a poster presentation. Nanoscale Horizon Presentation Prize is given to an outstanding presentation at the conference. He was awarded these prizes on the presentation of "Optical properties of transition metal dichalcogenides with microshperical optical cavity".

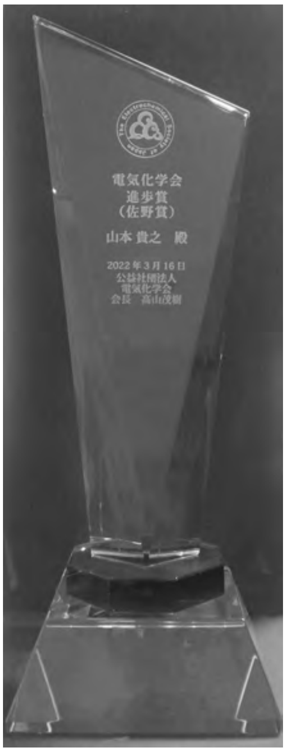
He presented about demonstration of optical resonances of light emission from transition metal dichalcogenides and van der Waals heterostructures in a shperical optical cavity in the previous symposium on March 1st, 2021 at Osaka University (online), In addition, this study will lead to advanced light emission devices with atomically semiconducting materials.

Young Researcher Award of The Electrochemical Society of Japan (Sano Award)

Chemical Reaction Complex Processes Research Section
Takayuki Yamamoto (Assistant Professor)

Assistant Professor Takayuki Yamamoto received Young Researcher Award of The Electrochemical Society of Japan (Sano Award) on March 16th, 2022. This award is annually given to young researchers who have achieved outstanding progress in the field of electrochemistry. He received this award for his work on "Next-Generation Rechargeable Batteries Utilizing Ionic Liquids and Various Charge Carriers".

In his award lecture online on March 17th, 2022, he presented new findings and progress on several rechargeable batteries including sodium and potassium secondary batteries with amide-based ionic liquid electrolytes and fluoride-shuttle batteries using fluorohydrogenate ionic liquids.



Research Encouragement Award at The 89th Workshop of Materials Tailoring Society

Chemical Reaction Complex Processes Research Secton
Alisha Yadav (D3)

The 89th worshop of Materials Tailoring Society was held on 6th–7th August 2021, Online, and was organized by Materials Tailoring Society.

The purpose of this workshop is to systemize the basic study of nanostructured interface creation that induces high-performance physical properties by non-equilibrium processing such as plasma and electrolytic processes and to also apply them to energy conversion and storage.

Ms. Alisha Yadav (D3) attended this workshop and made a poster presentation on the topic "Comparative studies on Graphite as Negative Electrode for Alkali Metal-ion Batteries using FSA-based Ionic Liquids", and received the Research Encouragement Award. She investigated the potassium storage behavior of graphite in K[FSA]–[C_3C_1pyrr][FSA] electrolyte at 313 K temperature through electrochemical and XRD measurements and observed the formation of various stages of K-GICs. She further compared the performance of graphite as negative electrode in Li-, Na-, and K-ion systems using M[FSA]–[C_3C_1pyrr][FSA] (x(M[FSA] = 0.20)) (M = Li, Na, K) electrolytes.

Best Student Poster Award in the 12th International Symposium of Advanced Energy Science

Chemical Reaction Complex Processes Research Section
Wataru Moteki (M2)

The 12th International Symposium of Advanced Energy Science was held on September 7–8, 2021, online Remote Conference. This event provides young researchers and students in the field related with energy an opportunity to present their works.

In the meeting, Mr. Wataru Moteki (M2) attended and made a poster presentation on the topic of “Electrodeposition of Crystalline Silicon Using a Liquid Zn electrode in KF–KCl Molten Salt”. He received the Best Student Poster Award.

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

Chemical Reaction Complex Processes Research Section
Wataru Moteki (M2)

The 3st Kansai Electrochemistry Workshop was held on 4th December 2021, on Webinar, which was held by the Kansai Branch of the Electrochemical Society of Japan. This event provides young researchers and students in the field of electrochemistry and its surrounding area an opportunity to present their works.

In the meeting, Mr. Wataru Moteki (M2) attended and made a poster presentation on the topic of “Crystalline Si electrodeposition using a liquid Zn electrode in a KF–KCl molten salt”. He received the Young Researcher’s Award.

JEOL RESONANCE Poster Award in ISMAR-APNMR-NMRSJ-SEST 2021

Structural Energy Bioscience
Research Section
Yudai Yamaoki (Assistant professor)

The ISMAR-APNMR-NMRSJ-SEST 2021 was held on online from 22nd to 27th August, 2021 as a joint conference of the 22nd International Society of Magnetic Resonance Conference, the 9th Asia-Pacific NMR Symposium, the 60th Annual Meeting of the Nuclear Magnetic Resonance Society of Japan 2021, and the 60th Annual Meeting of the Society of Electron Spin Science and Technology. ISMAR-APNMR-NMRSJ-SEST 2021 is the largest international conferences in the magnetic resonance research field and 920 front-line researchers were participated.

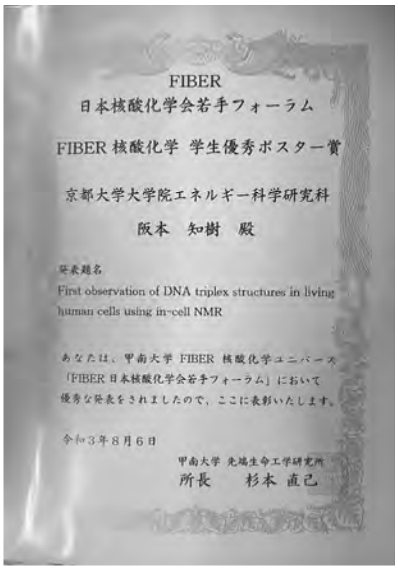
In this meeting, Yudai Yamaoki made poster presentation entitled “In-cell NMR analyses of the structure and dynamics of hairpin and G-quadruplex structures in the living human cells”. The intracellular environment is highly condensed with macromolecules. Under such cellular conditions, it has long been considered that dynamics of nucleic acids might be different from those under *in vitro* conditions, however there is no evidence. In the presentation, he used in-cell NMR technique that provide the information of structural dynamics of nucleic acids inside the living cell and revealed that the base-pair lifetime of some base pairs in the RNA hairpin and DNA G-quadruplex structures are different from that under *in vitro* conditions.

Yudai Yamaoki was awarded JEOL RESONANCE Poster Award from the committee of ISMAR-APNMR-NMRSJ-SEST 2021. JEOL RESONANCE Poster Award were given to five outstanding presentations in the joint conference.

Best Student Poster Award in Young Researchers Forum of FIBER and The Japan Society of Nucleic Acids Chemistry

Structural Energy Bioscience
Research Section
Tomoki Sakamoto (D1)

Young Researchers Forum of FIBER and The Japan Society of Nucleic Acids Chemistry was held on 5-6th August 2021 as an online forum. This forum was jointly organized by The Frontier Institute for Biomolecular Engineering Research (FIBER) and the Japan Society of Nucleic Acids Chemistry to deepen exchanges among researchers in nucleic acid chemistry and foster a younger generation of researchers. Tomoki Sakamoto made a poster presentation entitled "First observation of DNA triplex structures in living human cells using in-cell NMR" in this meeting. DNA, the carrier of genes, is known to form a triplex structure within a particular DNA sequence. It has been pointed out that such triplex structures are associated with diseases such as Friedreich's ataxia. In his presentation, he reported for the first time that DNA triplex structures could be formed in living human cells using in-cell NMR method, which can directly obtain information on molecules in living cells. The results obtained in this study will provide important information for developing DNA triplex structure-specific drugs.
Tomoki Sakamoto was awarded Best Student Poster Award in Young Researchers Forum of FIBER and The Japan Society of Nucleic Acids Chemistry. These awards were given to five students who gave outstanding presentations out of 87 participants



Local Co-Creation Project in Kinokawa; Grand Prize

Environmental Microbiology Research Section
Motohito Yoneda (Researcher)

Motohito Yoneda, a Researcher, was awarded the Grand Prize by the "Local Co-Creation Project in Kinokawa" sponsored by the government city of Kinokawa on March 20, 2022. This prize is given to those who created a new processed product brand rooted in the Kinokawa area.

He was awarded this prize for developing a new liquid seasoning by applying organic herbs grown by sowing arbuscular mycorrhizal strains. The characteristic of this seasoning is that it has a high aroma and lasts a long time. The products produced from this result will be distributed to the market as products certified by the government city of Kinokawa shortly.

< Picture stating receiving the prize “最優秀賞“, and Dr. Yoneda is wearing a lab coat. >

4. JOINT USAGE/RESEARCH PROGRAM

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

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

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

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

We propose a new concept of Zero Emission Energy as a typical model of Advanced Energy. IAE Zero Emission Energy Research aims at the realization of environmentally friendly energy system for sustainable society with minimum emission of environmental pollutants and with maximum utilization of energy and resources. Since FY2011, we had operated a project, “Joint Usage/Research Program on Zero Emission Energy”, which is the program authorized by the MEXT. We have started the second term of the Program from FY2016. Here, we aim to (1) promote interdisciplinary joint usage/research studies for

Poster of the 12th International Symposium

Zero Emission Energy Science & Technology, (2) promote education & practical training for young researchers and (3) explore future horizon of Advanced Energy System for sustainable development. IAE provides many unique & attractive facilities for the Joint Usage/Research not only in the field of advanced plasma & quantum energy but also in the field of soft energy.

Many researchers have participated in this program. In FY2021 Joint Usage/Research collaborations of total 105 subjects (including two workshop) on Zero Emission Energy were performed with more than 300 visiting participants from 30 all-Japan Universities and Institutions including graduate/undergraduate students. Researchers from 6 foreign Universities also participated in the program. The results of these collaborations are summarized in a report "IAE Joint Usage/Research Program on Zero Emission Energy 2021". The meeting to present some of remarkable results obtained in FY2021 was held online on March 14, 2022. If you have interest to this collection, please contact to the Office of Zero Emission Energy Research.

In addition to the Joint Usage/Research collaborations, we organized "The 12th International Symposium of Advanced Energy Science -Research Activities on Zero-Emission Energy Network-" on September 7–8, 2021. This symposium was held online due to the COVID-19. This symposium consists of oral and poster sessions, and satellite meeting. 162 scientists and students including 3 foreign and 1 domestic invited speakers participated in the symposium. (http://www.iae.kyoto-u.ac.jp/zero_emission_e/ZEcalendar/)

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

In FY2021, the evaluation of all of the second term was conducted by MEXT for all the Joint Usage/Research Center Programs. Our program was given "A" evaluation. We were also approved as the Joint Usage/Research Center for the third term, which will begin in FY2022.

List of Zero Emission Energy Joint Usage/Research Subjects in FY 2021

(Subject, Principal Researcher, IAE Key Person)

Elucidation of Hopping Conduction in Lithium Excess Solvate Ionic Liquids, Atsushi Kitada, Masato Katahira

Study on lignin degradation by infrared free electron laser, Takayasu Kawasaki, Heishun Zen

Study of formation process of solute clusters in stainless steel with ion irradiation, Ken-ichi Fukumoto, Kiyohiro Yabuuchi

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

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

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

Chemical state analysis of borocarbides, Ryuta Kasada, Kiyohiro Yabuuchi

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

Functionalization of amino sugar-containing polysaccharides using environmental microbes, Minoru Takeda, Masato Katahira

Interaction analysis between cellulase carbohydrate-binding module andlignin by ultra-high sensitivity NMR for biorefinery, Takashi Watanabe, Masato Katahira

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

NMR analysis on molecular mechanism of phase separation inhibition and elucidation of its physiological significance, Riki Kurokawa, Masato Katahira

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

Strucutral analysis of fluorine-containing compounds by NMR spectroscopy, Kazuhiko Matsumoto, Masato Katahira

Effect of high energy He ion implantation on hydrogen isotope behavior intungsten, Yasuhisa Oya, Kiyohiro Yabuuchi

The effects of dangling-bond on anodic dissolution of ceramics, Sosuke Kondo, Kiyohiro Yabuuchi

Development of biomaterial which improve gut microbiome and health of white-leg shrimp by using heat-stable carotenoid-producing Bacillus spores, Nguyen Thi Van Anh, Yumiko Takatsuka

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

Development of low-density stacked CNT target and fundamental process of the interaction by high-intensity laser irradiation, Ryutaro Matsui, Kazunari Matsuda

Electrodeposition of Si in Molten Salts Containing Silicate Ions towards the Production of Solar-Grade Silicon, Koji Yasuda, Toshiyuki Nohira

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

Advanced thermal diffusivity evaluation method using D3 miniature specimens at elevated temperature., Masafumi Akiyoshi, Kiyohiro Yabuuchi

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

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

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

Analysis of element distribution changes in solid lithium electrolytegenerated by electrodialysis using rf-GD-OES, Kazuya Sasaki, Keisuke Mukai

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

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

Development of Emissive Solid Materials Applicable to Luminescent Solar Concentrators, Masaki Shimizu, Hiroshi Sakaguchi

Development of pulsed laser deposition using infrared free electron laser, Takashi Nakajima, Heishun Zen

NMR analysis of peptides and nucleic acids that modulate biomolecularfunctions, Taiichi Sakamoto, Takashi Nagata

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

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

Carrier diffusion process in silicide kankyo semiconductors reveaed by mid-infrared free electron laser, Mamoru Kitaura, Heishun Zen

Structural study of DNA binding of the replication initiator ORC, Shou Waga, Masato Katahira

The temperature dependence of ductility in Al, Zr-added ODS ferritic steeltreated under different MA atmospheres, Noriyuki Iwata, Kiyohiro Yabuuchi

Study of material development and inteface desingn for all solid state Liion battery, Ikuma Takahashi, Keisuke Mukai

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

Study on the impact of phase reconfiguration in unbalanced distribution systems, Vannak VAI, Hideaki Ohgaki

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

Elusidation of ablation mechanism based on vibrational excitation in molding materials and surface modification by infrared free electron laser, Jun Fujioka, Heishun Zen

Clarification of hydrogen adsorption and desorption behavior for neutron multipliers for fusion applications, Jaehwan Kim, Keisuke Mukai

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

Design and investigation of complexes comprinsing atom-layered materials, Susumu Okada, Kazunari Matsuda

Study on Thermal Radiation of Quantum Materials for Highly Efficient and Functional Energy Conversion, Satoru Konabe, Yuhei Miyauchi

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

Surface processing of SiC achieved by combination of phonon excitation using FEL and electrochemistry, Kazuhiro Fukami, Heishun Zen

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

The study of material degradation evaluation with irradiation hardening in tungsten for divertor, Kouichi Tougou, Kiyohiro Yabuuchi

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

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

Development of tantalum added vanadium alloys for fusion reactors, Takeshi Miyazawa, Kiyohiro Yabuuchi

Spatially resolved measurement of atomic emission line spectra using NIR Zeeman spectroscopy, Taiichi Shikama, Shinichiro Kado

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

Study of the battery technology for Improving the Solar Home System (SHS) in Rural electrification, Nasrudin Abd Rahim, Hideaki Ohgaki

Development and application of organic spintronics materials toward energy-saviing devices, Yusuke Miyake, Hiroshi Sakaguchi

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

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

Clarification on retention processes of He and H in ion irradiated pyrochlore oxides, Bun Tsuchiya, Kiyohiro Yabuuchi

NMR analysis of the three-dimensional solution structure of the sequence-specific RNA-binding protein Musashi1 involved in translation control of the downstream target RNA, Takao Imai, Takashi Nagata

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

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

Time-series data analysis of Heliotron-J plasma by statistical modeling, Shigeru Inagaki, Kazunobu Nagasaki

Development of ultrasound-enhanced cell-internalization method and mechanism evaluation, Atsushi Harada, Eiji Nakata

Measurement of coherent edge radiation spectra during free-electron laser oscillations, Norihiro Sei, Hideaki Ohgaki

Study for the development of functional peptides using NMR, Hideki Kusunoki, Takashi Nagata

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

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

Effect of irradiation on Coated Materials for Tritium Barrier, Somei Ohnuki, Kiyohiro Yabuuchi

Quanitative relationship between plasma-produced reactive radical amount and biological/chemical reaction promotion, Hiroto Matsuura, Shinichiro Kado

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

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

Development of optical devices using the interface of layered material and nitride semiconductor, Shinichiro Mouri, Kazunari Matsuda

Ultra-Highly Sensitive DNA/RNA Sensor, Kazushige Yamana, Takashi Morii

Natural Convection Heat Transfer for Sugar Alcohols, Makoto Shibahara, Kiyohiro Yabuuchi

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

Design of Staple oligoemr based on thermodynamic analysis, Yousuke Katsuda, Takashi Morii

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

Microstructural evolution of ODS Ferritic Steels during cold working process for Next generation Nuclear components, Sanghoon Noh, Kiyohiro Yabuuchi

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

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

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

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

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

Development of high-speed camera image analysis method using magnetic field information, Nobuhiro Nishino, Shinichiro Kado

Development of a method for compsiting Li2TiO3 and nanocarbon by microwave irradiation, Sadatsugu Takayama, Keisuke Mukai

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

Dissociation of poly-amino acid aggregates by free electron laser irradiation, Kazuhiro Nakamura, Heishun Zen

Determination of the free energy of the late-blooming phase (3), Yoshitaka Matsukawa, Kiyohiro Yabuuchi

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

Fluorescenct analyses of biomolecules and metals using cephem compounds, Ippei Takashima, Eiji Nakata

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

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

Influence of irradiation defects on the tritium removal behavior from tungsten by hydrogen isotope exchange, Mingzhong Zhao, Kiyohiro Yabuuchi

Clarification of fine structure of environmentally compatible hydroxyapatite capsules, Takeshi Yabutsuka, Kiyohiro Yabuuchi

Conductivity Enhancement Mechanism of NASICON-type Lithium Ion Conductive Composite, Shigeomi Takai, Takashi Morii

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

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

Analyses of Electroretinograms from crayfish's compound eyes evoked by KU-FEL irradiation: Fast and Late reaction, Fumio Shishikura, Hideaki Ohgaki

Measurement of scintillation response by fast neutron, Kenichi Fushimi, Keisuke Mukai

Statistical analysis on edge turbulence fluctuation data in Heliotron-J, Yoshihiko Nagashima, Shinsuke Ohshima

Distributed Workshop on "Physics and control of non-linear and non-equlibrium plasma based on the concept of broad-band energy science", Yasuaki Kishimoto, Kazunari Matsuda

Study on how to make zero emmission infrastructure more social resilient by advanced ICT, Hidekazu Yoshikawa, Kazunori Morishita

KU-FEL User Symposium 2021, Mamoru Kitaura, Heishun Zen

Investigation for expeirimental simulation of space plasmas using magnetically confined configurations, Kenichi Nagaoka, Heishun Zen

5. COLLABORATION WORKS IN THE LABORATORY FOR COMPLEX ENERGY PROCESSES

Collaboration Works in
The Laboratory for Complex Energy Processes

1. Introduction

The laboratory was established for research on advanced energy by the collaborative projects among the researchers in the Institute of Advanced Energy to promote joint activity of our knowledge and wisdom to find solutions to these interdisciplinary energy/environmental problems. From such a viewpoint, the research targets of the laboratory are focused on two specific fields, (i) "advanced studies of science and technology on plasma energy and quantum energy" and (ii) "innovative studies of nano-bio functional materials for power generation". For this purpose, two sections (A2 and A3 mentioned below) are founded. In addition, A1 section promotes international or domestic collaborative research and assists activities such as academic meetings and seminars. In the fiscal year of 2021, the pandemic of COVID-19 had a significant impact on the actual implementation of the collaborative activity, because the traffic and actual meeting were strictly avoided.

Despite the difficulty in organizing the cooperative research program, however, close connection between related research fields in the institute have yielded unique and interesting outcomes from the collaboration. The laboratory takes charge of organizing and promoting the cooperative research project as a center of research activity in the Institute. The research teams were formed by mostly young generation staffs and students in the institute lead by associate professor or assistant professor, and participated in specific projects to carry out their subjects. The cooperative research activities will be published in a publication edited in the laboratory at the end of the fiscal year. Management of the technical staffs for large scale equipment are also under the responsibility of the laboratory.

A1 Division of International and Industrial Partnership

This division promotes international collaborative research on advanced energy to lead the field of energy science and technology as a worldwide pioneer. For this purpose, the symposium and the workshop organized by institution member are usually supported, however in this fiscal year, to reduce the risk of the infection was given the highest priority, and no meetings or exchange was planned.

A2 Division of Plasma and Quantum Energy Research

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

A3 Division of Soft Energy Science Research

This division promotes studies on emergent materials and systems for realizing next generation soft energy system. In particular, functional nano- and bio-materials to efficiently utilize solar energy and bio-energy are studied by integrating laser science, nanotechnology, and bio-technology. We aim at extending our research fields by utilizing the existing devices such as System for Creation and Functional Analysis of Catalytic Materials, SEMs, SPM, Solar Simulator, KU-FEL and various laser systems.

2. The cooperative research program

In the fiscal year of 2021, two categories were set up: (1) “Cooperative Research” for cross sectional research proposal by either Associate or Assistant Professor and (2) “Sprouting Research” for challenging research proposal by Assistant Professor. The submitted proposals were evaluated by the selection committee organized by a center director, a program chair and three division chairs. One “Cooperative Research” proposal and four “Sprouting Research” proposals were approved. The number of research subjects is listed in Table 1 according to the division. A brief summary of the cooperative research subjects carried out in FY2021 is shown in the next page.

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

The whole sum 5

Category			Total
A1	A2	A3	
0	1	4	5

The individual research subjects are as follows.

<u>Cooperative Research</u>

<u>A3</u>

"Development of chemical methods to stabilize DNA nanomaterials for handling biomass-related enzymes"

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

<u>Sprouting Research</u>

<u>A2</u>

"New approach for the study of plasma physic utilizing the open magnetic field region"

- S. Ohshima, S. Kobayashi (Inst. Adv. Energy, Kyoto Univ.)
- R. Matoike, A. Miyashita (Grad. Sch. Energy Sci., Kyoto Univ.)

<u>A3</u>

"Clarification of fundamental optical properties of moire superstructure"

- K.Shinokita (Inst. Adv. Energy, Kyoto Univ.)

"Electrochemical synthesis of alkaline earth metal-graphite interaction compounds and applications to rechargeable batteries"

- T. Yamamoto (Inst. Adv. Energy, Kyoto Univ.)

"Evaluation of the structure and dynamics of nucleic acids in living human cell"

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

The Laboratory Seminars

Laboratory Seminars

The Laboratory promotes topical academic seminars in order to strengthen the research activities in each research section and to enhance the mutual cooperation among a lot of academic fields. In the fiscal year of 2021, the aims and progress reports of five cooperative researches were presented and discussed, as summarized below. The Laboratory also planned a symposium on April 8, 2022 for presentation of the cooperative research results in FY2021.

(1) October 20, 2021
A. Rajendran
“Development of chemical methods to stabilize DNA nanomaterials for handling biomass-related enzymes”
Inst. Adv. Energy, Kyoto Univ.

(2) November 10, 2021
K. Shinokita
“Development of optical science in atomically-thin semiconductors”
Inst. Adv. Energy, Kyoto Univ.

(3) November 30, 2021
Y. Yamaoki
“Evaluation of the structure and dynamics of nucleic acids in living human cell”
Inst. Adv. Energy, Kyoto Univ.

(4) December 22, 2021
T. Yamamoto
“Development of next-generation rechargeable batteries using ionic liquid electrolytes”
Inst. Adv. Energy, Kyoto Univ.

(5) January 11, 2022
S. Ohshima
“New approach for the study of plasma physic utilizing the open magnetic field region”
Inst. Adv. Energy, Kyoto Univ

6. PROJECTS WITH OTHER UNIVERSITIES AND ORGANIZATIONS

NIFS Bilateral Collaboration Research Program on Heliotron J

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

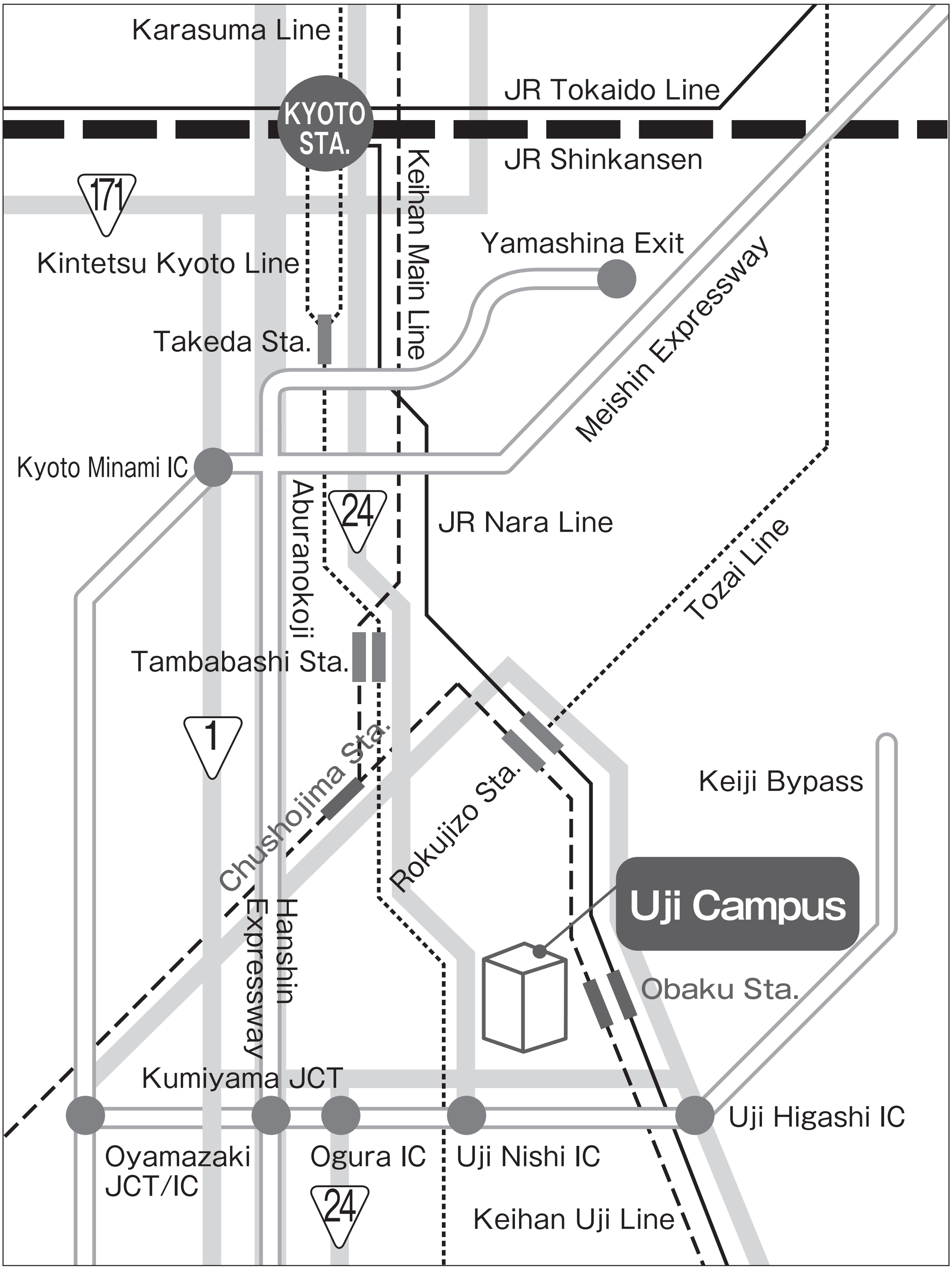
The main objective of the research in our Heliotron J group under this joint research program is to investigate experimentally/theoretically the transport and stability of fusion plasma in the advanced helical magnetic field and to improve the plasma performance through advanced helical-field control in Heliotron J. Picked up in FY2021 are the following seven key-topics; (1) transport study concerning field configuration control and relating plasma structure formation control, (2) control of plasma profile, plasma flows, plasma current for confinement improvement, (3) investigation of structure formation of plasma fluctuations in the core and peripheral region, (4) enhancement of operation region of high-density plasmas using novel fueling methods, (5) optimization of particle supply and heating scenario, (6) development of new technology in experiment and analysis.

Two results from this collaboration research in FY2021 are shortly reported below. The annual report for all the collaboration subjects in this program will be published by NIFS.

Magnetic configuration effect on energy confinement properties and profile structure formation: In the Heliotron J device, which has extensive and precise magnetic field controllability, the bumpiness component (toroidal mirror ratio) in the magnetic field spectrum is a characteristic control knob for neoclassical transport, MHD, and fast ion confinement to verify the effectiveness of the configuration optimization. We have recently expanded the magnetic field configuration range in the experiments and have focused on rotational transform control experiments. Controlling the rotational transform makes it possible to investigate the dependence of the confinement properties on the rotational transform and its physical mechanism that appears in the scaling laws. In addition, it is possible to control the rational surfaces, which determine the structure of the peripheral magnetic field by changing the rotational transform, thereby significantly changing the topology of the peripheral magnetic field. Experiments were performed by varying the central rotation transform from 0.46 to 0.63 while keeping the line-averaged density at about 1×10^{19} m^{-3}. The ECH injection conditions and magnetic field strength are adjusted to achieve central heating. The overall trend is that the confinement energy decreases with increasing rotational transform. To investigate the effect of rotational transform control on neoclassical transport, we compared the confinement time with the effective helical ripple, ε_{eff}. The effective helical ripple scan shows a gradually increasing trend with increasing rotational transform. However, the correlation with Wp is unclear. This suggests that rotational transform may affect turbulent transport as well as neoclassical transport. In the future, we plan to conduct neoclassical analysis and turbulence simulation analysis, including the effect of geodesic curvature.

Formation of electron internal transport barrier (e-ITB) in NBI only plasmas Role of preionization in NBI plasma start-up and stochastic acceleration phenomena: Producing plasmas using NBI only has never been successful in medium-sized helical devices. We have used non-resonant microwaves for pre-ionization and have successfully produced NBI plasmas. Pre-ionization generates a plasma of $n_e = 4\times10^{18}$ m^{-3}, and the carbon ion emission (OV) peak is observed at 3 ms after NBI injection. The dependence of the OV peak delay time on the density of the pre-ionized plasma is investigated. A numerical code for 0-dimensional NBI production has been developed. The simulation results agree with the experimental plasma evolution. The radiation barrier temperature of light impurities such as carbon and oxygen, and the threshold value for the density of pre-ionized plasma reproduces the measurement. The simulation results clearly show that the pre-ionizing plasma (1) produces enough NBI fast ions, which in turn (2) heats the background plasma and (3) ionizes the background gas to promote fast ion production, which contributes to the positive feedback. On the other hand, high-energy electrons exceeding 2 MeV are observed in the pre-ionized plasma from synchrotron radiation measurements. Since no resonance layer for microwaves of 2.45 GHz is located in the vacuum vessel, stochastic interaction between the microwave electric field and electrons (statistical acceleration) may be the mechanism of energetic electron generation. In Heliotron J, plasma production is usually performed by second harmonic ECH heating at 70 GHz, but in this case, the magnetic field strength must be fixed around 1.25T. The technique using pre-ionization enables NBI discharges at 0.6 T to 1.4 T, which can be combined with novel fueling methods such as pellet injection and high-intense gas puffing to perform operational scenarios for high-beta experiments.

7. HOW TO GET TO THE IAE



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

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

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