Title of Project : Research for quantum media conversion in diamond nano quantum system

Hideo Kosaka
(Yokohama National University, Faculty of Engineering, Professor)

Research Project Number : 16H06326 Researcher Number : 20361199
Research Area : Nano-structure physics
Keyword : Quantum information physics, Spintronics

【Purpose and Background of the Research】

Quantum communication network, which enables secure distribution of information including social security numbers, medical data, smart grid data, is necessary to be built towards big-data society based on internet of things (IoT).

In this research, we develop technologies for selective quantum state transfer from a photon to an integrated quantum memory, its long memory time, error correction, and quantum entanglement detection by geometric quantum manipulation of spin degenerate system. Quantum system in a nitrogen-vacancy center (NV center) is used to develop an integrated solid-state quantum memory with error resilience, which is necessary for realizing quantum information processing system.

【Research Methods】

The following targets are pursued with using an NV center in diamond, which shows superior advantage for quantum memories.

1. Quantum media conversion from a photon to a nitrogen nuclear spin with completely maintaining quantum state based on the quantum teleportation scheme.
2. Selective transfer of quantum state from a photon to an integrated quantum memory consisting of multiple carbon nuclei around an NV center.
3. Deterministic quantum entanglement detection by complete Bell state measurement between arbitrary nuclei in an integrated quantum memory.
4. Quantum error correction based on a logical qubit consisting of multiple nuclei.
5. Quantum wavelength conversion from a telecommunication wavelength to a diamond-absorption wavelength.

To achieve these targets, we develop our original scheme for geometric quantum manipulation of a degenerate logical qubit out of spin-1 electron system based on inherent interactions between a photon and an electron, or an electron and a nucleus.

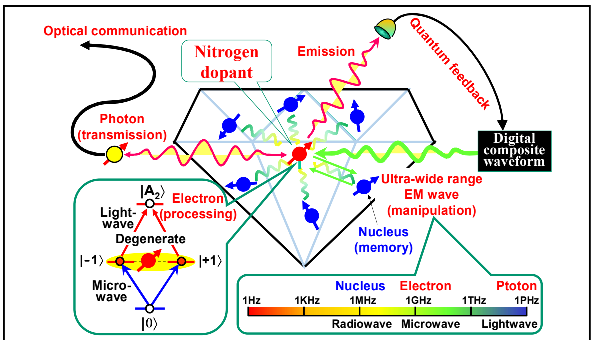

Fig. 1 Integrated quantum media conversion memory based on diamond NV center

【Expected Research Achievements and Scientific Significance】

The achievement of this project will be a breakthrough for building quantum communications to overcome the distance limit and for classical communications to overcome the capacity limit.

【Publications Relevant to the Project】

- Sen Yang, Hideo Kosaka, Jorg Wrachtrup, et.al., "High fidelity transfer and storage of photon states in a single nuclear spin", ***Nature Photonics***, nphoton.2016.103 (2016).
- Yuhei Sekiguchi, Hideo Kosaka, et.al., "Geometric spin echo under zero field", ***Nature Communications***, 7, 11668 (2016).
- Hideo Kosaka, et.al., "Entangled Absorption of a Single Photon with a Single Spin in Diamond", ***Phys. Rev. Lett.***, 114, 053603 (2015).

【Term of Project】 FY2016-2020

【Budget Allocation】 138,900 Thousand Yen

【Homepage Address and Other Contact Information】
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Title of Project : Assembly of nanostructure on insulating surfaces and investigation of gas reaction mechanism using atomic force microscopy

Yasuhiro Sugawara
(Osaka University, Graduate School of Engineering, Professor)

Research Project Number : 16H06327　Researcher Number : 40206404
Research Area : Scanning probe microscopy
Keyword : Atomic force microscopy, Nano-structure, Charge transfer, Gas reaction mechanism

【Purpose and Background of the Research】

The investigation of the physical and chemical properties of nanostructures on insulator surfaces is very important for those application to sensors, catalysis, and electronic devices. Nanostructures, composed of a few to several tens of atoms, exhibit strong quantum size effect. The electronic structure of the corresponding confined electrons differs completely from that of bulk materials. The presence of defects on insulator surfaces introduces unsaturated binding sites, which serve either as charge donors or acceptors. The electronic structure of nanostructures grown on insulator surfaces would be strongly influenced by charge transfers to or from the surface defects, dramatically changing the physical and chemical properties of the nanostructures. Therefore, in order to design and realize nanostructures with the desired novel functionality, e.g., a certain catalytic property, it is critical that we have a detailed understanding of the interaction between nanostructures and surface defects.

The objectives of this research are to clarify the charge transfer phenomena between defects and nanostructures on insulator surfaces and to clarify the relationship between the structure and the charge state of the nanostructures to the catalytic reaction mechanism on the atomic scale in reactive ambient environment.

【Research Methods】

(1) Elucidation of the defect structure and the charge state on insulator surface using atomic force microscopy and electrostatic force spectroscopy.

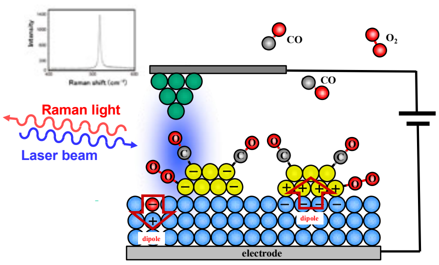

Figure 1 Experimental method

(2) Elucidation of the structure change in nanostructures and the charge state changes due to the reactive gas adsorption.
(3) Elucidation of the adsorption state of the adsorbed gas on the nanostructures using tip-enhanced Raman spectroscopy.
(4) Elucidation of the mechanism behind the catalytic reaction on nanostructures under reactive ambient environment conditions.

【Expected Research Achievements and Scientific Significance】

By investigating the physical and chemical properties of nanostructures on insulator surfaces, we can acquire knowledge on the electronic state and novel function in nanostructures. Such knowledge will provide a huge contribution to progress in “physics and chemistry of nanostructure on insulator surface in reactive ambient environment”. Furthermore, such knowledge will provide a huge contribution towards the realization of next-generation catalytic nanomaterials, fuel cells, and high sensitive gas sensors.

【Publications Relevant to the Project】

J. Bamidele, S. H. Lee, Y. Kinoshita, R. Turanský, Y. Naitoh, Y. J. Li, Y. Sugawara, I. Štich, and L. Kantorovich, “Vertical atomic manipulation with dynamic atomic-force microscopy without tip change via a multi-step mechanism”, Nature Communications, 5, 4476, 2014.
Y. J. Li, J. Brndiar, Y. Naitoh, Y. Sugawara, and Ivan Štich, “Atomic force microscopy identification of Al-sites on ultrathin aluminum oxide film on NiAl(110)”, Nanotechnology, 26, 505705, 2015.

【Term of Project】 FY2016-2020

【Budget Allocation】 139,100 Thousand Yen

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Title of Project : Microfluidic approach to single cell transcriptome analysis and its applications

Teruo Fujii
(The University of Tokyo, Institute of Industrial Science, Professor)

Research Project Number : 16H06328 Researcher Number : 30251474
Research Area : Interdisciplinary Science and Engineering
Keyword : Genomic engineering, Single cell analysis, Transciptome analysis

【Purpose and Background of the Research】

A population of cells either forming a tissue or being cultured has been analyzed so far as a group of homogeneous elements. It is, however, being revealed that those cells in a population show heterogeneous behaviors, as new analytical methods are rapidly becoming able to achieve measurements at the single-cell level. Recently, several attempts were made to understand cell-to-cell variation in gene expression levels, that is, single-cell transcriptome analysis based on next-generation sequencing (NGS) technologies. However, the number of cells analyzed at one time is highly limited because isolation and handling of large numbers of single cells is difficult with conventional methods. Here, we propose a novel microfluidic approach to drastically improve the throughput for single-cell transcriptome analysis, up to 10,000 cells per run, to comprehensively understand the cellular heterogeneity on the gene expression level.

【Research Methods】

We propose a novel method combining the electroactive microwell array (EMA), which has been developed by our group for parallelized analysis of large numbers of single-cells, with an advanced picoCAGE protocol that allows identify 5' ends of transcripts based on cap-analysis gene expression. To identify each cell, a different pair of index identifiers for the picoCAGE reaction will be spotted on an inner surface of each microwell by using microfluidic approaches.

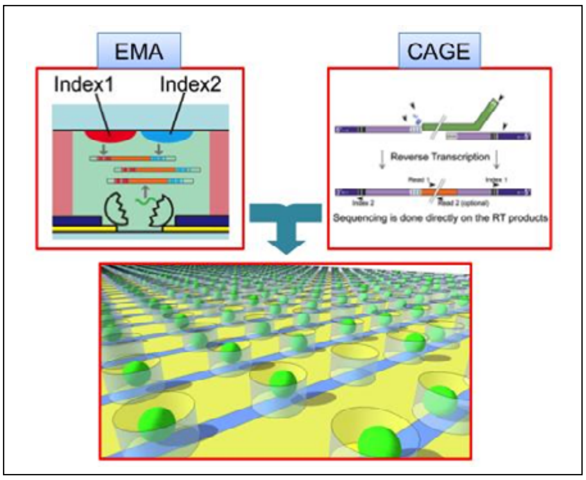

Figure 1 Single-cell transcriptome analysis

【Expected Research Achievements and Scientific Significance】

Large-scale single-cell analysis should be of interest for many biological studies and broadening the scope of biological understanding of cellular heterogeneity at the gene expression level. In this project, the present method is applied to the analysis of cervical cancer diagnosis and therapy. But it can be further extended to the analyses of biological and medical samples, such as rare cells, viable but not culturable microbes in various environments, drug resistant bacteria in early phase infection, etc., contributing to better understanding of environmental biodiversity as well as to the prevention of hospital-acquired infection.

【Publications Relevant to the Project】

Kim, S. H. and Fujii, T., "Efficient analysis of a small number of cancer cells at the single-cell level using electroactive double-well array," Lab on a Chip 16, pp. 2440 - 2449 (2016), selected as the outside front cover of the issue.
Plessy, C. et al., "Linking promoters to functional transcripts in small samples with nanoCAGE and CAGEscan", Nature Methods 7, pp. 528-534 (2010).

【Term of Project】 FY2016-2020

【Budget Allocation】 136,600 Thousand Yen

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Title of Project : Establishment of Cell Fiber Engineering For Next Generation of 3D Tissue Culture

Shoji Takeuchi
(The University of Tokyo, Institution of Industrial Science, Professor)

Research Project Number : 16H06329 Researcher Number : 90343110
Research Area : Science and Engineering (Interdisciplinary Science and Engineering)
Keyword : Nano micro biosystem

【Purpose and Background of the Research】

3D tissue construction *in vitro* is important not only for medical use but for many other applications including environmental monitoring, bio actuators and cultured meat. However, long-term culture of 3D tissues has been difficult so far due to the lack of nutrition in the central area of the tissue, which triggers cell death.

In this project, we develop a "cell fiber technology" that enables us to construct 3D tissue and to culture it for a long time, by understanding the mechanism to form cell fibers and analyzing details of constructed tissue properties. Also we verify the availability of this technology in various application fields, resulting in the establishment of a research platform of the cell fiber engineering.

【Research Methods】

We aim to achieve the following three points;

1. Understand the mechanism of production, control and handling of cell fibers to make it commodity technology.

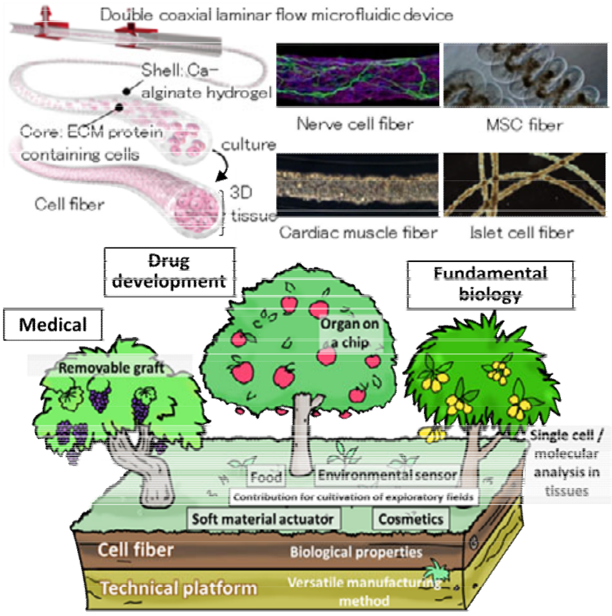

Fig.1 (Upper-left) Schematic illustration of cell fiber production. (Upper-right) cell fibers with various kinds of cells. (Lower) cell fiber engineering achieved through this project and expected effects.

2. Make "cell fiber database" that provides optimized culture conditions for various kind of cells as practical technical platform.
3. Show the possibility of cell fiber in basic biology (single cell/molecular analysis), pharmacology (drug testing, disease model) and medical fields (transplantation of tissue.).

We will make a team of researchers specializing in engineering, biology and medicine. Moreover, we will cooperate with the specialists of application fields to drive the project forward.

【Expected Research Achievements and Scientific Significance】

Cell fiber technology enables us to introduce appropriate ECM in the core of the fibers with cells, cells can be cultured in environment similar to *in vivo*. Additionally, cell fibers can be combined with larger scale tissue engineering technology such as bio-printing. We believe the cell fiber technology will be the world standard technical platform for next generation once we commodify this technique.

Through this project, we hope that cell fiber technology will change the conventional method of 3D tissue cultivation dramatically, providing various breakthroughs in basic biology, drug testing and medical treatment.

【Publications Relevant to the Project】

・H. Onoe, T. Okitsu, A. Itou, M. Kato-Negishi, R. Gojo, D. Kiriya, K. Sato, S. Miua, S. Iwanaga, K. Kuribayashi-Shigetomi, Y. Matsunaga, Y. Shimoyama, S. Takeuchi: Metre-long Cellular Microfibres Exhibit Tissue Morphologies and Functions, **Nature Materials**, vol. 12, pp. 584–590, 2013
・H. Onoe and S. Takeuchi: Cell-laden microfibers for bottom-up tissue engineering, **Drug Discovery Today**, vol. 20(2), pp. 236–246, 2015

【Term of Project】 FY2016-2020

【Budget Allocation】 144,900 Thousand Yen

【Homepage Address and Other Contact Information】

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Title of Project : Semiconductor Spin-currentronics

Masashi Shiraishi
(Kyoto University, Graduate School of Engineering, Professor)

Research Project Number : 16H06330 Researcher Number : 30397682
Research Area : Engineering Science
Keyword : Spin current, Semiconductor, Spintronics

【Purpose and Background of the Research】

Spin current (pure spin current without a charge flow and spin polarized current) in solids attracts tremendous attention in basic and applied physics, and much effort has been paid for its research. One main reason of the attractiveness of spin current is that people can fabricate spin devices of which size is below spin diffusion length thanks to a development of nanotechnologies (whereas the charge current is a conservative current, the spin current is not, and thus spin dissipates with a length scale of spin diffusion length). In the earlier stage of spintronics, a study of spin current is focusing only on nonmagnetic metals. However, recently, spin current in semiconductors, such as Si, Ge, GaAs and Graphene, can be generated and propagated at room temperature, which allows advanced studies on it.

Researchers have been facing with difficulty in injecting and propagating spins in semiconductors at room temperature, and in addition, unfortunate confusion about a reliability of a measuring method of spin current, a 3-terminal method, has been hindering a progress of spin-currentronics in semiconductors. Now, the heated discussion is settled, but studies on spin-currentronics using a various semiconductor materials with artificial nano-structures and using novel semiconductors such as transition metal dichalcogenides (TMDs) have not been implemented. Furthermore, an application-oriented study based on semiconductor spin-currentronics is still in the early development stage.

【Research Methods】

In this research project, we focus on (1) inorganic semiconductors (group-IV[Si, Ge] and compound [GaAs, SiC]), (2) novel atomically flat semiconductors, such as transition metal dichalcogenides (WSe2 and so on) and graphene, and (3) topological insulators (BiSbTeSe, TlBiSe and so on) as potential "semicondcutors" for spintronics applications. In terms of devices structures, quantum-wells, 2-dimensional electron gases in compound and oxide semiconductors, in addition to bulk semiconductors. The research strategies are as follows:

I. Understanding of spin current properties in semiconductors by using a novel high-frequency method and conventional electrical, dynamical and thermal methods, and of underlying physics of semiconductor spin-currentronics.
II. Clarification of correlation between spin relaxation and carrier densities in semiconductors, especially in TMDs and topological insulators.
III. Creation of novel spin devices by using conventional inorganic semiconductors, TMDs and topological insulators.

【Expected Research Achievements and Scientific Significance】

Because of the unwanted confusion described above, progress of semiconductor spintronics was not so dramatic comparing with that of metallic spintronics, where GMR heads and MRAMs were in practical use. In the course of this project, we can establish a steadfast basis of semiconductor spintronics and obtain a direction for practical application of semiconductor spin devices.

【Publications Relevant to the Project】

1) S. Dushenko, H. Ago, K. Kawahara, T. Tsuda, S. Kuwabata, T. Takenobu, T. Shinjo, Y. Ando and M. Shiraishi, "Gate-tunable spin-charge conversion and a role of spin-orbit interaction in graphene", Phys. Rev. Lett. 116, 166102 (2016).
2) S. Dushenko, M. Koike, Y. Ando, M. Myronov and M. Shiraishi, "Experimental demonstration of room-temperature spin transport in n-type Germanium epilayers", Phys. Rev. Lett. 104, 196602 (2015).
3) Yu. Ando, T. Hamasaki, T. Kurokawa, F. Yang, M. Novak, S. Sasaki, K. Segawa, Yo. Ando and M. Shiraishi, "Electrical Detection of the Spin Polarization Due to Charge Flow in the Surface State of the Topological Insulator Bi1.5Sb0.5Te1.7Se1.3", Nano Lett. 14, 6226 (2014).

【Term of Project】 FY2016-FY2020

【Budget Allocation】 134,400 Thousand Yen

【Homepage Address and Other Contact Information】

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Title of Project : Development and application of valley-spin photonics in atomically thin layered materials

Kazunari Matsuda
(Kyoto University, Institute of Advanced Energy, Professor)

Research Project Number : 16H06331 Researcher Number : 40311435
Research Area : Applied physics
Keyword : Optical properties, Nanoscale control physics

【Purpose and Background of the Research】

Since the realization of atomically thin layered materials, the studies of these materials cause the paradigm-shift in material and optical sciences. There is a coupling between valley in the momentum space and spin degree of freedom in the atomically thin materials, called as valley-spin. This valley spin would open the frontier of research fields, which is different from charge and spin in the conventional electronics and photonics.

In this project, we will study the novel quantum optical phenomena related to the valley-spin and its coherent control by state of art optical spectroscopy in the transition metal dichalcogenides, and metal-monochalcogenides (Fig. 1). We would like to develop the new research field of valley-spin photonics for optical and material science research fields.

【Research Methods】

We will develop the element technology for generation, detection, and control of valley-spin in the atomically thin layered materials toward the valley-spin photonics. In this approach, we will study as follows, 1) fabrication of high quality atomically thin layered materials and its artificial hetero-structure, 2) valley-spin generation, detection, and coherent control by advanced optical spectroscopy, 3) realization of valley-spin optical devices.

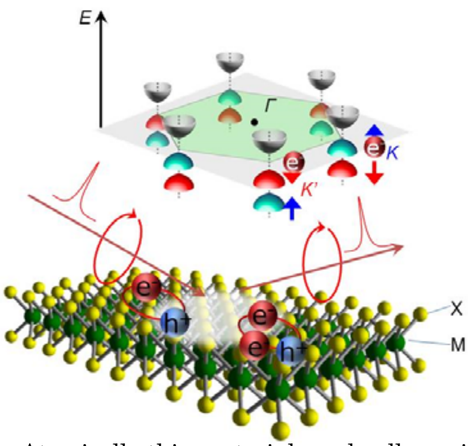

Fig.1 Atomically thin materials and valley-spin photonics

【Expected Research Achievements and Scientific Significance】

In the atomically thin layered materials, the novel quantum optical phenomena will be emerged, because of the huge enhancement of quantum confinement of electrons in the very thin (two-dimensional) layer. We can also apply the valley-spin degree of freedom in these materials. These are based on the new strategy in the material and optical science. Moreover, the low-energy consumption quantum optical devices will be realized by the valley-spin current. Thus, this project is important not only in the viewpoint of fundamental science but also in the future green technology.

【Publications Relevant to the Project】

・D. Kozawa, R. Kumar, A. Carvalho, K. K. Amara, W. Zhao, S. Wang, M. Toh, R. M. Ribeiro, A. H. Castro Neto, K. Matsuda and G. Eda, Photocarrier relaxation pathway in two-dimensional semiconducting transition metal dichalcogenides, Nat. Commun. **5**, 4543 (2014).
・Y. Miyauchi, M. Iwamura, S. Mouri, T. Kawazoe, M. Ohtsu, and K. Matsuda, Brightening of excitons in carbon nanotubes on dimensionality modification, Nat. Photonics **6**, 715 (2013).
・S. Mouri, Y. Miyauchi, and K. Matsuda, Tunable photoluminescence of monolayer MoS_2 via chemical doping, Nano Lett. **13**, 5944 (2013).

【Term of Project】 FY2016-2020

【Budget Allocation】 142,800 Thousand Yen

【Homepage Address and Other Contact Information】

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Title of Project : Microscopic understanding of interface spin-orbit coupling and development of perpendicular magnetic anisotropy devices

Seiji Mitani
(National Institute for Materials Science, Research Center for Magnetic and Spintronic Materials, Group Leader)

Research Project Number : 16H06332 Researcher Number : 20250813
Research Area : Applied Physics
Keyword : Spintronics, Magnetism, Surface & Interface, Ultrathin film, Spin-Orbit Coupling

【Purpose and Background of the Research】

Spin-orbit coupling (SOC) at the interfaces of magnetic heterostructures is the physical origin of interface perpendicular magnetic anisotropy that is indispensable for next generation magnetic memory technologies. It is also important for the new research fields such as electric field control of magnetism and the so-called spin-orbitronics. However, there remains a serious problem that microscopic understanding is lacking in interface SOC. As a result, there are a lot of difficulties in designing materials and predicting properties in these research fields.
In this study, we are aiming at understanding the microscopic mechanisms of interface SOC, via systematic studies in which sample preparation of atomically controlled magnetic heterostructures, spectroscopic analyses based on photoemission and XMCD, and first-principles calculations (for site-resolved spin and orbital states etc.) are combined. Our interests are also on effect of Rashba SOI in the magnetic heterostructures and novel methods to elucidate orbital states. One of the final targets is to achieve giant interface perpendicular magnetic anisotropy and its new functionalities.

【Research Methods】

An important point of this study is to make "model" heterostructures that enable us to directly compare the experimental results with the first-principles calculations. For this purpose, we employ the epitaxial growth and monoatomic layer control techniques that have been accumulated in our previous research activities.
Photoemission spectroscopy and XMCD meas-urements are mainly performed as a microscopic analysis, and we also attempt to develop a new method to determine orbital states in materials.
In first-principles calculations, atomic site-dependent spin and orbital states are analyzed for obtaining microscopic understanding of interface SOI. Further, material design and functionality prediction will also be performed.

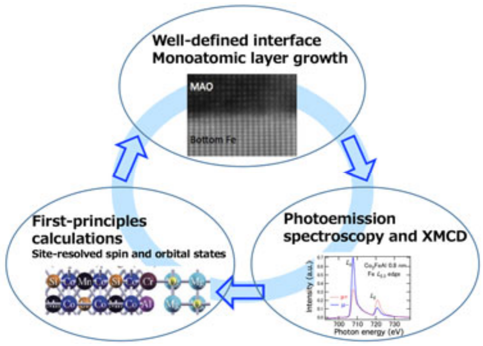

Fig. 1. Method of the study.

【Expected Research Achievements and Scientific Significance】

Understanding of the microscopic mechanisms of interface SOC is expected to obtain sufficiently. It contributes to the progress of related new and important fields. We also expect to attain giant magnetic anisotropy and its sensor/memory devices.

【Publications Relevant to the Project】

- J. W. Koo et al., "Large perpendicular magnetic anisotropy at Fe/MgO interfaces", Appl. Phys. Lett. **103**, 192401 (2013):
- J. Okabayashi et al., "Perpendicular magnetic anisotropy at the interface between ultrathin Fe film and MgO studied by angular-dependent X-ray magnetic circular dichroism", Appl. Phys. Lett. **105**, 122408 (2014):
- Y. Miura et al., "A first-principles study on magnetocrystalline anisotropy at interfaces of Fe with non-magnetic metals", J. Appl. Phys. **113**, 233908 (2013).

【Term of Project】 FY2016-2020

【Budget Allocation】 145,000 Thousand Yen

【Homepage Address and Other Contact Information】

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Title of Project : Advanced Single-Atom Spectroscopy

Kazutomo Suenaga
(National Institute of Advanced Industrial Science and Technology, Nano-Materials Research Institute, Prime Senior Researcher)

Research Project Number : 16H06333 Researcher Number : 00357253
Research Area : Interdisciplinary Science and Engineering
Keyword : Electron microscopy, Individual atoms, single molecules, Low-dimensional materials

【Purpose and Background of the Research】

It has remained a challenge for scientists to see and identify individual atoms since Dalton first proposed distinct atoms in his atomic theory in 1800. Recent development of electron microscopes has enabled us to obtain spectrum from individual atoms by providing an atomically small electron probe and a high-performance spectrometer. In this project, we aim to develop the single atom spectroscopy technique for higher performance with higher sensitivity, higher precision and higher efficiency so that one can monitor changes in spin state or oxide state of single atoms. The project will contribute to the fundamental researches in the wide field such as physics, biology, chemistry and materials.

【Research Methods】

The following three research theme are proposed, (i) High-speed chemical map to track individual atoms, (ii) High-precision spectroscopy for single atom electron states, and (iii) in situ spectroscopy to detect fine structure changes in near-edge fine structure for single atom spectrum. To realize them we improve the environments of TEM, chromatic aberration of lenses, stability and brightness of electron source and performance of spectrometer.

【Expected Research Achievements and Scientific Significance】

(i) Tracking individual atoms in chemical map leads to understand the dynamics of lattice defect that is a key for device properties in low-dimensional materials. (ii) High-precision single-atom spectroscopy allows us to detect single atoms at higher reliability and the wider elements detectable in the periodic table. It is important to get spin/oxide states of wider range of elements, especially for transition atoms or noble atoms. (iii) *in situ* ELNES measurements allow to monitor chemical reaction or phase transformation at atomic level. Especially, a molecule in which Fe atom locates its center is known to react oxygen and the spin state of Fe atoms is claimed to be a key to catch or release the oxygen molecules. One will be able to monitor such a biological activity at single atom basis.

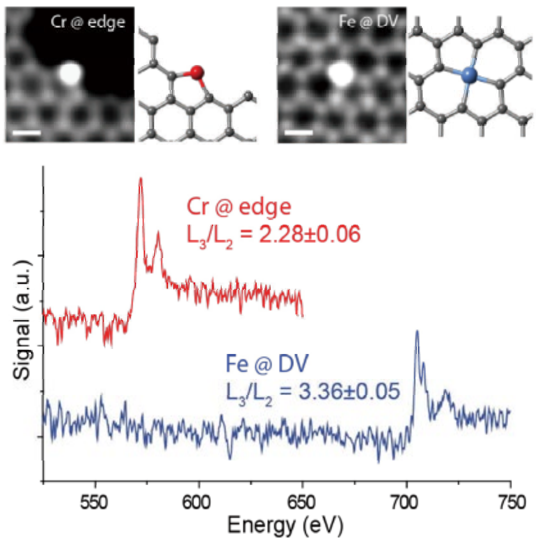

Figure. Single atom spin state spectroscopy. The branching ratio of *L*-absorption edge does correspond to the charge transfer between d-subbands of specific 3d transition metals. Here in the figure above, a Cr atom at graphene edge and a Fe atom at divacancy (DV) in graphene both show a high-spin state judging from the measured L_{23} branching ration.

【Publications Relevant to the Project】

・K. Suenaga et al., "Element-selective single atom imaging" *Science* 290 (2000) pp. 2280-2282
・K. Suenaga and M. Koshino, "Atom-by-atom spectroscopy at graphene edge", *Nature*, **468** (2010) pp.1088-1090

【Term of Project】 FY2016-2020

【Budget Allocation】 130,900 Thousand Yen

【Homepage Address and Other Contact Information】

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Title of Project : High-performance nanolaser biosensor with an ion-sensitivity

Toshihiko Baba
(Yokohama National University, Graduate School of Engineering, Professor)

Research Project Number : 16H06334 Researcher Number : 50202271
Research Area : Optical Engineering/ Photon Science
Keyword : Photonic Crystal

【Purpose and Background of the Research】

GaInAsP semiconductor photonic crystal nanolasers are simply fabricated and easily operated at near infrared by room-temperature photopumping. By functionalizing the device surface with an antibody, and so on, they act as biosensors which detect biomolecules in an analyte solution.

In a previous project (Grant-in-Aid for Scientific Research (S), 2012–2016), we detected various bio-samples such as standard proteins, biomarker proteins for cancers and Alzheimer disease, environmental toxin, and living cells. In particular, we succeeded in sensitive detection of proteins from ≤ fM order ultralow concentrations and their selective detection in contaminated samples with a selectivity of $>10^9$. The high performance cannot be explained by a principle as a refractive index sensor; it was rather suggested to relate with ions in the solution and surface charge on the device.

Based on this discovery, we set the following two purposes in this study: 1) investigation and utilization of iontronic effects in the nanolaser (Fig. 1), which have never been studied for photonic sensors, and 2) development of medical diagnostic system with improved and stabilized performance.

【Research Methods】

Regarding the iontronic effects, we theoretically analyze the electrostatic interaction, nano-fluidic effect, and electro-optic effects in the semiconductor. We compare them with experimental observations obtained by using multi-probe microscope and high-sensitivity infrared camera. We also observe the behaviors of molecular-level adsorption and optimize the functionalization for each target protein.

Regarding the medical diagnostic system, we employ a unified functionalization system using atomic layer deposition. We test the optimized device particularly for detecting proteins related with schizophrenia, which are taken from blood of patients. Integrating nanolasers and simple microfluidic device, we develop a quantitative measurement system with a disposable sensor chip.

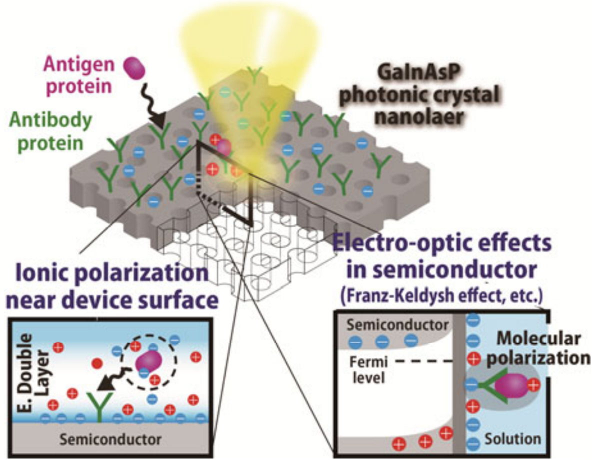


Figure 1 Schematic of photonic crystal nanolaser biosensor and iontronic effects

【Expected Research Achievements and Scientific Significance】

Conventional photonic sensors including surface plasmon and microcavities have been thought to sense the environmental index, although it has not fully been confirmed. In this study, we discuss a novel principle, which we expect to provide more advanced performance and functions.

【Publications Relevant to the Project】

K. Watanabe, Y. Kishi, S. Hachuda, T. Watanabe, M. Sakemoto, Y. Nishijima and T. Baba, Appl. Phys. Lett. **106**, 021106 (2015).
T. Baba, MRS Commun. **5**, 555 (2015).
M. Sakemoto, Y. Kishi, K. Watanabe, H. Abe, S. Ota, Y. Takemura and T. Baba, Opt. Exp. **24**, 11232 (2016).
S. Hachuda, T. Watanabe, D. Takahashi and T. Baba, Opt. Exp. **21**, 12815 (2016).

【Term of Project】 FY2016-2020

【Budget Allocation】 130,400 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.baba-lab.ynu.ac.jp/babalabe.htm

Title of Project : New development of algebraic geometry viewed from theoretical physics

Atsushi Moriwaki
(Kyoto University, Graduate School of Science, Professor)

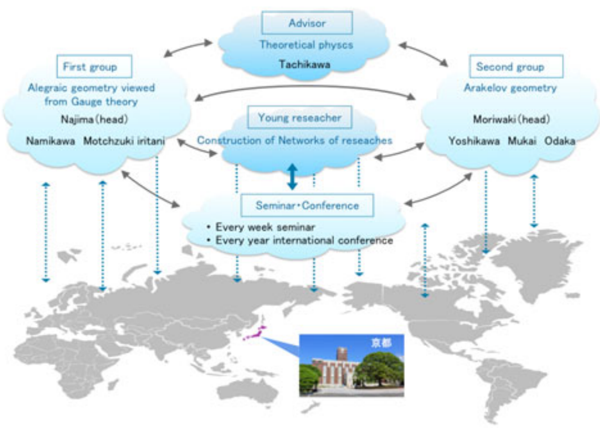
Research Project Number : 16H06335 Researcher Number : 70191062
Research Area : Mathematical and Physical Science, Mathematics, Algebra
Keyword : Algebraic Geometry

【Purpose and Background of the Research】

As pointed out by Prof. Dodd, algebraic geometry is an experimental field of mathematical theory. Nowadays it is also an experimental field of theoretical science. Especially interactions with supersymmetric gauge theory starting from 80's and the mirror symmetry of Calabi-Yau manifolds inspired by superstring theory during 90's were the most impressive achievements. Beside them, we have a lot of developments of algebraic geometry related to mathematical physics such as the theory of symplectic manifolds, Seiberg-Witten invariant, Gromov-Witten invariant, Donaldson-Thomas invariant and so on.

As above, perspectives from mathematical physics are recently necessary methods to develop algebraic geometry. Moreover, new research subjects of algebraic geometry arise from the borders around mathematical physics.

Fortunately, in Kyoto University, we have a lot of algebraic geometers deeply related to mathematical physics. We coordinate the colleagues as a research team and try to find surprising phenomena and new theories connected with mathematical physics, which lead to recent developments of algebraic geometry and contribute to construct an international center of this area at Kyoto.



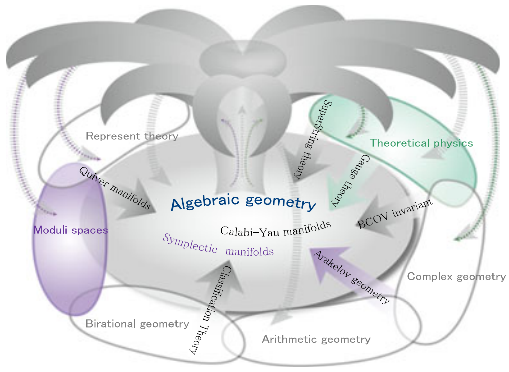
【Research Methods】

We assign two teams to our Research group. The first team consists of Nakajima, Namikawa, Mochizuki, Iritani, who study algebraic geometry viewed from gauge theory. The second team consists of Moriwaki, Mukai, Yoshikawa, Odaka, who study arithmetic geometry around mathematical physics. Tachikawa will give advises to two teams as a theoretical physicist.

We employ a young and excellent researcher, who will work in order to join achievements of two teams and construct international networks of our research area.

【Expected Research Achievements and Scientific Significance】

We hope that we will obtain significant results of algebraic geometry relevant to mathematical physics. These fruits will give a big influence on not only algebraic geometry but also theoretical physics.



【Publications Relevant to the Project】

・H. Nakajima, Instantons on ALE spaces, quiver varieties, and Kac-Moody algebras, Duke Math. 76 (1994) 365--416.
・A. Moriwaki, ``Arakelov geometry", Translations of Mathematical Monographs, vol 244, (2014), American Mathematical Society.

【Term of Project】 FY2016-2020

【Budget Allocation】 61,700 Thousand Yen

【Homepage Address and Other Contact Information】

https://www.math.kyoto-u.ac.jp/ja/people/profile/moriwaki
moriwaki@math.kyoto-u.ac.jp

Title of Project : Multiple Zeta Values and Functions

Masanobu Kaneko
(Kyushu University, Faculty of Mathematics, Professor)

Research Project Number : 16H06336 Researcher Number : 70202017
Research Area : Algebra
Keyword : Number Theory, Arithmetic Geometry, Low-dimensional Topology

【Purpose and Background of the Research】

Multiple zeta values and multiple zeta functions are defined by the following nested infinite series.

$$\zeta(k_1,\ldots,k_r) := \sum_{0<m_1<\cdots<m_r} \frac{1}{m_1^{k_1}\cdots m_r^{k_r}}$$

When the arguments are all positive integers, this is called the multiple zeta value, whereas as a function of complex variables, this is called the multiple zeta function. When the number of variables is one, this is nothing but the celebrated Riemann zeta function. We call here in general "multiple zetas" for those values and functions including more generalized versions. It was Euler who initiated the study of these objects, but it is since about two decades that active research has been explored in connection to various areas in mathematics as well as mathematical physics.

During the period of our research project, we try to reveal connections between various results and conjectures on multiple zeta values that have been made since two decades, and try to find a unified point of view, which may probably be still hidden behind. Also, we develop analytic and p-adic theory of multiple zeta functions, and together with the theory of multiple zeta values, we will be trying to contribute new development in the area of multiple zetas.

【Research Methods】

Main topics of research will be:

--- Relations and algebraic structures of multiple zeta values,

--- Analytic and p-adic theories of multiple zeta functions,

--- Finite multiple zeta values, p-adic multiple zeta values, and motivic multiple zeta values,

--- Multiple polylogarithms,

--- Multiple zeta values and quantum invariants from the viewpoint of arithmetic topology,

--- Poly-Bernoulli numbers,

--- Understandings from the Galois side and the combinatorics side.

Members of the project will conduct independent as well as joint works on some of these topics, communicating from time to time with each other on their progress.

We will occasionally have seminars, workshops, and conferences in order to meet with each other and discuss our research progress.

【Expected Research Achievements and Scientific Significance】

Although the progress in the area since these two decades is enormous, there still remain many unsolved problems and conjectures in the field of multiple zetas like the Broadhurst-Kreimer conjecture. Certainly we will have a better understanding toward such conjectures and of mutual connections among those coming from different backgrounds.

Recent works on finite multiple zeta values, desingularized multiple zeta functions, multiple zeta functions associated to root systems, are promising examples of fruitful establishments. Applications to other branches, such as an application of poly-Bernoulli numbers to combinatorics, will also be expected.

【Publications Relevant to the Project】

- M. Kaneko, K. Ihara and D. Zagier, Derivation and double shuffle relations for multiple zeta values, Compositio Math. vol. 142-02, pp 307--338, (2006).
- M. Kaneko, K. Tasaka, Double zeta values, double Eisenstein series, and modular forms of level 2, Math. Ann. vol. 367, pp 1091-1118, (2013).

【Term of Project】 FY2016-2020

【Budget Allocation】 75,400 Thousand Yen

【Homepage Address and Other Contact Information】

http://www2.math.kyushu-u.ac.jp/~mkaneko/kibans/en/index.html

Title of Project : Fusion of Birational Geometry and Theory of Periods; A New Era for Studies of Mirror Symmetry

Atsushi Takahashi
(Osaka University, Graduate School of Science, Professor)

Research Project Number : 16H06337 Researcher Number : 50314290
Research Area : Mathematics, Geometry
Keyword : Complex Geometry, Birational Geometry, Mirror Symmetry

【Purpose and Background of the Research】

A geometric object has quantities reflecting its characteristics. For a rectangle, (height) × (width) and (height) ÷ (width) represent its size and shape. For another rectangle whose width is the inverse of the original one, its size and shape become the original shape and size. One has a pair of rectangles replacing the role of the size and shape. Mirror symmetry is, such as in this example, a symmetry exchanging two kinds of geometric features.

Mirror symmetry is an equivalence between two topological string theories called A- and B-models, associated to symplectic geometry and algebraic geometry, which yields qualitative and quantitative conjectures, relates wide range of mathematics and deepens classical one along with new findings. It is important to elucidate the mathematical truth behind, with ``physical ideas, objects and methods".

There are two particularly important issues. One is to prove the homological mirror conjecture, an equivalence between two categories associated to A- and B-models. The other is a derivation from the homological mirror conjecture of the classical one, an equivalence between Gromov-Witten theory and the deformation theory. It is to develop the theory of B-periods for categories, including primitive forms and flat (Frobenius) structures. Towards these issues, many important results have been obtained.

On the other hand, for a further understanding of birational geometry, especially, the minimal model theory, studies by categorical and mixed-Hodge theoretical methods have been extensively done. Quite recently, there appeared a new approach to study derived categories, the categorical dynamics, which also shows the importance of such methods.

By fusion of birational geometry and theory of periods, we evolve both of them drastically, deepen further understanding of mirror symmetry and contribute to traditional important problems.

【Research Methods】

Settlement of various problems in the following:

1. Fundamental studies of nc-Hodge structures and the categorical dynamics. Basic research toward the theory of quantum primitive forms.
2. Studies of (nc-) birational geometry, especially the minimal model theory, by the categorical and the (nc-) Hodge-theoretical methods.
3. Further understanding of mirror symmetry and period mappings relating GW-invariants, primitive forms and Weyl group invariants.

The plan will be carried out in the following way:

① Individual and joint research by our research system, consisting of research team members, cooperation researchers and collaborators.
② The activation and the further development by the employment of post-doctoral fellows.
③ Research origination and exchanges by our seminars, workshops and annual conferences.

【Expected Research Achievements and Scientific Significance】

Not only large contribution in the state-of-the-art studies of mirror symmetry, our research will lead to a lot of new knowledge in traditional problems with a history of more than 100 years. Provision of invariants and methods to birational geometry and elucidation of the interactions among singularities, orbifolds and root systems, are expected.

【Publications Relevant to the Project】

・ Wolfgang Ebeling, Sabir M. Gusein-Zade, Atsushi Takahashi, Orbifold E-function of Dual Invertible Polynomials, Journal of Geometry and Physics 106 (2016), 184 – 191.
・ Yuuki Shiraishi, Atsushi Takahashi, On the Frobenius Manifolds for Cusp Singularities, Advances in Mathematics 273 (2015), 485 – 522.

【Term of Project】 FY2016-2020

【Budget Allocation】 79,900 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.math.sci.osaka-u.ac.jp/~takahashi/project.htm
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Title of Project : Stochastic Analysis on Infinite Particle Systems

Hirofumi Osada
(Kyushu University, Graduate School of Mathematics, Professor)

Research Project Number : 16H06338 Researcher Number : 20177207
Research Area : Probability Theory
Keyword : Infinite Particle Systems, Stochastic Analysis, Random Matrices, Solvable Models, Stochastic Geometry

【Purpose and Background of the Research】

Infinite particle systems are objects typically appearing in statistic physics, and ensembles of infinite-many particles consisting of finite-number of species. Below we suppose they consist of a single species. We regard infinite particle systems as an element of configuration spaces and denote their equilibrium states as point processes. Their random time evolutions are described by infinite-dim stochastic differential equations with symmetry.

The purpose of the present research is to establish a stochastic analysis of infinite particle systems based on the new theory of infinite dimensional stochastic differential equations with symmetry.

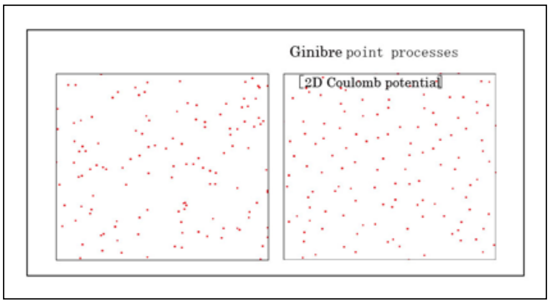
This stochastic analysis can be applied to essentially all Gibbs measures, point processes of eigen values of random matrices, and zero points of random analytic functions, and so on. In particular, stochastic systems with very long range and extremely strong interaction potentials.

We investigate novel and special phenomena arising from long range and strong interactions. In particular, we study phase transition on inverse temperature β and their critical phenomena.

At the same time, we study the algebraic structure of infinite particle systems as solvable models for $\beta=2$ in one space dimension.

【Research Methods】

Our team is consisting of one representative, and 6 cooperators, post doctors, students, and others. We will study: 1) New theory of stochastic analysis of infinite particle systems, 2) Universality of stochastic dynamics, 3) Dynamical rigidity 4) Lattice Gasses, 5) Stochastic partial differential equations, 6) Random media.



Poisson/Ginibre

【Expected Research Achievements and Scientific Significance】

We post the typical examples of two dimensional infinite particle systems such as Poisson and Ginibre point processes. The former has no interactions, while the latter has a very long range and extremely strong interaction potentials. In fact, Ginibre is the one of the main objects of our research.

We expect such strong interactions yield novel, unexpected, and interesting phenomena. Existing methods confront difficulty to treat such strong interacting systems, our new theory overcomes this difficulty.

【Publications Relevant to the Project】

- Infinite-dimensional stochastic differential equations, related to random matrices, Hirofumi Osada, Probability Theory Related Fields (2012) 153:471–509
- Interacting Brownian motions in infinite dimensions with logarithmic interaction potentials, Hirofumi Osada, The Annals of Probability 2013, Vol. 41, No. 1, 1–49
- Interacting Brownian motions in infinite dimensions with logarithmic interaction potentials II: Airy random point field, Hirofumi Osada, Stochastic Processes and their Applications 123 (2013) 813–838

【Term of Project】 FY2016-2020

【Budget Allocation】 90,100 Thousand Yen

【Homepage Address and Other Contact Information】

http://www2.math.kyushu-u.ac.jp/~osada/public-2_html/index.html

【Grant-in-Aid for Scientific Research (S)】

Science and Engineering (Mathematical and Physical Sciences)

Title of Project : New development of mathematical theory of turbulence by collaboration of the nonlinear analysis and computational fluid dynamics

Hideo Kozono
(Waseda University, Faculty of Science and Engineering, Professor)

Research Project Number : 16H06339 Researcher Number : 00195728

Research Area : Partial Differential Equations, Nonlinear Analysis

Keyword : Navier-Stokes Equations, Harmonic Analysis, Functional Analysis, Global Well-posedness, Asymptotic Analysis

【Purpose and Background of the Research】

The Navier-Stokes equations have been investigated widely in both theoretical and experimental fields. The mathematical study on the Navier-Stokes equations was founded by Leray.
The principal investigator Kozono and Kagei obtained several remarkable results in area of pure mathematical analysis.It turns out that the numerical simulation recently gives corresponding results which guarantee from viewpoint of fluid dynamics. In comparison with the numerical simulation, the advantage of the technique of harmonic analysis makes it possible to handle the asymptotic behavior of physical quantities as the parameter goes to infinity.
Such a mathematical method to deal with the exact quantity as the limit of those in finite regions gives us an essential breakthrough in the numerical simulation in theory of turbulence.
On the other hand, Kaneda together with Yoshimatsu has performed of the computational science and statistical theory of turbulence study. He has the results on the realization of the Direct Numerical Simulation (=DNS) in the world maximum scale about the uniformly isotropic turbulence. In addition, he proceeds to the DNS of the high Reynolds number with the world maximum size about the turbulence between two parallel flat boards.
Kaneda is evaluated as the leader developing the spectrum statistics theory of turbulence.

【Research Methods】

This project aims to establish a new theory of nonlinear dynamics for super large degree of freedom including the turbulence in the fluid mechanics in terms of the nonlinear analysis and the computational fluid dynamics. So, we propose the following four projects (i), (ii), (iii) and (iv);
(i) Harmonic analysis, singular limit and estimates of effect on the finiteness
(ii) Mathematical analysis of boundary layer and viscosity limit
(iii) Elucidation of the universal law of turbulence; small and large scales
(iv)Information abridgement technique, prediction possibility and reliable evaluation

The method dealing with infinity and the mathematical analysis such as the limiting procedure give us the elucidation of the turbulence phenomenon requiring a large-scale calculation.
We will improve a poor turbulence theory without rigorously mathematical convention, and then construct a new knowledge of turbulence with information abridgement technique.
As a result, reliable turbulence theory which do not depend on a law learned by experience or by intuition excessively will be largely accelerated.

【Expected Research Achievements and Scientific Significance】

It is well-known that the Clay Math. Institute proposes seven important Millennium problems, where the existence of the global classic solution to the Navier-Stokes equations is selected.
On the other hand, our DNS of the uniformly isotropic turbulence is by far the larger computational performance so that it can deal with the turbulent fluid with the high Reynolds number without any error of the experiment and indeterminacy.
Our study is based on the DNS of such a world highest standard of Kaneda's research group, and we are going to overcome difficulty of turbulence with the high Reynolds number.
In this way, our research projects develop the modern mathematical analysis, the applied mathematics, computational science and hydrodynamics and will lead the relevant subjects to the world-wide level.

【Publications Relevant to the Project】

・ Kozono, Harmonic analytic research on stationary and nonstationary problems for the incompressible Navier-Stokes equation. (Japanese) Sugaku 67 (2015), no. 2, 113-132.
・Kozono, Amann, Giga etal., Recent Developments of Mathematical Fluid Mechanics, Birkhaeser-Verlag 2016.

【Term of Project】 FY2016-2020

【Budget Allocation】 123,600 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.math.sci.waseda.ac.jp/math/

Title of Project : Precise determination of the proton charge radius by electron scattering off proton at ultra-low momentum transfer region

Toshimi Suda
(Tohoku University, Research Center for Electron-Photon Science, Professor)

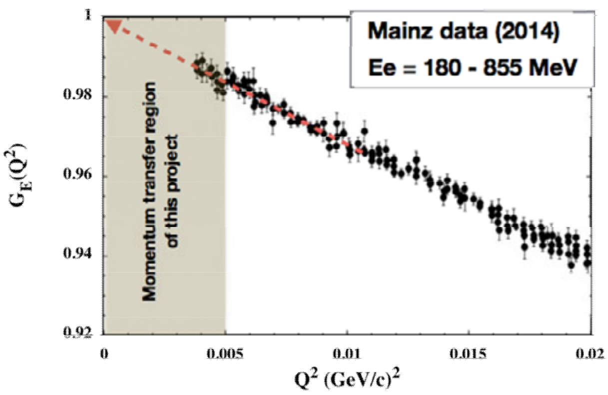
Research Project Number : 16H06340 Researcher Number : 30202138
Research Area : Nuclear Physics (Experiment)
Keyword : Elastic electron scattering, proton charge radius, ultra-low momentum transfer

【Purpose and Background of the Research】

The purpose of this research is a precise determination of the proton charge radius. The proton radius is under hot debates today known as "*Proton Charge Radius Puzzle*". We will determine the radius by elastic electron scattering at the smallest momentum transfer region ever accessed. Such measurements enable us to determine the radius in the least model dependent way.

The proton charge radius provided by elastic electron scattering and the Lamb shift measurement of atomic hydrogen has been 0.88 fm, whereas the radius extracted from the spectroscopy of muonic-hydrogen atoms is found to be 0.84 fm. This is the puzzle. Since the proton size is one of the most fundamental physical quantities, much effort including careful re-analysis of the past data and reducing uncertainties in theoretical interpretation is underway. The puzzle, however, still remains, and the origin of this discrepancy is not yet clear.

This research aims at providing the most precise radius by means of electron scattering. We will conduct a series of measurements of elastic electron scattering off proton at an ultra-low momentum transfer region, $0.0003 \le Q^2 \le 0.005$ $(\mathrm{GeV/c})^2$, where Q is the four-momentum transfer. As shown in the figure below, the minimum Q^2 accessed so far was 0.004 $(\mathrm{GeV/c})^2$ in the Mainz experiment. This project will reduce the minimum Q^2 further down to 0.0003 $(\mathrm{GeV/c})^2$. This allows us to extract the radius in a model independent way, since the radius is defined to be the derivative of the charge form factor, $G_E(Q^2)$, at $Q^2 = 0$.



【Research Methods】

The experiments will be performed using the 60 MeV electron linear accelerator of Research Center for Electron Photon Science (ELPH), Tohoku University. Making full use of the advantages of this low-energy and small accelerator, the charge and magnetic form factors are experimentally separated by so-called Rosenbluth separation method, which requires frequent changes of the beam energies.

The key for success of this research is to control systematical uncertainties to be an order of 10^{-3}, since the change of $G_E(Q^2)$ in the momentum transfer range is only a few %. The CH_2 target will be employed for this purpose, since the charge radius of carbon is precisely known in the 10^{-3} level. We will be able to determine absolute elastic cross section off proton with high precision by the relative measurements to that of carbon.

【Expected Research Achievements and Scientific Significance】

Our measurements will cover the lowest momentum transfer region, so that the proton charge radius is determined in the least model-dependent way. We will measure the *absolute* cross section, and extract the charge form factor from the cross section by means of the *Rosenbluth separation*, both of which are in sharp contrast to the Mainz experiments. The results of our project will, thus, provide the most reliable proton radius data for those determined by electron scattering.

【References Releveant to the Project】

・ R. Pohl et al., Nature **466** (2010) 213.
・ A. Antognini et al., Science **229** (2013) 417.

【Term of Project】 FY2016-2020

【Budget Allocation】 128,500 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.lns.tohoku.ac.jp
suda@lns.tohoku.ac.jp

Title of Project : Study of binary neutron star merger by high cadence optical observations

Toshikazu Shigeyama
(The University of Tokyo, Graduate School of Science, Associate Professor)

Research Project Number : 16H06341 Researcher Number : 70211951
Research Area : Physics
Keyword : Astrophysics, gravitational wave, binary neutron star

【Purpose and Background of the Research】

The advanced LIGO (aLIGO), gravitational wave detectors in USA began to detect gravitational waves from celestial objects. If gravitational wave signals from a binary neutron star merger are detected, then it is expected that the electro-magnetic counter part could be detected and lead to better understanding of extremely dense matter in the neutron stars in addition to a test of the theory of general relativity.

【Research Methods】

In our study, we will develop an extremely wide-field camera loading a high sensitivity CMOS censor Tomoe Gozen1 (the field of view=9 degree, Tomoe in the following), and install it on the Schmidt telescope in the Kiso observatory of University of Tokyo. We will perform quick follow up observations of gravitational wave events by this camera aiming at the detection of the optical counter parts. In parallel with this preparation, we will also strengthen a system to analyze data from another gravitational wave detector KAGRA, which is now under construction in Japan and will operate in a few years.

From the theoretical point of view, we will construct models to predict and reproduce the optical counter parts emitted from binary neutron.

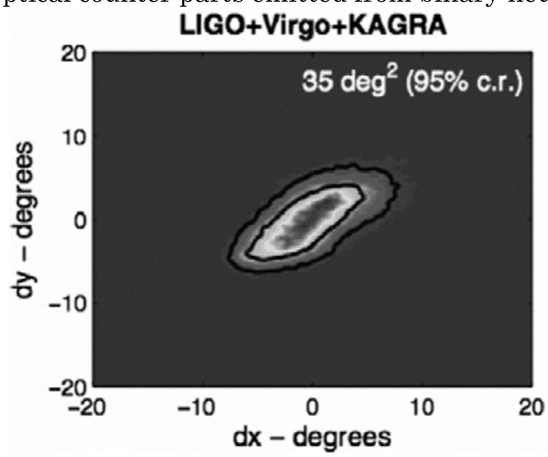


Fig. 1 Predicted localization of a gravitational wave source

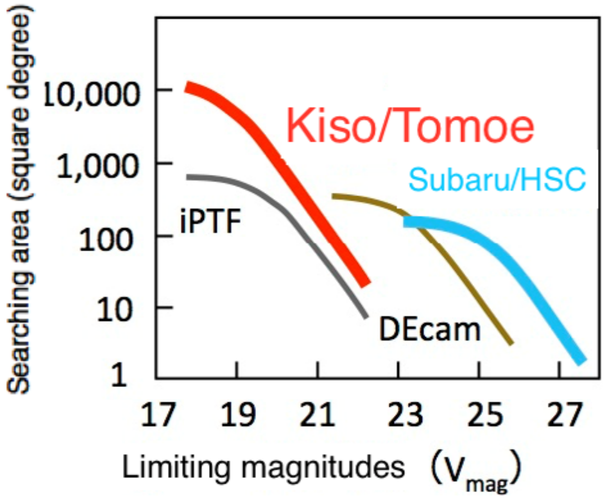


Fig. 2 Searching area achieved by one hour exposure as a function of limiting magnitude.

【Expected Research Achievements and Scientific Significance】

By comparing theoretical models with observational results thus obtained, we will deduce the chemical compositions, mass, and kinetic energy of the ejecta from a binary neutron star merger, which will constrain the properties of extremely dense matter in neutron stars. At the same time, we will explore the role of this kind of events as a source of elements heavier than iron.

【Publications Relevant to the Project】

・Sekiguchi, Y. et al. Physical Review D 91, 064059 (2015)
・Tsujimoto & Shigeyama, Astronomy & Astrophysics, 565, L5 (2014)

【Term of Project】 FY2016-2020

【Budget Allocation】 98,300 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.ioa.s.u-tokyo.ac.jp/tomoe

Title of Project : Identification of Gravitational Wave Sources with X-ray Transient Monitor and Study of Black Hole Formation Mechanism

Daisuke Yonetoku
(Kanazawa University, College of Science and Engineering, Professor)

Research Project Number : 16H06342 Researcher Number : 40345608
Research Area : Mathematical and Physical Science
Keyword : Astrophysics (Experiment), Gravitational Wave, X-ray, Satellite, Black Hole

【Purpose and Background of the Research】

In this research, we will strongly contribute to construct and develop the gravitational wave (GW) astronomy.

The first detection of gravitational wave has been done by GW observatory LIGO in United States on Sep. 15, 2015. Since we obtained a new method "GW" to observe the universe, we expect to realize a brand new astronomy with simultaneous observations with both GW and electro-magnetic wave, especially for the moment of black hole formation and related phenomena in surrounding environments.

However, the localization accuracy by GW observation only is too poor to identify the origin of GW sources. Therefore, in this research, we will perform synchronous observations with GW detections using a wide field X-ray imaging detector and a gamma-ray trigger system aboard micro satellite planning to launch in FY2018. We will promptly send alert messages of X-ray and gamma-ray observation, and we strongly encourage follow-up observations by optical, infrared, radio (multi-wavelength) large observatories.

【Research Methods】

The wide field observation with over 1/10 of entire sky can be realize only in X-ray and gamma-ray, so we enable to detect transient phenomena coincide with GW detections. In this research, we will develop flight model of X-ray and gamma-ray detectors (Figure1). We also install the alert system, and organize the follow-up observations (Figure 2).

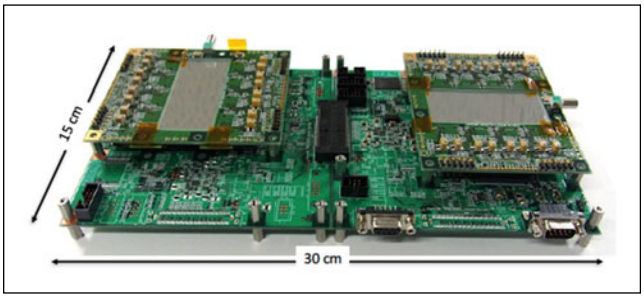


Figure 1. Proto-type model of wide field X-ray imaging detector. We develop the flight model in this research.

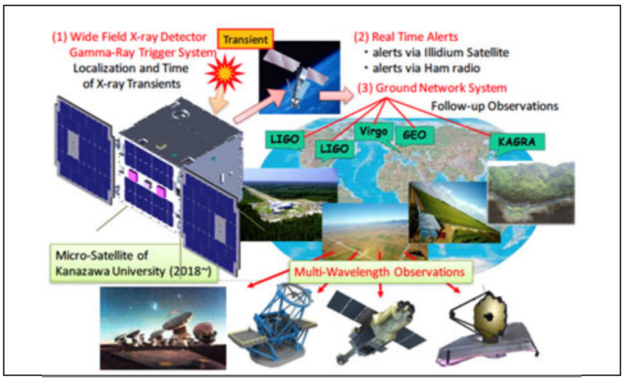


Figure 2. A complete picture of this research.

【Expected Research Achievements and Scientific Significance】

Several models of black hole formation are discussed, for example a direct collapse model and a massive magnetar model as an intermediate state of its formation. Using the time difference between GW and X-ray/gamma-ray detections, we will enable to discuss the process of black hole formation. Moreover, the main energy source of relativistic outflow (jet), i.e. a neutrino driven or a magnetic driven models, will be distinguished. We will realize advanced astrophysics with GW and electro-magnetic wave observations.

【Publications Relevant to the Project】

"Establish of Gravitational Wave Astronomy with Gamma-Ray Burst and X-ray Transient Monitor", D. Yonetoku, et al., UNISEC, 5, 2, pp.19-27 (2014)
"X-raying extended emission and rapid decay of short gamma-ray bursts", Y. Kagawa, D. Yonetoku et al., ApJ, 811, 8 (2015)

【Term of Project】 FY2016-2020

【Budget Allocation】 140,800 Thousand Yen

【Homepage Address and Other Contact Information】

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【Grant-in-Aid for Scientific Research (S)】

Science and Engineering (Mathematical and Physical Sciences)

Title of Project : Search for new physics in rare kaon decays

Taku Yamanaka
(Osaka University, Graduate School of Science, Professor)

Research Project Number : 16H06343 Researcher Number : 20243157
Research Area : Particle physics (experiment)
Keyword : Particle physics (experiment), kaons, J-PARC, new physics beyond the standard model

【Purpose and Background of the Research】

After the Big Bang, the same numbers of particles and anti-particles were created, but after the Universe has cooled down, anti-particles are extremely rare. This means that there was a CP-violating process that changed the balance between the particles and anti-particles. The standard model for particle physics cannot explain such CP-violation that created the matter-dominant universe.

The purpose of this research is to search for new physics beyond the standard model that breaks the CP symmetry.

We will use the $K_L \to \pi^0 \nu\nu$ decay as a probe to search for CP-violating new physics. First, this decay violates the CP symmetry. Second, the branching ratio predicted by the standard model is small (3×10^{-11}), and its theoretical uncertainty is also small (2%), making the decay mode sensitive to new physics effects. If the branching ratio is different from the standard model prediction, it signifies the existence of new physics.

【Research Methods】

We will use the J-PARC high intensity proton accelerators to produce kaons, and look for the decay with the KOTO detector shown in Fig. 1. The two photons from the π^0 decay are observed with the CsI calorimeter placed downstream. To ensure that there are no other observable particles besides the two photons, the decay region is surrounded by detectors such as NCC, FB, MB, and CV.

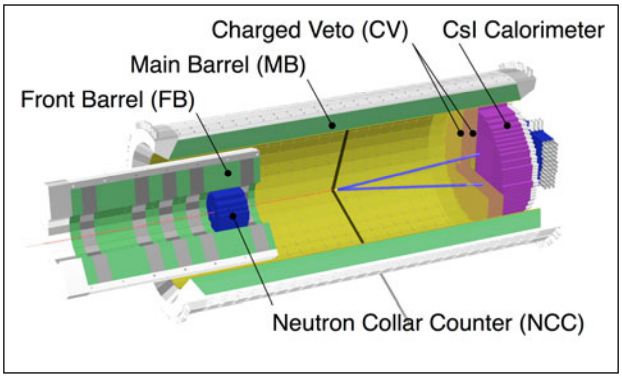


Fig. 1 KOTO detector

In 2013, we collected the first data for 4 days and achieved a sensitivity equivalent to the past best experiment. In 2015 we collected 20 times more data. We will increase our sensitivity by increasing the proton beam intensity, and by applying the following upgrades.

To suppress a new background caused by neutrons hitting the calorimeter directly, we will install 4000 new photo-sensors in front of the calorimeter. The timing difference between the sensor and existing PMTs on the back measures the interaction depth of the incident particles to distinguish between photons and neutrons.

To collect data at high beam power, we will upgrade our data acquisition system. It utilizes new ATCA technology to build events and apply online cuts by counting the number of particles hitting the calorimeter.

【Expected Research Achievements and Scientific Significance】

If the branching ratio is larger than 1×10^{-10}, we can claim the existence of new physics with the 3σ significance. Combined with the results from CERN NA62 experiment that measures branching ratio of the $K^+ \to \pi^+ \nu\nu$ decay, and KEK Belle II experiment, we can constrain models and parameters for the new physics. Even if we do not observe the decay, we can still constrain some new physics models.

【Publications Relevant to the Project】

- T. Masuda *et al.*, "Long-lived neutral-kaon flux measurement for the KOTO experiment", PTEP 2016, 013C03-1~23 (2016).
- T. Yamanaka, "The J-PARC KOTO Experiment", PTEP 2012, 02B006-1~7 (2012).

【Term of Project】 FY2016-2020

【Budget Allocation】 133,800 Thousand Yen

【Homepage Address and Other Contact Information】
http://koto.kek.jp

Title of Project : Searching for a sterile neutrino at J-PARC MLF

Takasumi Maruyama
(High Energy Accelerator Research Organization (KEK), Institute of Particle and Nuclear Studies, Associate Professor)

Research Project Number : 16H06344 Researcher Number : 80375401
Research Area : Physics
Keyword : Experimental research for the elementary particle physics

【Purpose and Background of the Research】

The discovery of the neutrino oscillation phenomena provides the Novel Prize to Dr. Takaaki Kajita and Dr. Art Mcdonald in 2015. The neutrino oscillations provide the flavor (electron, muon, tau, (sterile)) changing of neutrinos as a function of their energy and flight length. This research aims to search for the sterile neutrino flavor in the oscillation with high precision.

The sterile neutrinos have no weak interactions, thus the standard model of the elementary particle physics can't explain them. Once the existence of the particle is established, the standard model should be changed drastically based on the fact.

The search for the sterile neutrino is performed using the neutrino oscillation between active and sterile neutrinos. There are some indications for the phenomena with the experiments using neutrinos from accelerator, reactor and radioactive source, but the definite conclusion of the existence has not yet been obtained. This research aims to have a conclusion with the fastest time-scale among the planned experiments in the world.

【Research Methods】

Figure1 shows the setup of the experiment, which consists of MLF building and a detector. From right hand side, 3GeV protons are injected to the mercury target, which creates not only neutrons for life and material science but also number of

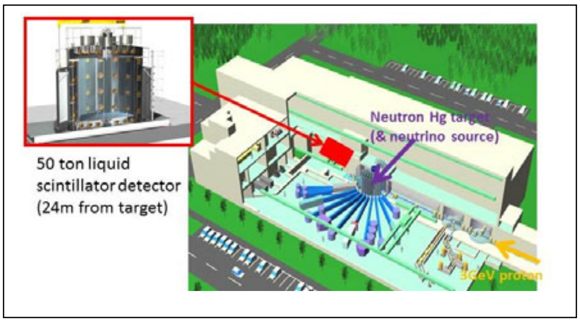


Fig1 setup at MLF

neutrinos. After the proton injections to the target, μ^+ is created and stopped, and it decays to e^+, ν_e and anti-ν_μ. We put the detector with 50 tons of liquid scintillator to the red box in the figure (on the 3rd floor of the MLF) and the baseline from the target is about 24 meters. We search for the anti-ν_μ to anti-ν_e oscillation with 24 meters. This oscillation phenomena with such a short distance is only happened in the case that sterile neutrinos exist.

【Expected Research Achievements and Scientific Significance】

Figure2 shows the sensitivity of this research. The horizontal axis shows the oscillation fraction

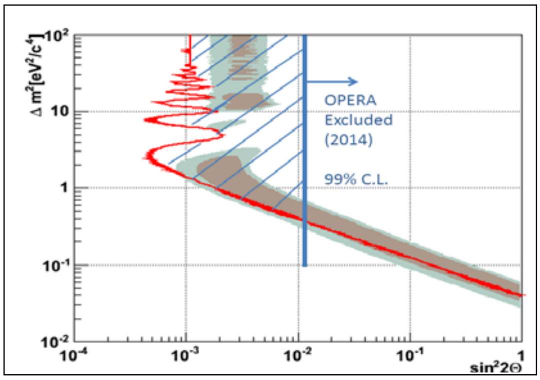


Fig.2 sensitivity

from anti-ν_μ to anti-ν_e, and the vertical axis shows the squared of eigen-state mass difference of 4th and other neutrinos. The shaded region can be searched with this experiment while the brown (99%C.L) and the green (90%) show the indication regions from prior experiments. We can conclude most of the region of interest with 90%C.L.

【Publications Relevant to the Project】

- S. Ajimura et al, PTEP 2015 6, 063C01 (2015)
- M. Harada et al, arXiv:1310.1437 (proposal)

【Term of Project】 FY2016-2020

【Budget Allocation】 140,100 Thousand Yen

【Homepage Address and Other Contact Information】

http:// research.kek.jp/group/mlfnu/

Title of Project : Materials Design and Exploration of Functions for Strongly Correlated Materials – Challenges to Non-Equilibrium and Non-Periodic Systems

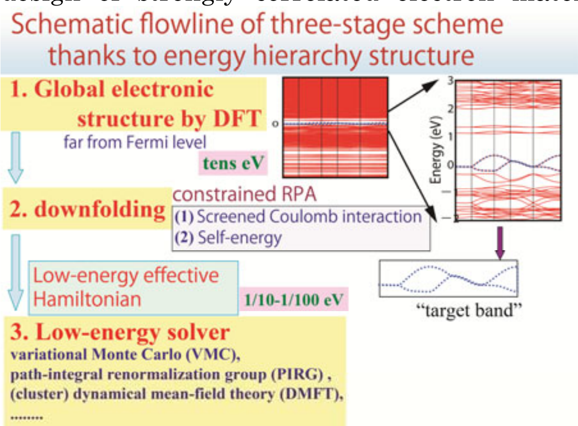
Masatoshi Imada
(The University of Tokyo, Graduate School of Engineering, Professor)

Research Project Number : 16H06345 Researcher Number : 70143542
Research Area : Physical Sciences
Keyword : Strongly Correlated Materials, Non-equilibrium Systems, Interfaces, First-Principles

【Purpose and Background of the Research】

Electron correlations have been one of the central fields to cultivate novel concepts in basic science, which have novel functions and potential applications as well. However, strongly correlated materials were faced with difficulties in theoretical and computational tools for their studies. Recently this challenge has been greatly explored and a powerful method called multi-scale ab initio scheme for correlated electrons (MACE) (bottom figure) has been pursued and successfully applied.

In this project, we extend this scheme to 1. non-equilibrium phenomena and 2. non-periodic systems such as surface, interface and quasicrystals and pioneer frontiers of strong correlation physics. Above all, a. non-equilibrium high-temperature superconductivity, b. principles for efficient solar cells, c. theories to analyze time-resolved experimental probes, d. high-temperature superconductivity on interfaces and thin films, e. topological mobile and tunable interfaces such as magnetic domain walls, f. anomalous thermal and electronic conduction of quasicrystals, and g. magnetism at grain boundaries of permanent magnets are suitable subjects to be pursued by developing our methods. Mechanisms and functions of novel phenomena in charge-spin-lattice coupled systems will be studied with emphasis on transition metal compounds based on MACE towards the goal of materials design of strongly correlated electron materials.



【Research Methods】

[Methodologies] (1) We implement methods for non-equilibrium states and excitations by extending variational Monte Carlo (VMC), and dynamical mean- field (DMFT) methods as well as many-body perturbation methods including the vertex corrections. (2) We improve methods to treat non-periodic systems (surfaces, interfaces and quasi-crystals) by taking account of structural relaxations. (3) We extend VMC and DMFT for electron-phonon interaction, spin-orbit interaction and multi-orbital systems. Emergent excitations as well conventional collective excitations are examined. Open source codes will be released after developing codes for general use.

[Application to materials design] We clarify mechanisms of non-equilibrium high-temperature superconductivity, general principles for materials design of efficient solar cell design. After taking account of lattice relaxation and electron-phonon interaction, designing high- temperature superconductivity at interfaces and thin films and functional topological interfaces are explored.

【Expected Research Achievements and Scientific Significance】

Basic science and materials design of strongly correlated systems will be developed based on first principles methods.

【Publications Relevant to the Project】

・F. Aryasetiawan, M.Imada *et al.*, "Frequency-Dependent Local Interactions and Low-Energy Effective Models from Electronic Structure Calculations" Phys. Rev. B **70** (2004) 195104.
・M. Imada and T. Miyake, "Electronic Structure Calculation by First Principles for Strongly Correlated Electron Systems" J. Phys. Soc. Jpn. **79** (2010) 112001.

【Term of Project】 FY2016-2020

【Budget Allocation】 85,400 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.solis.t.u-tokyo.ac.jp/index.html
imada@ap.t.u-tokyo.ac.jp

Title of Project : Molecular quantum liquids in strongly correlated electron systems

Reizo Kato
(RIKEN, Condensed Molecular Materials Laboratory, Chief Scientist)

Research Project Number : 16H06346 Researcher Number : 80169531
Research Area : Mathematical and Physical Sciences
Keyword : Molecular solid/Organic conductor, Strongly correlated electron system, Superconductivity

【Purpose and Background of the Research】

Materials where the electrons are strongly correlated form one of highly important research fields of this century in terms of both basic science and application. In the strongly correlated electron systems, several degrees of freedom including charge, spin, lattice, and orbital are simultaneously active and competing with each other. This causes plenty of uncharted electronic states that are waiting our investigation. Among them, “quantum liquids” that exhibit neither long-range order (as solid) nor complete uniformity (as gas), characterize essential behavior of the strongly correlated electron system.

The molecular π electron system is suitable for the study of quantum liquids, thanks to “simple and clear electronic structures”, “soft crystal lattice”, “low carrier density”, and “controllability by chemical modifications”.

In this project, we will quest for three types of quantum liquids in molecular π electron systems, 1) Quantum spin liquid, 2) Fractional Hall liquid in multi-layer Dirac electron system, 3) Non-Fermi liquid in the vicinity of the field-induced Mott transition.

【Research Methods】

1) Quantum spin liquid (QSL)

Based on NMR, ESR, low-temperature X-ray diffraction, vibrational spectroscopy, and theoretical studies on the molecular QSL with a triangular lattice, $EtMe_3Sb[Pd(dmit)_2]_2$, and related materials, we figure out the QSL phase with neighboring unconventional electronic phases.

2) Fractional Hall liquid in multi-layer Dirac electron system

We aim to observe an unconventional fractional Hall effect in a hole-doped organic conductor α-$(BEDT\text{-}TTF)_2I_3$. Another goal is development of new Dirac electron systems based on single-component molecular conductors.

3) Non-Fermi liquid in the vicinity of the field-induced Mott transition

By studying the filling-controlled Mott transition in the field-effect transistor (FET) with a thin single crystal, we will reveal non-Fermi liquid and superconducting phases in a universal phase diagram around the Mott insulator.

【Expected Research Achievements and Scientific Significance】

This comprehensive and interdisciplinary research project is expected to provide basic understanding of the strongly correlated electron system and to open new field of materials science that constructs basis of molecular electronics and devices.

【Publications Relevant to the Project】

・"Development of π-Electron Systems Based on $[M(dmit)_2]$ (M= Ni and Pd; dmit: 1,3-dithiole-2-thione-4,5-dithiolate) Anion Radicals", R. Kato, *Bull. Chem. Soc. Jpn.*, **87**, 355-374 (2014).
・"Quantum Hall Effect in Multilayered Massless Dirac Fermion Systems with Tilted Cones", N. Tajima, T. Yamauchi, T. Yamaguchi, M. Suda, Y. Kawasugi, H. M. Yamamoto, R. Kato, Y. Nishio, and K. Kajita, *Phys. Rev. B*, **88**, 075315/1-6 (2013).
・"A Strained Organic Field-Effect Transistor with a Gate-Tunable Superconducting Channel", H. M. Yamamoto, M. Nakano, M. Suda, Y. Iwasa, M. Kawasaki, and R. Kato, *Nature Commun.*, **4**, 2379/1-7 (2013).

【Term of Project】 FY2016-2020

【Budget Allocation】 142,600 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.riken.go.jp/lab-www/molecule/index-e.html

Title of Project : Physical properties of uppermost mantle structure and the Mohorovicic seismic discontinuity

Katsuyoshi Michibayashi
(Shizuoka University, Faculty of Science, Department of Geosciences, Professor)

Research Project Number : 16H06347 Researcher Number : 20270978
Research Area : Mathematical and Physical Sciences
Keywords : Earth and Planetary Science, Geology, Ocean-floor Science, Lithosphere, Mantle

【Purpose and Background of the Research】

We study the physical properties (e.g., the development of textures, elastic properties, electron conductivity, and permeability) of mantle-derived materials (i.e., rocks) such as trench peridotites in the Izu–Bonin–Mariana Trench and peridotites in the Oman ophiolite of the Arabian Peninsula in order to understand the structural development of the uppermost mantle and the Mohorovicic seismic discontinuity within the lithospheric mantle of Earth.

The trench peridotites in the Izu–Bonin–Mariana Trench preserve the uppermost mantle structures that formed during fore-arc spreading at the time of the initiation of subduction of the Pacific plate beneath the Philippine Sea plate.

The peridotites in the Oman ophiolite represent the uppermost lithospheric mantle of an oceanic plate that formed at a fast-spreading ridige such as those in the eastern part of the Pacific plate. We investigate the physical factors controlling the structural development of the uppermost mantle by comparing these two types of the peridotites.

【Research Methods】

We use a polarizing microscope to analyze thin sections of the peridotites oriented parallel to the lineation and perpendicular to the foliation, thereby revealing their microstructures, including grain size, grain shape, and mineral modes.

Electron microscopes can be used to measure the crystallographic orientations and chemical compositions of rock-forming minerals such as olivine, pyroxene, and spinel, by which we determine environmental conditions (e.g., temperature and pressure) as well as volatile contents (e.g., water and carbon dioxide).

In the field, we study the physical properties of the crust–mantle boundary by logging bore holes drilled by the Oman Drilling Project. We use the submersible *Shinkai6500* to explore the fore-arc mantle exposed at the deepest ocean floor in the Izu–Bonin–Mariana trench.

Our goal is to construct the best lithological model of the uppermost mantle based on these data.

【Expected Research Achievements and Scientific Significance】

We will obtain the most relevant data in Earth Science in terms of understanding the uppermost mantle and the Mohorovicic seismic discontinuity. We will then develop the most advanced physical model of the seismic velocity structure of oceanic plates, such as the Pacific plate, based on marine geophysical observations. Furthermore, we will support the Mantle Drilling Project, which aims to understand the uppermost lithospheric mantle of the Pacific plate, a typical oceanic plate on Earth.

【Publications Relevant to the Project】

Michibayashi, K. et al., **2016**. Natural olivine crystal-fabrics in the western Pacific convergence region: a new method to identify fabric type. ***Earth and Planetary Science Letters***, 443, 70-80.

Harigane, Y., **Michibayashi, K.** et al., **2013**. The earliest mantle fabrics formed during subduction zone infancy. ***Earth and Planetary Science Letters***, **377-378**, 106-113.

Michibayashi, K. and Oohara, T., **2013**. Olivine fabric evolution in a hydrated ductile shear zone at the Moho Transition Zone, Oman Ophiolite. ***Earth and Planetary Science Letters***, 377-378, 299-310.

【Term of Project】 FY2016-2010

【Budget Allocation】 141,700 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.ipc.shizuoka.ac.jp/~sekmich/
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Title of Project : Development of near-real-time volcanology based on in-situ observation experiments of shallow magmatic processes

Michihiko Nakamura
(Tohoku University, Graduate School of Science, Professor)

Research Project Number : 16H06348 Researcher Number : 70260528
Research Area : Mathematical and Physical Sciences (Earth and Planetary Science)
Keyword : Magma, Igneous rocks, Volcanic eruption Magma, Igneous rocks, Volcanic eruption

【Purpose and Background of the Research】

In shallow volcanic conduits, magma viscosity rapidly increases through crystallization of minute crystals (nanolites) due to decompression-induced liquidus temperature increase and resulting large undercooling (Figure 1). How magmas run through this "decompression-freezing interval" determines whether a volcanic eruption occurs or not, and how explosive the eruption will be. In this project, we investigate the rate of viscosity increase due to decompression-induced crystallization based on in-situ observation experiments. The driving force of magma ascent and explosions is bubble formation in magmas, thus is determined by volume of bubbles. Experimental investigation of outgassing mechanism is therefore another end of this study. Application of these results to a fluid-dynamic model of conduit flow would make it possible to forecast eruption transition at "near-real-time" according to pressure-time paths of magmas in actual intrusion events.

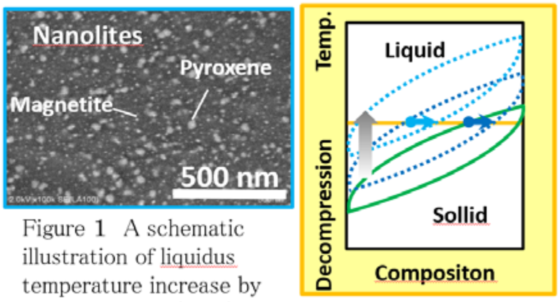

Figure 1 A schematic illustration of liquidus temperature increase by decompression (right) and nanolites in an erupted product of the 2011 Shinmoe-dake eruption (left).

【Research Methods】

By introducing high-temperature heating stages to electron microscopes (TEM, FE-SEM), we will conduct in-situ measurements of nucleation and growth rates of crystals from undercooled magmas at a wide scale range down to nanometer. Obtained rates will be utilized to determine bifurcation conditions of eruption styles for the Shinmoedake and other active volcanoes. Outgassing degree and rheological properties of andesitic–basaltic magmas will be measured by a newly developed experimental apparatus. Combining these results, we will be able to calculate temporal change of magma viscosity and resulting eruption behavior.

【Expected Research Achievements and Scientific Significance】

In the case of mafic magmas, vesiculation microstructure and outgassing degree will depend on the shear strain rate because of the effect of surface tension; this is expected to affect the results of conduit flow modeling significantly. Our research will enable near-real-time assessment of physical properties and resulting behavior of intruded magmas in coming volcanic activities.

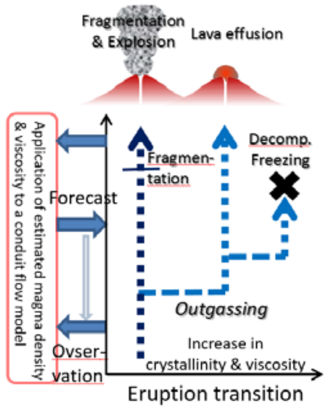

Figure 2 Improvement of eruption models through the observation-forecast-varidation cycle

【Publications Relevant to the Project】

- Okumura, S., Nakamura, M., Uesugi, K., Nakano, T., Fujioka, T., Coupled effect of magma degassing and rheology on silicic volcanism, Earth Planet. Sci. Lett., 362, 163-170, doi:10.1016/j.epsl.2012.11.056, 2013.
- Mujin, M., Nakamura, M., A nanolite record of eruption style transition, Geology, 42, 611-614, doi:10.1130/G35553.1, 2014.
- Nakamura, M., Material sciences on magma ascent processes, Japan Geoscience Letters, 11, 3-5, 2015.

【Term of Project】 FY2016-2020

【Budget Allocation】 136,100 Thousand Yen

【Homepage Address and Other Contact Information】

http://epms.es.tohoku.ac.jp/arcmag/
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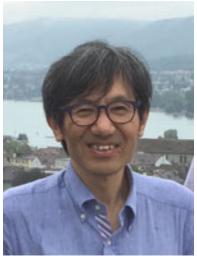


Title of Project : Physicochemical analysis of early solar system based on formation kinetics of refractory inclusions of meteorites

Hisayoshi Yurimoto
(Hokkaido University, Faculty of Science, Professor)

Research Project Number : 16H06349 Researcher Number : 80191485
Research Area : Geochemistry/Cosmochemistry
Keyword : Geochemistry, Cosmochemistry, Meteorites, Solar system, Protoplanetary Disk

【Purpose and Background of the Research】

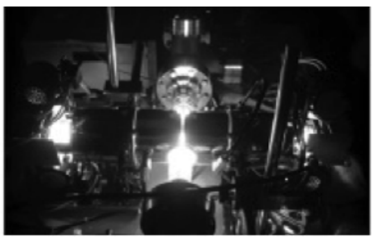
We have evidence of high temperature processes in the early solar system to condense solid materials from vapor and to melt solid precursors in the protoplanetary disk from studies of refractory inclusions (CAIs and AOAs) in primitive chondrites. The processes have not been observed by astronomical observations of protostars and protoplanetary disks. Therefore, the physicochemical conditions and the astrophysical setting have not well constrained.

In this study, we study physicochemical conditions of the high temperature processes generated in the early solar system by material synthesis experiments in laboratory according to analysis of isotopic mineralogy and petrology of refractory inclusions in primitive chondrites. This study is specially focused determination of total pressure, water vapor pressure, and gas/dust ratios in the inner edge of the protoplanetary disk.

【Research Methods】

Following is plans of laboratory experiments to determine physiochemical conditions (temperature, pressure and water vapor partial pressure) of CAI and AOA formation in the early solar system.

Synthetic laboratory experiments to reproduce petrographic texture and the isotopic spatial distribution of inter- and intra-minerals observed in natural CAIs are conducted. These experiments are crystallization experiments of CAI melt under low pressure and low water vapor pressure conditions to exchange oxygen isotopes. We used $H_2{}^{18}O$ vapor for these experiments. According to these experiments, we will determine partial pressure of water vapor of surrounding atmosphere. Then, we will calculate total pressure of CAI forming region using oxygen fugacity observed by natural CAI minerals.



We also conduct vaporization experiments of CAIs under low pressure H_2-H_2O condition. We realize elemental fractionation factor, isotopic fractionation factor and evaporation coefficient for CAI formation. Using these parameters, condensation timescale for natural CAIs is inferred as a function of temperature and pressure. Oxygen isotopic exchange rates and self-diffusivity of oxygen in crystals are determined by this experiment. Therefore, we can infer that CAI condensation time, condensation temperature, condensation pressure and dust/gas ratio in the early solar system using elemental and oxygen isotopic zoning observed in natural CAIs for condensation origin.

【Expected Research Achievements and Scientific Significance】

An expected research achievement is the first determination of physicochemical conditions of refractory materials formation at the beginning of solar system formation experimentally.

【Publications Relevant to the Project】

・Kawasaki, N., Kato, C., Itoh, S., Wakaki, S., Ito, M. and Yurimoto, H. (2015) ^{26}Al–^{26}Mg chronology and oxygen isotope distributions of multiple melting for a Type C CAI from Allende. *Geochim.Cosmochim. Acta* **169**, 99-114.
・Takigawa A., Tachibana S., Nagahara H. and Ozawa K. (2015) Evaporation and condensation kinetics of corundum:The origin of the 13-μm feature of oxygen-rich AGB Stars. *Astrophys. J. Suppl.*, **218**, doi:10.1088/0067-0049/218/1/2.

【Term of Project】 FY2016-2020

【Budget Allocation】 140,700 Thousand Yen

【Homepage Address and Other Contact Information】
http://vigarano.ep.sci.hokudai.ac.jp

Title of Project : Fabrication and Characterization of Novel Nano-Materials Using One- and Two-dimensional Reaction Fields

Hisanori Shinohara
(Nagoya University, Graduate School of Science, Professor)

Research Project Number : 16H06350 Researcher Number : 50132725
Research Area : Fundamental Chemistry
Keyword : Carbon nanotubes, Graphene, Reaction Fields

【Purpose and Background of the Research】

Based on our past achievements and background in nano-peapods studies, it is not until relatively recently that we discovered very fascinating materials, *i.e.*, various nanowires encapsulated carbon nanotubes (cf.Fig.1). We found that nanowires (whose size varies from single-chain nanowires to several hundreds-chain nanowires depending upon the diameter of host carbon nanotubes) can easily be fabricated during a high-temperature annealing of simple aromatic hydrocarbons. This is the first example that pure nanowires of various sizes are prepared within carbon nanotubes, in which electronic and magnetic properties are expected to exhibit some unique properties such as ferromagnetism and superconductivity due to substantial charge transfers between nanowires and carbon nanotubes.

【Research Methods】

Of the most important targeted goals of the present projects is not only to fabricate the present novel nano-carbon materials but to characterize them in terms of simultaneous measurements of structures and electron transport properties. This can only be realized by a specially designed technique where HRTEM, FET and Raman spectroscopy measurements are performed on exactly the same individual nano-peapod and/or nanowires carbon nanotubes. Furthermore, by using the two-dimensional space between two layers of graphene, one can "sandwich" nanomaterials in two-dimensional fashion (Fig.2). In addition, the present project investigates also the development and fabrication of such a combined experimental set-up.

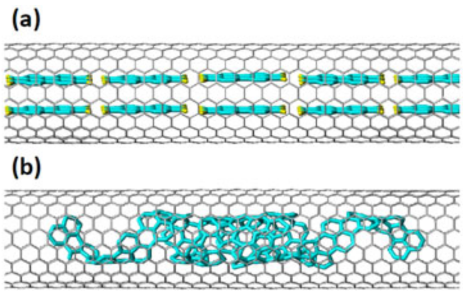


Fig. 1 Inner space

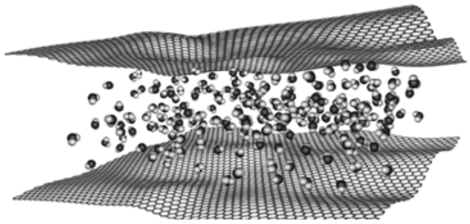


Fig.2 2D-Inner space

【Expected Research Achievements and Scientific Significance】

By using the present experimental techniques, we are able to fabricate both one- and two-dimensional brand-new nanomaterials within carbon nanotubes and between the two layers of graphene, respectively.

【Publications Relevant to the Project】

- "Template Synthesis of Linear-Chain Nano- diamonds inside Carbon Nanotubes" Y.Nakanishi *et al.* ***Angew.Chem.Int.Ed.*** 54, 10802-10806 (2015).
- "Core-Level Spectroscopy to Probe the Oxidation State of Single Europium Atoms" L.H.G.Tizei *et al.* ***Phys.Rev.Lett.*** 114, 197602-1-5 (2015).

【Term of Project】 FY2016-2020

【Budget Allocation】 108,200 Thousand Yen

【Homepage Address and Other Contact Information】

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noris@nagoya-u.jp

Project Title : Studies on Chemical Synthesis of Polyketide-Derived, Biologically Active Complex Natural Products

Keisuke Suzuki
(Tokyo Institute of Technology, School of Science, Department of Chemistry, Professor)

Research Project Number : 16H06351　Researcher Number : 90162940
Research Area : organic chemistry
Keyword : natural products, polyketide, complexity, diversity, dimeric structure, hybridization

【Purpose and Background of the Research】

Even by the cutting-edge organic synthesis that provides now facile access to various useful compounds in scientific and industrial fields, certain classes of compounds remain inaccessible, due to the skeletal, functional, and stereochemical complexity. A typical example is the complex architectures derived from the type-II polyketide biosynthesis, constituting an attractive class of compounds with potential bioactivities. In this five-year project, we will address synthetic studies of such natural products by focusing on the development of new synthetic strategies and tactics, hoping eventually to achieve the total syntheses.

【Research Methods】

We sought a hint from natural biosynthesis and considered how the complexity and diversity of natural product structure evolved, recognizing three factors, 1) modification of the basic building unit A within itself, giving analogues A_1, A_2, A_3…, 2) oligomerization, in particular dimerization, of A, and 3) hybridization with other biosynthetic constructs B, C, giving A–B–C. Centering attention to the type-II polyketide biosynthesis, intensive study will be carried out on the chemical synthesis of biologically active complex natural products.

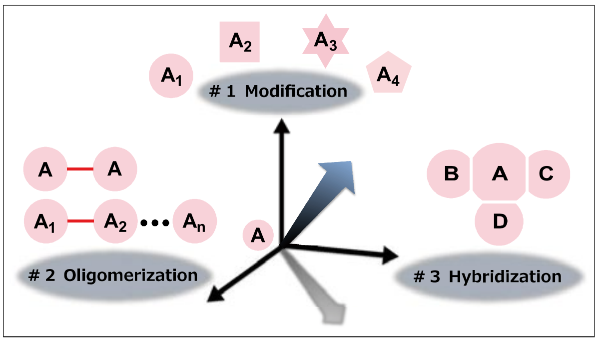

Fig.1 Structural diversity of natural products

【Expected Research Achievements and Scientific Significance】

This project will explore new synthetic strategies and tactics that will allow access to complex structures that are unavailable from natural source or through conventional organic synthetic methods.

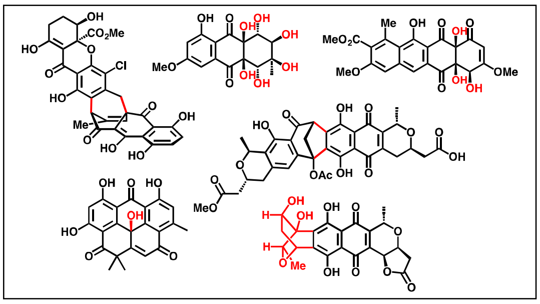

Fig 2. Selected synthetic targets

【Publications Relevant to the Project】

- "Total Synthesis of the Antibiotic BE-43472B", Y. Yamashita, Y. Hirano, A. Takada, H. Takikawa, K. Suzuki, *Angew. Chem. Int. Ed.* 2013, *52*, 6658–6661.
- "Synthesis and Determination of the Absolute Configuration of Cavicularin by a Symmetrization/Asymmetrization Approach", H. Takiguchi, K. Ohmori, K. Suzuki, *Angew. Chem. Int. Ed.* 2013, *52*, 10472–10476.
- "Synthesis of the Pluramycins 2: Total Synthesis and Structure Assignment of Saptomycin B, K. Kitamura, Y. Maezawa, Y. Ando, T. Matsumoto, K. Suzuki, *Angew. Chem. Int. Ed.* 2014, *53*, 1262–1265.

【Term of Project】 FY2016-2020

【Budget Allocation】 141,800 Thousand Yen

【Homepage Address and Other Contact Information】
http://www.chemistry.titech.ac.jp/~org_synth

Title of Project : New Organic Chemistry and Material Science of Curved π-Conjugated Molecules

Shigeru Yamago
(Kyoto University, Institute for Chemical Research, Professor)

Research Project Number : 16H06352 Researcher Number : 30222368
Research Area : Organic chemistry
Keyword : Synthetic organic chemistry, Supramolecular chemistry, Nano carbon materials

【Purpose and Background of the Research】

Cyclic π-conjugated molecules with a curved surface as exemplified in fullerenes or carbon nanotubes (CNTs) have attracted significant attention as an active component for organoelectronic and optoelectronic materials. However, the available structure of the carved π-conjugated molecules has been quite limited as the bulk synthesis relies on physical methods. Therefore, the development of a new, selective, and practical method for bottom-up organic synthesis of novel curved π-conjugated would have significant impact both for fundamental organic chemistry and material science.

In this research project, novel curved π-conjugated molecules will be designed and synthesized in order to utilize CPP derivatives for organoelectronic materials. Through the synthesis of new molecules including host-guest complexes of curved π-conjugated molecules and the analyses of physical properties, their applications to organoelectronic devices will be examined.

【Research Methods】

The followings are four representative research topics.

(1) **Synthesis**: By using both early- and late-stage functional group introductions, new π-extended and/or functionalized cyclic π-conjugated molecules will be synthesized.

(2) **Formation of π-layered structure**: Construction and functionalization of the hierarchically ordered structure consisted of the curved molecules will be investigated based on the host-guest interaction.

(3) **Evaluation of physical properties**: Physical properties of the excited and charged states of the molecules will be clarified by time-resolved spectroscopy and theoretical calculation.

(4) **Evaluation as electronic materials**: The correlation between molecular structure, aggregation structure and physical properties will be clarified by charge transport calculation, charge mobility measurement, and aggregate structure analysis.

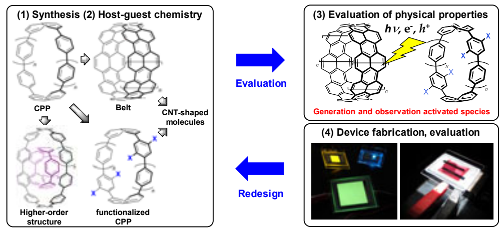

Figure 1. Main research topics

【Expected Research Achievements and Scientific Significance】

Synthesis of cyclic and curved π-conjugated molecules is a significant challenge in organic synthesis as the currently available methods are quite limited. This research will provide new curved conjugated molecules based on an innovative synthetic method and assembly by the host-guest chemistry. Furthermore, the potentials of the curved molecules for the active layer of organoelectronic devices will be clarified by the elucidation of physical properties. Through the research, a new field of organic chemistry and material science of curved π-conjugated molecules would be established.

【Publications Relevant to the Project】

"Organoplatinum-Mediated Synthesis of Cyclic π-Conjugated Molecules: Towards a New Era of Three-Dimensional Aromatic Compounds", S. Yamago, *et al. Chem. Rec.*, **14**, 84-100 (2014).

"Cycloparaphenylenes and carbon nanorings", S. Yamago, *et al. Polycyclic Arenes and Heteroarenes: Synthesis, Properties, and Applications*, Qian, M. Ed., John Wiley & Sons Ltd, Chichester, UK, **2015**, pp143-162.

【Term of Project】 FY2016-2020

【Budget Allocation】 145,600 Thousand Yen

【Homepage Address and Other Contact Information】

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Title of Project : Novel Energy and Information Conversions, Created by Solid-State Electrochemical Processes

Kunio Awaga
(Nagoya University, Graduate School of Science, Professor)

Research Project Number : 16H06353 Researcher Number : 20202772
Research Area : Materials Chemistry
Keyword : Electronic Functions, Surface and Interface, Solid State Electrochemistry

【Purpose and Background of the Research】

Development of novel information and energy conversions using ubiquitous materials and methods has attracted much attention. From this perspective, solid-state electrochemistry, which has innovated various rechargeable batteries and dye-sensitized solar cells, is receiving a new spotlight. In this project, we will develop novel energy and information conversions, by using the methodology of solid-state electrochemistry in organic electronics.

【Research Methods】

This project consists of three research themes.

Plan A. Bidirectional research between organic electronics and solid-state electrochemistry. We synthesize the porous compounds, such as metal-organic frameworks (MOFs) and covalent-bond frameworks (COFs), which possess structural robustness for ion doping/dedoping in electro-chemical processes. These materials are examined as cathode active materials for rechargeable Li batteries (Fig. 1). On the other hand, we try to establish novel molecular magnetism. Through the continuous valence control of the MOFs and COFs by means of electrochemistry, we realize new functions such as para-ferromagnetic switching.

Plan B. Electrochemical organic electronics. The electric double layers (EDLs) at solid-liquid interfaces can produce a huge electric field reaching to ~10^9 V/m. In this project, we make use of the EDLs in organic electronics and develop organic transistors and effective organic photocells. We develop the [Metal|Semiconductor|Insulator|-Metal] photocells, to effectively covert pulsed light into transient photocurrent, and to realize novel technology for energy and information conversions.

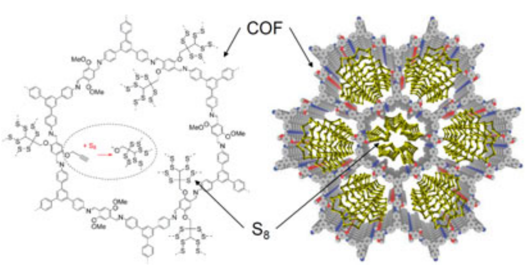

Fig. 1 Hybridization between COF and S_8, and its application to Li-S battery.

Plan C. Development of operando measurements and theory for solid-state electrochemical processes. To systematically conduct the research plans A and B, we work on various operando measurements under solid-state electrochemical reactions, such XAFS, XRD, solid-state NMR, and magnetic and electric measurements. We also improve the theoretical treatments for these processes, by combing molecular dynamics and molecular orbital calculations.

【Expected Research Achievements and Scientific Significance】

The expected research achievements are (i) high-energy-density molecule-based rechargeable batteries consisting of ubiquitous materials, (ii) electrochemically-controlled molecular magnets, and (iii) effective optoelectronic conversions using transient photocurrent. By exchanging the materials and methodology between solid-state electrochemistry and organic electronics, we would like establish a win-win relation between the two.

【Publications Relevant to the Project】

・"Discovery of a “Bipolar Charging” Mechanism in the Solid-State Electrochemical Process of a Flexible Metal–Organic Framework," Z. Zhang, H. Yoshikawa and K. Awaga, *Chem. Mater.*, 2016, **28**, 1298.
・"Organic optoelectronic interfaces with anomalous transient photocurrent", L. Hu, X. Liu, S. Dalgleish, M.M. Matsushita, H. Yoshikawa and K. Awaga, *J. Mater. Chem. C*, 2015, **3**, 5122.

【Term of Project】 FY2016-2020

【Budget Allocation】 143,000 Thousand Yen

【Homepage Address and Other Contact Information】

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Title of Project : Development of Functional Organosuperbase Catalysts Enabling Molecular Recognition

Masahiro Terada
(Tohoku University, Graduate School of Science, Professor)

Research Project Number : 16H06354 Researcher Number : 50217428
Research Area : Synthetic chemistry
Keyword : Asymmetric synthesis, Organocatalyst, Selective synthesis, Catalyst design/reaction, Reaction field

【Purpose and Background of the Research】

The development of advanced molecular transformations with considering environmentally friendly system has become significantly important subject in synthetic organic chemistry, a fundamental and important research field for manufacturing. Brønsted bases have been extensively employed for activation of reactants having an acidic proton. Most of these bases are metal salts derived form alkaline metals or alkaline earth metals. Whereas organobases were commonly utilized as a reagent for molecular transformations, however applicable transformations have been quite limited because of these less basicity. In recent years, intensive interest has been devoted to the development of organosuperbases. However these metal salts and organosuperbases were utilized under equimolar conditions, little attention has been paid to the catalytic use of these fascinating molecules. We focused on the utilization of these organosuperbase as a catalyst and the development of functional organosuperbase catalysts enabling molecular recognition, namely chiral organosuperbases. The purpose of this research is that the design and synthesis of chiral organosuperbases and its application to develop stereoselective transformations.

【Research Methods】

It is well known that phosphazenes exhibit higher order basicity when conjugate system was introduced to the iminophosphorane unit via an imino functionality. In our research proposal, we design and synthesis of organosuperbases, which enable molecular recognition, and apply these organosuperbase catalysts to develop efficient enantioselective transformations. In order to introduce efficient recognition system and strong basicity to the catalyst molecules, we designed the following type of molecular frameworks. To make the catalyst molecule having C_2 symmetry, we introduced phosphazene or guanidine units to both ends of the iminophosphorane core. The other approach is the introduction of acidic functionality as a hydrogen bond donor site to the fundamental organosuperbase framework resulting in the formation of bifunctional organosuperbase catalysts. We are planning to apply these organosuperbases to catalytic system which has never been established by using conventional organocatalysts. In addition, we also conduct the theoretical studies to elucidate the origin of the stereochemical outcome and catalytic cycles.

【Expected Research Achievements and Scientific Significance】

With the aim at initiating innovation to the industrial processes, we will establish unprecedent and remarkable catalytic activity, high selectivity, and construction of catalyst-recycling system.

【Publications Relevant to the Project】

- "Development of a Chiral Bis(guanidino)iminophosphorane as an Uncharged Organosuperbase for the Enantioselective Amination of Ketones" T. Takeda, M. Terada, *J. Am. Chem. Soc.*, **2013**, *135*, 15306-15309.
- "Enantioselective Addition of a 2-Alkoxycarbonyl-1,3-dithiane to Imines Catalyzed by a Bis(guanidino) iminophosphorane Organosuperbase" A. Kondoh, M. Oishi, T. Takeda, M. Terada, *Angew. Chem. Int. Ed.*, **2015**, *54*, 15836-15839.
- "Construction of Vicinal Quaternary Stereogenic Centers by Enantioselective Direct Mannich-Type Reaction Using a Chiral Bis(guanidino) iminophosphorane Catalyst" T. Takeda, A. Kondoh, M. Terada, *Angew. Chem. Int. Ed.*, **2016**, *55*, 4734-4737.

【Term of Project】 FY2016-2020

【Budget Allocation】 143,500 Thousand Yen

【Homepage Address and Other Contact Information】

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Title of Project : New polymer film processing based on the amplified conversion triggered from the free surface

Takahiro Seki
(Nagoya University, Graduate School of Engineering, Professor)

Research Project Number : 16H06355 Researcher Number : 40163084
Research Area : Functional polymer chemistry
Keyword : Free surface, polymer thin films, photoalignment, surface morphing, modeling

【Purpose and Background of the Research】

We have been conducting systematic explorations on the photoalignment and surface morphing of photoresponsive liquid crystalline polymer films. Very recently, we found that mesogens in liquid crystalline polymer films can be photoaligned by a surface skin layer of photoresponsive polymer. Alternatively, we also found that large mass transfer is induced on polymer films when another kind of polymer droplet is placed by inkjet printing followed by softening procedure via heating or light irradiation. Based on these new findings, a new project is constituted to create new technology of polymer film processing triggered from the free (air) surface.

【Research Methods】

The research method is constituted of two approaches based on 1) polymer chemistry and 2) polymer physics. 1) Polymer chemistry approach: Attempts will be made to switch the mesogen orientation reversibly by light using the surface skin layer. Mesogen orientations will also be controlled using small molecules at the free surface. 2) Polymer physics approach: Since no knowledge is obtained for the mass transfer process triggered by the hetero-interface, systematic accumulation of data changing the polymer properties is needed. At the same time, physics model will be considered to explain this phenomenon. Collaborations will be made with researchers at University of Hyogo, Tokyo University of Science, and National Composite Center of Nagoya University.

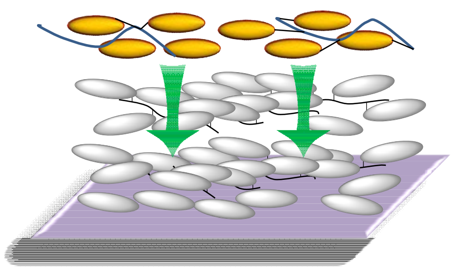


Figure 1 Liquid crystal control from the free surface.

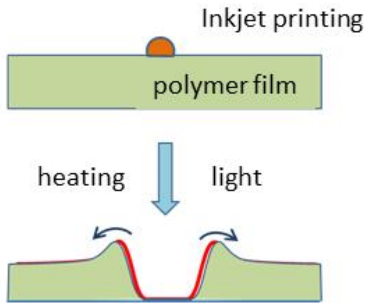


Figure 2 Mass transfer in polymer film triggered by another polymer deposited at the free surface

【Expected Research Achievements and Scientific Significance】

Numerous data have been accumulated for the material processing controlled from the nature of solid surfaces, however polymer processing utilizing the free surface has been hardly studied. The systematic research in this strategy is strongly needed. New proposals of new processing methods for polymer and liquid crystal thin film technologies are expected to be provided.

【Publications Relevant to the Project】

・K. Fukuhara, S. Nagano, M. Hara, T. Seki, Free-surface molecular command systems for photoalignment of liquid crystalline materials, *Nat. Commun.*, **5**, 3320 (2014).
・T. Nakai, D. Tanaka, M. Hara, S. Nagano, T. Seki, Free surface command layer for the photoswitchable out-of-plane alignment control in liquid crystalline polymer films, *Langmuir*, **32**, 909-914 (2016).

【Term of Project】 FY2016-2020

【Budget Allocation】 138,200 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.apchem.nagoya-u.ac.jp/06-BS-2/sekilabo/index.html

Title of Project : Regulation and mechanistic investigation of gene expression by artificial genetic switches

Hiroshi Sugiyama
(Kyoto University, Graduate School of Science, Professor)

Research Project Number : 16H06356 Researcher Number : 50183843
Research Area : Chemical Biology
Keyword : Gene Regulation, DNA nanostructure, Functional Py-Im polyamide conjugates

【Purpose and Background of the Research】

This study elucidates a mechanism of the epigenetic gene regulation by our original chemical biology approach.

Principally, for the somatic cell reprogramming and pluripotent stem cell differentiation, we supplement an epigenetic gene activation function to sequence-specific DNA-binding Py-Im polyamide. Successively, we establish a direct imaging technology to visualize key dynamic modifications in nucleosome structures corresponding to gene expression at a single molecule level.

Using these two distinct chemical biology approaches, we push forward the coordinating research like two wheels to elucidate the mechanism of epigenetic gene regulation and to progress the concept of artificial gene switch.

【Research Methods】

In our research, it is important to uncover molecular mechanism and dynamic structural changes associated with gene expression.

1) To develop functional Py-Im polyamide conjugates for inducing cell reprogramming from the human somatic cell through epigenetic gene regulation.
2) To develop functional Py-Im polyamide conjugates for precise epigenetically controlled human iPS cell differentiation.

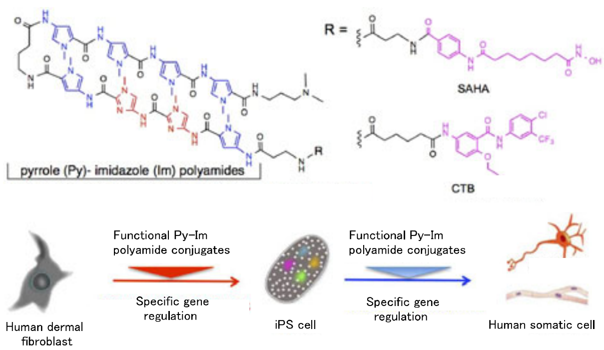


Figure 1. The structure and concept of functional Py-Im polyamide conjugates

3) To regulate gene expression by targeting molecules that alters G-quadruplex or triplex structures.
4) To visualize biological molecular motions and states by direct imaging technology using AFM.
5) To clarify the mechanism related to gene regulation by the analysis of nucleosome adaptations and related functions.

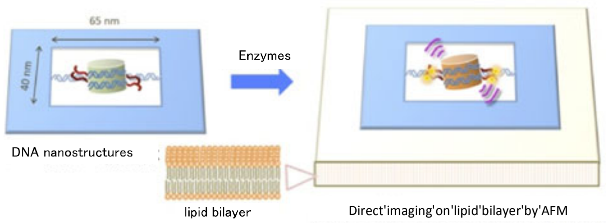


Figure 2. The concept of single molecular analysis of nucleosome using DNA nanostructures

【Expected Research Achievements and Scientific Significance】

Successful development of our coordinated approaches will lead to innovative therapy for refractory congenital gene diseases and cancer. Furthermore, we reveal mechanistic details of epigenetic control of gene expression using DNA nanostructure-based direct imaging technique, which in turn will advance this technology.

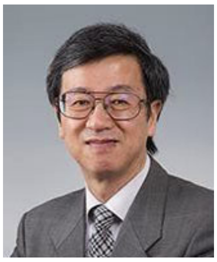
【Publications Relevant to the Project】

- Suzuki, Y.; Endo, M.; Sugiyama, H. *et al.*, *Nature Commun.*, 2015, *6*, 8052.
- Suzuki, Y.; Endo, M.; Sugiyama, H. *et al.*, *J. Am. Chem. Soc.* **2014**, *136*, 211-218.
- Pandian, G. N.; Taniguchi, J.; Sugiyama, H. *et al.*, *Sci. Rep.* **2014**, *4*, 3843.
- Han, L.; Pandian, G. N.; Sugiyama, H. *et al.*, *Angew. Chem. Int. Ed.* **2013**, *52*, 13410-13413.

【Term of Project】 FY2016-2020

【Budget Allocation】 133,700 Thousand Yen

【Homepage Address and Other Contact Information】
http://kuchem.kyoto-u.ac.jp/chembio/



Title of Project : Establishment of Scientific Basis of the Strength and Reliability of Materials Based on the Order of Atom Arrangement and Its Application to the Explication of the Degradation Process of Various Materials

Hideo Miura
(Tohoku University, Graduate school of Engineering, Professor)

Research Project Number : 16H06357 Researcher Number : 90361112
Research Area : Engineering
Keyword : Mechanics of Materials in Nano- and Micro-Scale

【Purpose and Background of the Research】

Initial strengthened micro textures of heat-resistant materials disappear due to the increase of operating temperature and mechanical stress for improving the thermal efficiency of various power and chemical plants. The purpose of this study is to develop the observation method of the change of the micro texture from the viewpoint of the order of atom arrangement. The degradation process of the quality of grains and grain boundaries is measured quantitatively in various materials and the strain-induced anisotropic diffusion of component elements is analyzed by applying molecular dynamics for clarifying the dominant factors of the degradation process at elevated temperatures.

【Research Methods】

The crystallinity of grains and grain boundaries was evaluated in this study by *IQ* (Image Quality) value obtained from EBSD (Electron Back-Scatter Diffraction) analysis. The amplitude of *IQ* value varies due to various damages such as vacancies, dislocations, impurities, local strain, and so on. Thus, this *IQ* value is effective for analyzing the grade of damage of atomic configuration, in other words, the order of atom arrangement. In addition, the strength of a grain and a grain boundary is measured separately by developing a micro test system in an electron microscope.

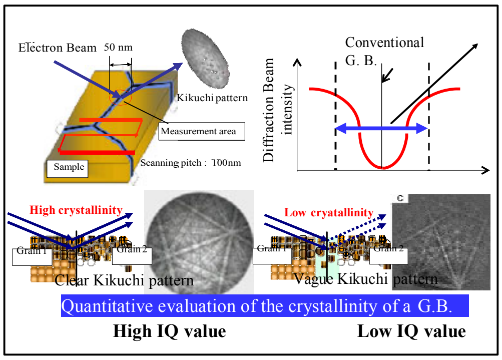


Fig. 1 Quantitative analysis of the crystallinity of a grain boundary

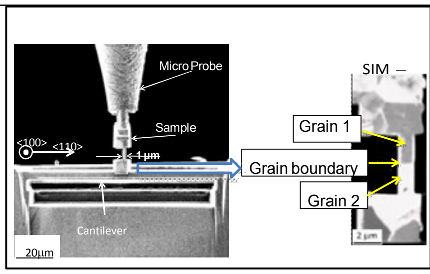


Fig. 2 Micro test system for measuring the strength of a grain and a grain boundary

【Expected Research Achievements and Scientific Significance】

The degree of disorder of atom arrangement caused by various defects such as vacancies, dislocations, the change of local composition, and so on is evaluated quantitatively. In particular, the stress-induced anisotropic diffusion of component element is validated as a dominant factor of the degradation and it is found that there is critical stress at which the accelerated diffusion starts to occur. This IQ is effective for evaluating the order of degradation of atom arrangement of various materials at elevated temperatures.

【Publications Relevant to the Project】

・N. Murata, N. Saito, K. Tamakawa, K. Suzuki, and H. Miura, J. of Electronic Packaging, vol. 137 (3), (2015), pp. 031001～031008.
・Suzuki, K., Murata, N., Saito, N., Furuya, R., Asai, O, and Miura H., Jap. J. of Applied Physics, vol. 52, (2013), pp. 04CB01-1～04CB01-8.

【Term of Project】 FY2016-2020

【Budget Allocation】 80,800 Thousand Yen

【Homepage Address and Other Contact Information】

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Title of Project : Development of zoom condenser system for X-ray free electron laser by high precision deformable reflective optics

Kazuto Yamauchi
(Osaka University, Graduate School of Science and Engineering, Professor)

Research Project Number : 16H06358 Researcher Number : 10174575
Research Area : Mechanical engineering
Keyword : Precision machining, Shape metrology, X-ray optics

【Purpose and Background of the Research】

X-ray focusing optics is highly demanded both in 3rd-generation synchrotron radiation (SR) sources and X-ray free-electron lasers. We are studying X-ray mirror devices based on precision metrology and fabrication process developments, and have established nanofocusing optics for cutting-edge SR beamlines. In these optical systems, an advanced function to adaptively change the beam size enables multiple analysis in X-ray microscopy.

In this research, we aim to realize a zoom condenser system consisting of two-stage Kirkpatrick-Baez (KB) mirrors with four precision deformable mirrors, which can work under diffraction-limited condition. In addition we are planning to provide adaptive focusing optical system with single stage KB mirrors to a SPring-8 beamline within 3 years to clarify the future problems as a milestone.

【Research Methods】

We try to realize mirror fabrication process to satisfy the Rayleigh's criterion, in which optical path difference due to the shape error of the mirror is smaller than $\lambda/4$ (λ: employed X-ray wavelength). For the adaptive shape control, we employ piezoelectric actuators with appropriate drift reduction method. In parallel, we develop an at-wavelength wavefront determination method to perform in-situ wavefront correction to maintain the diffraction-limited performance at any beam size.

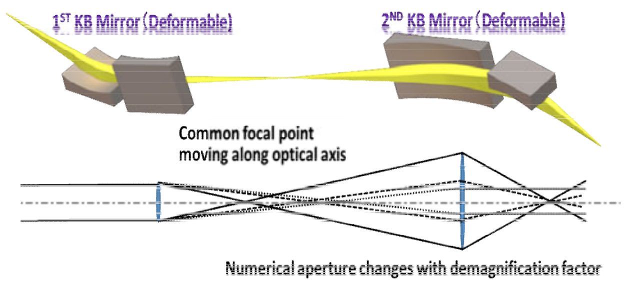

Fig. 1 Schematic drawing of zoom condenser system consisting of two-stage KB mirrors.

【Expected Research Achievements and Scientific Significance】

In coherent diffraction imaging which is one of the most important XFEL applications, the sizes of specimen and beam have significant relationship; beam size has to be nearly the same as the specimen size to maximize the photon density on it. So far, the specimen is selected mainly from the available beam size not from the scientific demand. The zoom condenser system can provide appropriate beam-size and can enhance the capability of XFEL.

Of course, the mirror figuring method plays significant roles for high precision manufacturing.

【Publications Relevant to the Project】

[1] S. Matsuyama, H. Nakamori, T. Goto, T. Kimura, K. P. Khakurel, Y. Kohmura, Y. Sano, M. Yabashi, T. Ishikawa, Y. Nishino K. Yamauchi, Nearly diffraction-limited X-ray focusing with variable-numerical-aperture focusing optical system based on four deformable mirrors, Scientific Reports 6, 24801 (2016)
[2] K. Yamauchi, M. Yabashi, H. Ohashi, T. Koyama, and T. Ishikawa, Nanofocusing of X-ray free-electron lasers by grazing-incidence reflective optics. Journal of Synchrotron Radiation, 22 (2015) 592-598
[3] H. Mimura, H. Yumoto, S. Matsuyama, T. Koyama, K. Tono, Y. Inubushi, T. Togashi, T. Sato, J. Kim, R. Fukui, Y. Sano, M. Yabashi, H. Ohashi, T. Ishikawa, and K. Yamauchi, Generation of 1020 W/cm2 Hard X-ray Laser Pulses with Two-Stage Reflective Focusing System, Nature Communications, 5 (2014) 3539

【Term of Project】 FY2016-2020

【Budget Allocation】 141,800 Thousand Yen

【Homepage Address and Other Contact Information】

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Title of Project : Photoelectric conversion system of spin-information utilizing semiconductor quantum dots

Akihiro Murayama
(Hokkaido University, Graduate School of Information Science and Technology, Professor)

Research Project Number : 16H06359 Researcher Number : 00333906
Research Area : Electronic materials/Electric materials
Keyword : Electronic materials (semiconductor, magnetic), Quantum structure, Fabrication method

【Purpose and Background of the Research】

Electrical injection of spin-polarized electrons from ferromagnetic metallic electrodes into III-V compound semiconductor quantum dots (QDs) will be studied, where QDs are used to fabricate optical active layers for photoelectric conversion of spin information. In QDs, electron-spin states can be conserved during an emission process, enabling us to transform spin information into circular polarization of light and vice versa.

We study spin-polarized light emitting diodes based on QDs by investigating ultrafast spin injection into the QDs and spin transport in semiconductor barriers. Optical resonators for efficient photoelectric conversion are fabricated along with circularly polarized stimulated emitters and spin-polarized photo-diodes using QDs.

The above research is aimed at establishing a technology base for photoelectric conversion of spin-information utilizing QDs [Fig. 1].

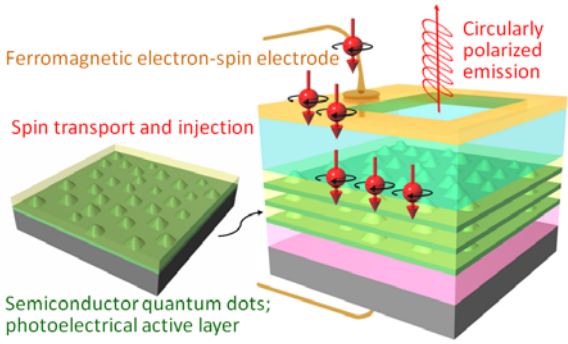

Figure 1 A schematic of photoelectric spin-conversion device utilizing QD active layers

【Research Methods】

We fabricate coupled QD structures with two-dimensional (2D) electron systems of quantum wells (QWs) and achieve efficient spin capture as well as ultrafast spin injection [Fig. 2]. Spin transport in semiconductor barriers is also studied. Quantum structures for room-temperature operation can be designed based on the temperature dependences of spin states and the relaxation in spin injection. Nanoscale optical resonators suitable for efficient photoelectric spin conversion are fabricated along with investigating the basic properties of circularly polarized stimulated emitters and spin-polarized photo-diodes using QD active layers.

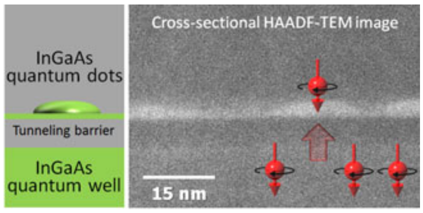

Figure 2 A QD structure coupled with a QW

【Expected Research Achievements and Scientific Significance】

Spin-polarized wavefunctions and the dynamics in QDs coupled with 2D electron systems, and subsequent energy relaxation are essential for spin injection into QDs, which will be an important achievement in material science. Photoelectric spin conversion at room temperature will facilitate future applications of semiconductor spintronics, which stays in a basic state of research to date.

【Publications Relevant to the Project】

・X.-j. Yang et al., "Ultrafast spin tunneling and injection in coupled nanostructures of InGaAs quantum dots and quantum well",
Applied Physics Letters **104**, 01240:1-4, 2014.
・T. Yamamura et al., "Growth-temperature dependence of optical spin-injection dynamics in self-assembled InGaAs quantum dots",
Journal of Applied Physics **116**, 094309:1-7, 2014.

【Term of Project】 FY2016-2020

【Budget Allocation】 142,500 Thousand Yen

【Homepage Address and Other Contact Information】

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Title of Project : Origin elucidation of problems in interface electric charge transportation phenomenon by using scanning nonlinear dielectric microscopies

Yasuo Cho
(Tohoku University, Research Institute of Electrical Communication, Professor)

Research Project Number : 16H06360 Researcher Number : 40179966
Research Area : Electrical and electronic engineering
Keyword : Scanning nonlinear dielectric microscopy, Interfacial electric charge transfer, Local DLTS

【Purpose and Background of the Research】

Interfacial charge transfer effects have been commonly and frequently used in great number of electronic devices including SiC-MOS devices. However, the interfacial (or channel) electron mobility of such devices has been much less than that expected from the theoretical values and this is their common problem now. Although this problem is the large obstacle for obtaining high performance next generation electronics devices, unfortunately, it has not been solved for a long time, yet. The main reason why the problem has been unsolved is that the origin of low interfacial charge mobility is unknown due to the lack of the local and nondestructive investigation methods for evaluating such interfaces.

To obtain such local and nondestructive method, we will newly develop several multifunctional and high performance scanning nonlinear dielectric microscopy (SNDM).

Using these SNDM, we will clarify the origin of several problems in interfacial charge transfer effects. Then, based on the obtained knowledge, we will achieve great improvement in the performance of electronics devices.

【Research Methods】

At first, we will newly develop several multifunctional and high performance SNDM. In particular, SNDM for local DLTS (Deep Level Transient Spectroscopy) method, scanning nonlinear dielectric para-magnetic resonance microscopy (SNDMR) will be newly developed. Moreover, we will make further advancement of the performance of recently developed scanning nonlinear dielectric potentiometry (SNDP), noncontact-scanning nonlinear dielectric microscopy (NC-SNDM) and super higher order scanning nonlinear dielectric microscopy (SHO-SNDM). Combining and using these high performance SNDM series, we will clarify the origin of the interface state density and scattering defects that degrade the channel carrier mobility by measuring and evaluating the interfaces employed in targeting devices.

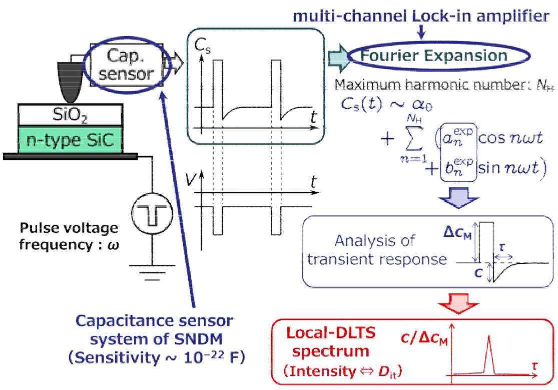

Figure1 Principle of proposed local DLTS method

【Expected Research Achievements and Scientific Significance】

We will clarify the origin of several problems in interfacial charge transfer effects. Then, based on the obtained knowledge, we will achieve great improvement in the performance of electronics devices by feed backing the obtained knowledge about the origin of degradation of interface qualities to the fabrication processes. Thus, we will be able to fabricate new high performance device with quite high channel electron (career) mobility.

【Publications Relevant to the Project】

K. Yamasue and Y. Cho, Rev. of Scientific Instrum., Vol.86 (2015) pp. 093704-1-8
N. Chinone, T.Nakamura and Y. Cho, “J. Appl. Phys., Vol.116 (2014) pp.084509-1-7.

【Term of Project】 FY2016-2020

【Budget Allocation】 149,700 Thousand Yen

【Homepage Address and Other Contact Information】

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Title of Project : Creation of 2D-Atomically-Thin-Layered Hetero-junctions and their Applications to Novel Terahertz Photonic Devices

Taiichi Otsuji
(Tohoku University, Research Institute of Electrical Communication, Professor)

Research Project Number : 16H06361 Researcher Number : 40315172
Research Area : Engineering, Interdisciplinary Science and Engineering
Keyword : Electron device, Quantum device, Millimeter and terahertz waves, Graphene, Nanophysics

【Purpose and Background of the Research】

Terahertz (THz) is an unexplored electromagnetic frequency band in which conventional electronic and photonic devices cannot operate well due to the substantial physical limitations originating from the transit time delays and/or phonon decoherence. In such a situation, graphene, a carbon atomic monolayer sheet, has attracted attention thanks to its extremely high carrier transport properties of relativistic Dirac Fermions. Recently, study on atomically-thin van der Waals (vdW) heterostructures consisting of graphene, h-BN, and/or transition-metal dichalcogenide (TMD) like MoS_2 has been emerging. We theoretically found that a gated double-graphene-layered (G-DGL) heterostructure can mediate THz photon- and plasmon-assisted resonant tunneling between the GLs, enabling various functionalities in the THz domain with extremely higher quantum efficiencies by orders than ever. The key to make them in practical engineering is to develop the continuous hetero-epitaxial growth (C-H-Epi-G) technology.

This research is aimed to create the C-H-Epi-G technology for the 2D vdW heterojunction systems, and to devise highly efficient various THz functional devices by exploiting unprecedented physical phenomena exhibited among their complex quantum systems governed by electrons, photons, plasmons, as well as phonons (Fig. 1).

【Research Methods】

First, the G-DGL structure consisting of the DGL core shell and the external gate is created as the platform of device implementation. Second, the photon-assisted and plasmon-assisted resonant tunneling are introduced into the G-DGL as the physical operation mechanisms to manifest the advantage of the performances of THz amplification, oscillation, detection, and nonlinear wave control over the existing technologies. Third, the double resonance of the graphene plasmons and the tunneling is introduced as an advanced physical operation mechanism to obtain further improved performances of these functionalities (Fig. 2).

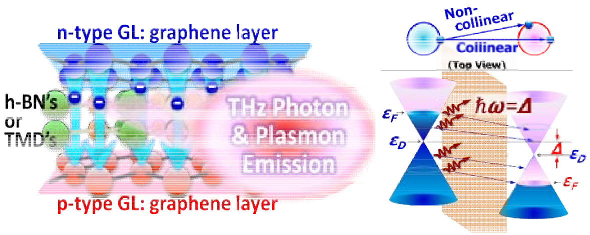

Fig. 2 Photon- and plasmon-assisted resonant tunneling in the G-DGLs for THz emitters.

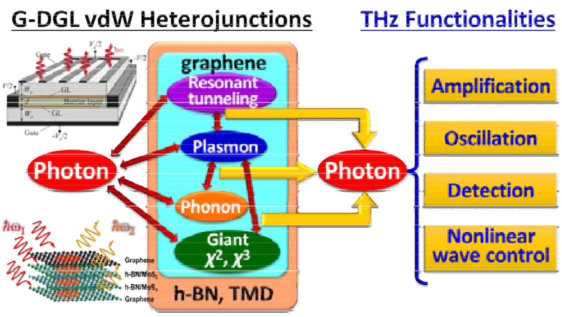

Fig. 1 Nonlinear complex quantum phenomena in G-DGL vdW heterojunctions and their applications to THz functional devices.

【Expected Research Achievements and Scientific Significance】

Introduction of unprecedented physical mechanisms of complex quantum systems in the G-DGL is unique and has a great merit and impact to enable ultra-highly efficient THz functionalities.

If successful this study, 100-Gbit/s-class ultra-fast THz wireless communications, such as Trans-fer-Jet that can transfer ultra-high-capacity media instantly, is expected to bring industrial revolution to the future of ubiquitous ICT societies.

【Publications Relevant to the Project】

・T. Otsuji et al., “Active graphene plasmonics for terahertz device applications,” **J. Phys. D 47**, 094006 (2014).
・V. Ryzhii et al., "Double-graphene-layer terahertz laser," **Opt. Exp. 21**, 31569-31579 (2013).

【Term of Project】 FY2016-2020

【Budget Allocation】 144,600 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.otsuji.riec.tohoku.ac.jp

Title of Project : Innovative Water Treatment System Combining Pretreatments and Membrane Separation for Sustainable Supply of Safe High-quality Water

Yoshihiko Matsui
(Hokkaido University, Faculty of Engineering, Professor)

Research Project Number : 16H06362 Researcher Number : 00173790
Research Area : Engineering, Civil and Environmental Engineering
Keyword : Water and Wastewater Systems

【Purpose and Background of the Research】

To address water-related issues, a need is recognized for advanced water-supply technologies that would allow safe and secure use of even low-quality water resources at a reduced cost and with greater energy efficiency and could be managed and maintained simply. Toward this, we apply superfine adsorbent particles produced with a nano-milling technology and pore surface control; metastable regions of polyvalent metal salts to polymer technologies, thereby improving coagulation performance; vacuum ultraviolet (VUV) light-accelerated oxidation. We combine these and membrane separation, and develop innovative water treatment system, which offers high separation and decomposition capabilities.

【Research Methods】

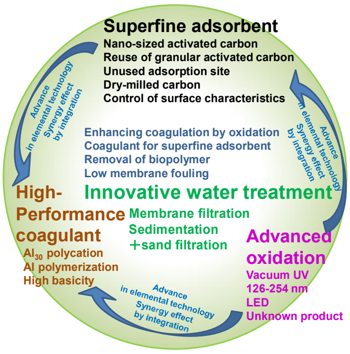

Fig. 1 Research plan.

We start with examining elemental technology of adsorption, coagulation and oxidation, and develop prototype materials and equipment and then apply a variety of assessment methods, including direct measurement and model estimations, to evaluate the basic characteristics of these materials and equipment. Further, we consider synergistic effects from their combinations.

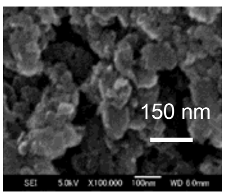

Fig. 2 Superfine powdered activated carbon.

1) We attempt the production of super-fine particles of activated carbon by milling and consider the agglomeration properties and change in adsorption capacity, along with the potential for reuse of spent granular activated carbon. 2) By optimizing production conditions such as reaction temperatures, we produce ultra-high basicity coagulants that better removes, arsenic, viruses, and bio-polymers that lead to membrane fouling. 3) Applying VUV light of various wavelengths accelerates the OH radical oxidation reaction, allowing investigation of non-biodegradable substance decomposition and the impact on coagulation improvement. 4) We investigate the affinity of superfine powdered activated carbon (SPAC) and ultra-high basicity flocculants to membrane, as well as their residual features, for application to the development of membrane separation and sedimentation with sand filtration.

【Expected Research Achievements and Scientific Significance】

The combination of membrane separation with SPAC, ultra-high basicity coagulant, VUV-accelerated oxidation, and their component technologies will bring about innovation to the separation and reaction process. This will produce innovative water purification systems that can be applied to low-quality water resources, at low cost and with little energy. This represents a significant contribution toward a stable supply of water that is safe for consumption and daily use.

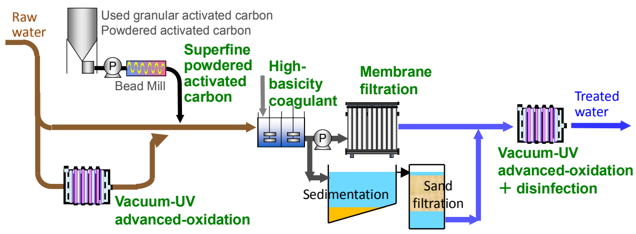

Fig. 3 Combined use of superfine powdered activated carbon, high-basicity coagulant, vacuum-UV advanced-oxidation and membrane filtration.

【Publications Relevant to the Project】

・Kimura, M., et al, N., Minimizing residual aluminum concentration in treated water by tailoring properties of polyaluminum coagulants, Water Research, 47(6), 2075-2084, 2013.
・Matsui, Y., et al., Characteristics of competitive adsorption between 2-methylisoborneol and natural organic matter on superfine and conventionally sized powdered activated carbons, Water Research, 46(15), 4741-4749, 2012.

【Term of Project】 FY2016-2020

【Budget Allocation】 100,800 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.eng.hokudai.ac.jp/labo/risk/

【Grant-in-Aid for Scientific Research (S)】
Science and Engineering (Engineering)

Title of Project : Development of Preservation/Renovation Techniques for Seismic Performance Improvement and Authenticity of Historical Buildings

Takayoshi Aoki
(Nagoya City University, Graduate School of Design and Architecture, Professor)

Research Project Number : 16H06363 Researcher Number : 10202467
Research Area : Architecture, Building structures/Materials, Architectural history/environment
Keyword : Historical buildings, authenticity, seismic performance, Preservation/Renovation technique

【Purpose and Background of the Research】

Large-scale earthquakes occur frequently, and many historical buildings including the cultural heritages were severely damaged. Although repair and reinforcement become an urgent need, effective methods have not been established, and these have to be conducted individually. This research program is to develop novel techniques for diagnosis, repair and reinforcement of historical buildings by verifying the integrated knowledge developed in the world. In addition, this research aims to present guidelines for the preservation of cultural and modernization heritages, and to develop techniques to enhance their earthquake resistance capacity and durability in consideration of the authenticity.

Airship hangar (1917)

Handa red brick (1898)

【Research Methods】

1) Extract the problems from the existing examples of investigation, diagnosis, repair and reinforcement conducted to historical buildings.
2) Clarify the problems related to investigation, diagnosis, repair and reinforcement methods from the investigation studies on historical buildings.
3) Based on 1) and 2), evaluate the durability improvement and reinforcement technique from the viewpoint of reinforcing effect, construction precision, landscape, durability, extent of injury, authenticity, reversibility, economics and so on.
4) Evaluate effectiveness and scope of non-, minor- and destructive testing methods such as optical measurement, drilling, flat jack, microtremor measurement and monitoring and so on.
5) Clarify material deterioration especially caused by salt deposition from measurement of environment, moisture state, and analysis of salt.
6) Clarify degradation mechanisms and prediction of materials, and propose an effective repair method based on the exposure test and accelerated weathering test, using deterioration suppressing materials and surface protection measure.
7) Verify the repair and reinforcement effect by monitoring.
8) Based on the above investigations, develop repair material and reinforcement method, and present the guidelines.

【Expected Research Achievements and Scientific Significance】

Preservation/renovation techniques developed in this research will be a useful guide in the maintenance and repair of historical buildings to preserve them for future generation. In addition, research results are applicable to RC infrastructure and building stock. Furthermore, the evaluation of PML (probable maximum loss) and development of BCP (Business Continuity Plan) expect an incentive toward “preventive maintenance” measures from “ex-post measures” technique of historical buildings.

【Publications Relevant to the Project】

・D. Sabia, T. Aoki, R. Cosentini, R. Lancellotta, Model Updating to Forecast the Dynamic Behavior of the Ghirlandina Tower in Modena, Italy, Journal of Earthquake Engineering, Vol.19, Issue 1, pp.1-24, 2015.
・T. Aoki, N. Yuasa, H. Hamasaki, Y. Nakano, N. Takahashi, Y. Tanigawa, T. Komiyama, et al, Safety Assessment of the Sanctuary of Vicoforte, Italy, Journal of Materials and Structural Integrity, Vol.5, No.2/3, pp.215-240, 2011.

【Term of Project】 FY2016-2020

【Budget Allocation】 136,300 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.sda.nagoya-cu.ac.jp/aoki/

Title of Project : Infrared Energy Harvester by Artificially Structured Heterojunction

Tadaaki Nagao
(National Institute for Materials Science, International Center for Materials Nanoarchitectonics, Group Leader)

Research Project Number : 16H06364 Researcher Number : 40267456
Research Area : Materials Engineering
Keyword : Infrared Light, Thermal Radiation, Physical Properties, Optical Nanomaterials

【Purpose and Background of the Research】

All the objects on earth have thermal energy and thus emit or absorb infrared light to exchange mutually their thermal energy. If the spectrum of thermal radiation and absorption is flexibly controlled by adopting artificial surface nanostructures, many devices for the energy application will be realized. For example, single-band infrared light emitters, material-specific infrared sensors, and energy harvesting device that collect thermal radiation from the environment as well as waste heat in industry and houses will be realized and contribute to the developments of sensors, energy conservation and low carbon emission.

In this project, we focus ourselves on the phenomena related to the thermal properties of matter such as phonons, localized infrared plasmons, as well as low-energy electronic excitations to clarify the energy transfer among them and establish the guiding principles for developing the heterojunctions or infrared resonators with artificially enhanced energy conversion efficiency. For example, we will develop the methodology for designing and fabricating metal-semiconductor heterojunction combined with polaritonic resonator with optimized energy conversion efficiency between the phonon excitation and electronic excitation, which will enable us to collect or emit infrared light with high efficiency and further convert it to other types of energies. By appropriately designing and combining semiconductors with elemental or compound materials with excellent infrared absorption, optimization of energy transfer between infrared plasmon polariton, low-energy electronic excitations and phonons will be achieved.

【Research Methods】

By designing appropriately the nanoscale and mesoscale structures, thermal absorption and emission of the objects can be modified largely from those of the blackbody. We will characterize the generation, absorption, propagation, and damping of these artificial structures by our spectroscopic techniques such as photoluminescence spectroscopy, ultrafast spectroscopy, infrared microscopy, and scanning near-field microscopy. The knowledge will be adopted for establishing the methodology for realizing the high-efficiency transduction of infrared radiation to the electrical or near-infrared energy and thus leading to the development of high-sensitivity sensors and energy harvesting system.

【Expected Research Achievements and Scientific Significance】

The understanding for the mechanism of the energy conversion between electricity, heat, and thermal radiation at the surface/interface of materials will be deepened and new knowledge will be accumulated. The methodology for artificially controlling these energy conversion processes will be established, and will lead us to the realization of environmental energy harvesting devices and self-powered sensor networks.

【Publications Relevant to the Project】

- S. Ishii, S.R. Pasupathi, T. Nagao, “Titanium Nitride Nanoparticle as Plasmonic Solar Heat Transducers,” J. Phys. Chem. C **120**[4], 2343-2348 (2016).
- T. Dao, K. Chen, S. Ishii, A. Ohi, T. Nabatame, M. Kitajima, and T. Nagao, “Infrared perfect absorbers fabricated by colloidal mask etching of Al-Al2O3-Al trilayers,” ACS Photonics **2**, 964-970 (2015).
- K. Chen, T. Dao, S. Ishii, M. Aono, and T. Nagao, “Infrared aluminum metamaterial perfect absorbers for plasmon-enhanced infrared spectroscopy,” Advanced Functional Materials **42**, 6637-6643(2015)

【Term of Project】 FY2016-2020

【Budget Allocation】 141,400 Thousand Yen

【Homepage Address and Other Contact Information】
http://samurai.nims.go.jp/NAGAO_Tadaaki-j.html
NAGAO.Tadaaki@nims.go.jp

Title of Project : Research on supreme fatigue property in steel: importance of microstructurally-small fatigue crack

Kaneaki Tsuzaki
(Kyushu University, Graduate School of Engineering, Professor)

Research Project Number : 16H06365 Researcher Number : 40179990
Research Area : Structural and functional materials
Keyword : fatigue, fatigue crack arresting, strain aging, martensitic transformation, steel

【Purpose and Background of the Research】

Fatigue is one of most prevalent and historical causes of failure that affects all metals and alloys. Developing materials with strong resistance to fatigue is a critical challenge for our society, since fatigue failure severely restricts the long-term and safe application of advanced structural materials in various fields such as energy conversion, fusion power, light weight mobility, fuel cells and hydrogen-based industry cycles.

Recently, we have proposed two high strength materials with supreme fatigue properties: (1) precipitation-hardened aluminum alloy with distinct fatigue limit; (2) austenitic steel with superior low-cycle fatigue life.

It is well known that the fatigue limit of carbon steels is not the critical stress for crack nucleation but for crack propagation. It means that when a fatigue crack is nucleated, it can be stopped during further fatigue stress cycling at a relatively low stress level. In these circumstances, it is found in the case of material (1) that matrix strengthening near the crack tip is a key of appearance of the fatigue limit and atomic diffusion of a particular element affects the strengthening.

Low-cycle fatigue is a type of fatigue phenomenon where a large stress/strain is applied so that the number of cycles to failure (fatigue life) becomes less than 10,000 cycles. Typically, the fatigue life is reported to be around 2,000 cycles at a total strain range of 2 %. In contrast, we have achieved fatigue life of more than 10,000 cycles for material (2) where martensitic transformation from FCC to HCP occurs around a crack tip.

These new findings strongly encourage us to research and find a new design concept for material development with strong resistance to fatigue. In this research project, we make challenge to build up a new concept to develop advanced steels with supreme fatigue properties based on our new findings.

【Research Methods】

In the first half term of the project, FY2016 and 2017, the mechanisms contributing to the supreme fatigue properties of the materials (1) and (2) will be investigated in details. Atomic diffusion causing matrix hardening called dynamic strain aging and shear type transformation allowing reversible deformation to take place dynamically around a crack tip during fatigue would be essential for the mechanisms.

In the second half term, FY2018 to FY2020, we will attempt to apply our obtained knowledge of mechanisms to the development of new steels: (a) austenitic stainless steels with high fatigue limit; (b) austenitic steel without deterioration of fatigue life even under hydrogen circumstance. Additionally, a new but fundamental research field called ‘microstructurally-small fatigue crack’ will be established.

【Expected Research Achievements and Scientific Significance】

Fatigue-resistant steel as well as hydrogen-resistant steel is a new type of steel which will be appreciated by society, i.e., hydrogen-based industry cycles. The fatigue crack propagation mechanism, especially for so-called microstructurally-small crack, with dynamic phenomenon of diffusion and transformation will give us a new fundamental research field of mechanical engineering and materials science.

【Publications Relevant to the Project】

Yun-Byum Ju, Motomichi Koyama, Takahiro Sawaguchi, Kaneaki Tsuzaki, Hiroshi Noguchi : “In situ microscopic observations of low-cycle fatigue-crack propagation in high-Mn austenitic alloys with deformation-induced ε-martensitic transformation”, *Acta Materialia*, **112** (2016), 326-336.

【Term of Project】 FY2016-2020

【Budget Allocation】 151,000 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.mech.kyushu-u.ac.jp/~force/

Title of Project : Breakthrough toward "second-generation" grain boundar engineering

Sadahiro Tsurekawa
(Kumamoto University, Faculty of Advanced Science and Technology, Professor)

Research Project Number : 16H06366 Researcher Number : 40227484
Research Area : Materials Science and Engineering
Keyword : Microstructural control, grain boundary, dislocation

【Purpose and Background of the Research】

Bulk properties of polycrystalline materials are significantly affected by grain boundaries. Tadao Watanabe has proposed the concept of grain boundary engineering for providing desirable properties of polycrystalline materials" in 1983 / 1984 on the basis of the structure-dependent grain boundary properties, which is nowadays known to be useful for achieving enhanced bulk properties like creep resistance and corrosion resistance (Fig. 1). As mentioned above, "first generation" grain boundary engineering achieved certain results. However, there still remain some issues to be settled for further establishment of grain boundary engineering: *e.g.*, grain boundary engineering is not commonly applied to the materials with a high stacking fault energy.

Motivation of this project is to achieve a breakthrough toward "second generation" grain boundary engineering. We will deal with two major issues as follows:

<u>Issue 1</u>: Comprehensive understanding of grain boundary phenomena to strengthen fundamental base of grain boundary engineering

- Local mechanical properties near the grain boundary – Understanding Hall-Petch relation on the basis of the interaction between grain boundary and dislocations.
- Structure and properties of non-equilibrium grain boundaries

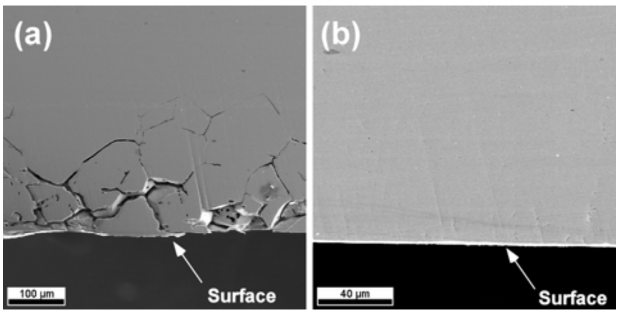

Fig.1 Effect of grain boundary control on corrosion in austenitic stainless steel (SUS304): (a) Conventionally processed, (b) grain boundary engineered. (S.Tsurekawa *et al.*, Acta Mater., 54,3617, (2006).)

<u>Issue 2</u>: Guiding principle for grain boundary control of materials with high stacking fault energy

【Research Methods】

(1) Orientation controlled bicrystals are used for nanoindentation tests to study the local mechanical properties near the grain boundaries, and for *in-situ* deformation / observation in TEM to examine the relation between the dislocation motion and mechanical response.
(2) Quantitative evaluation of grain boundary microstructure using the fractal and percolation theory.

【Expected Research Achievements and Scientific Significance】

The achievements of this study make it possible to apply the grain boundary engineering to a wide-rang of materials, and would promote an innovation for development of new advanced materials based on grain boundary functions. In addition, we propose a new elements strategy because grain boundary engineering can achieve enhanced properties even for conventional materials without using further allying elements.

【Publications Relevant to the Project】

- T. Watanabe, S. Tsurekawa, The Control of Brittleness and Development of Desirable Mechanical Properties in Polycrystalline Systems by Grain Boundary Engineering, Acta Mater., 47, 4171–4185, 1999.
- S. Tsurekawa, Y. Chihara, K. Tashima, P. Lejček, Local plastic deformation in the vicinity of grain boundaries in Fe-3 mass% Si alloy bicrystals and tricrystal, J. Mater. Sci., 49, 4698 – 4704, 2014.

【Term of Project】 FY2016-2020

【Budget Allocation】 137,900 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.msre.kumamoto-u.ac.jp/~mice/
turekawa@kumamoto-u.ac.jp

Title of Project : Fabrication of fluidic ceramics with supercritical fluid technology toward dynamic thermal management

Tadasumi Adschiri
(Tohoku University, WPI-AIMR, Professor)

Research Project Number : 16H06367 Researcher Number : 60182995
Research Area : Engineering
Keyword : supercritical fluid, nano fluid, thermal management

【Purpose and Background of the Research】

Recently many methods have been developed for producing nanoparticles. However, the application based on the nanoparticles has not yet appeared. One of the main reason is the difficulty in controlling dispersibility of nanoparticles in organic solvents, or in polymers. Supercritical hydrothermal synthesis, which Adschiri had developed, enables synthesis of nanoparticles covered by organic molecules with high concentration. Since the surface is just like organic molecules, the nanoparticles shows high affinity to polymers. In addition, by tuning the particle size distribution properly, the hybrid nano-polymers (80 vol%) that shows fluidity could be fabricated ("fluidic ceramics"). This technology opened a door toward new hybrid materials. Many companies have started R&D for developing nano hybrid materials. However, the science for the fluidic ceramics had not yet been established.

The aim of this study is 1) to elucidate the mechanism of this fluidity of the hybrid materials, and establish the method to design the fluidic ceramics, and 2) to develop a high performance "thermal management materials".

【Research Methods】

1) Elucidation of the mechanism of organic modification on nanoparticles by using radiation analyses.
2) Estimation of phase behavior of nanoparticulate systems by combining computer science and chemical engineering thermodynamics. PVT of nanoparticles are measured, from which particle-particle interactions will be estimated. The interaction parameters thus evaluated will be used to predict the phase behavior of the nanoparticulate systesm.
3) Mathematic analysis (Persistent Homology) is introduced to describe the disordered structure of nanoparticles. This expression will be used to correlate the structure and fluidity (viscosity) of the fluidic cermaics.
4) A thermal management materials, namely fluidic ceramics with high heat conductivity, is designed, based on the above elucidated mechanisms. The nanoparticles modified with optimized molecules will be synthesized by the supercritical hydrothermal reactor.

【Expected Research Achievements and Scientific Significance】

1) A new science of rheology based on the relation between disordered structure and fluidity.
2) A designing method to design the organic modified nanoparticles, which shows high fluidity.
3) A method to describe disordered structure of nano particulate systems with the Persistent Homology.
4) Fabrication of a high performance "thermal management materials":
 a) New materials that shows high fluidity and high thermal conductivity.
 b) Transparent flexible nano-composit films with which the transmittance/reflection of light can be manipulated with the temperatures.

【Publications Relevant to the Project】

・ Byrappa K, T.Adschiri, "Hydrothermal technology for nanotechnology", Progress in Crystal Growth and Characterization of Materials, 53 117-166 (2007)
・ J.Zhang, S.Ohara, M.Umetsu, T.Naka, Y.Hatakeyama, T.Adschiri, "Colloidal ceria nanocrystals tailor-made crystal morphology in supercritical water" , Adv. Mater., 19, 203-206 (2007)

【Term of Project】 FY2016-2020

【Budget Allocation】 140,700 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.wpi-aimr.tohoku.ac.jp/ajiri_labo/english/index.html
ajiri@tagen.tohoku.ac.jp

Title of Project : Creating Soft-Batteries by Simple and Rapid Processes and Innovating Capacity by Reversible Structure Change

Suguru Noda
(Waseda University, School of Advanced Science and Engineering, Professor)

Research Project Number : 16H06368 Researcher Number : 50312997
Research Area : Engineering
Keyword : materials processes, secondary batteries, carbon nanotubes, three-dimensional interfaces

【Purpose and Background of the Research】

Electric energy storage has increasing demands for portable devices, vehicles, emergency power sources and renewable power. Batteries are currently made by coating active materials on metallic foils with conductive fillers and binders. These non-capacitive components account for significant mass fractions of current batteries. Mass and cost of batteries will be minimized if electrodes are built on stable separators with minimal use of such components.
We premise volume change of high-capacity materials and create porous/sponge electrodes with conserved/reversibly changing volumes using light-weight, flexible and conductive carbon nanotubes (CNTs). A chemical engineer leads the project with electrochemists to realize batteries with innovative capacity via simple, rapid, and high-yield production processes.

【Research Methods】

High capacity materials degrade due to volume change during charge-discharge. Huge energy and power densities have been reported for various nanostructures, however for impractically thin layers neglecting heavy and thick metal foils. Thick electrodes need to be produced by simple processes from inexpensive sources quickly at high yields.
We have realized several μm thick, gradient, porous Si-Cu films with excellent anode performance in 1 min by rapid vapor deposition (RVD) (Fig. 1). We will create three-dimensional current collectors of metal foils with directly connected CNTs and realize porous electrodes with conserved volume.
We have realized semi-continuous production of >100 μm-long, >99 wt%-pure few-wall CNTs in 0.3 s residence time at 70% yield by fluidized bed. Such CNTs form light-weight, flexible, sponge-like films via dispersion-filtration without any binders (Fig. 2). We will capture capacitive materials within them and create light-weight, practically thick sponge electrodes with reversibly changing volume.
Finally, soft batteries with innovative capacity will be developed by combining these porous/sponge electrodes with separators/electrolytes.

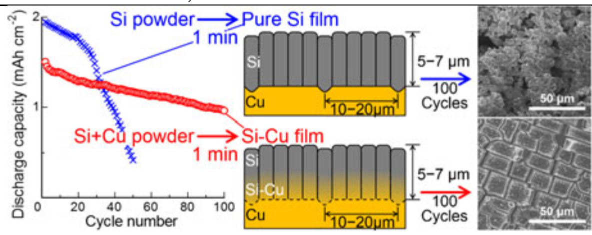

Fig. 1. Porous and gradient Si-Cu anodes by RVD.

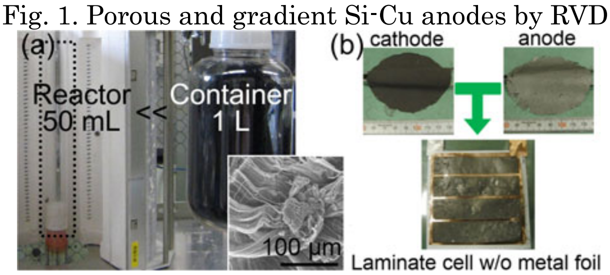

Fig. 2. Production of long CNTs for batteries.

【Expected Research Achievements and Scientific Significance】

Novel design with practical production process will realize soft batteries with innovative capacity at low cost. Porous/sponge electrodes will be applied to and improve current batteries.

【Publications Relevant to the Project】

・D.Y. Kim, H. Sugime, K. Hasegawa, T. Osawa, and S. Noda*, "Sub-millimeter-long carbon nanotubes repeatedly grown on and separated from ceramic beads in a single fluidized bed reactor," Carbon **49**(6), 1972–1979 (2011).
・K. Hasegawa and S. Noda*, "Lithium ion batteries made of electrodes with 99 wt% active materials and 1 wt% carbon nanotubes without binder or metal foils," J. Power Sources **321**, 155–162 (2016).

【Term of Project】 FY2016-2020

【Budget Allocation】 142,900 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.f.waseda.jp/noda/

【Grant-in-Aid for Scientific Research(S)】
Science and Engineering (Engineering)

Title of Project : Creation of Transdermal Drug Delivery Systems Using Solid-in-oil Nano-dispersion Technique

Masahiro Goto
(Kyushu University, Graduate School of Engineering, Professor)

Research Project Number : 16H06369 Researcher Number : 10211921
Research Area : Process engineering, Biochemical engineering
Keyword : Drug delivery system(DDS)

【Purpose and Background of the Research】

Transcutaneous immunization is a novel vaccination strategy that delivers the vaccine antigens into the intact skin topically to induce protective immune responses. Needle-free vaccination approach has a global priority due to the risk-reduction of needle prone accidents and the injection-related pain or angst. Since a transcutaneous vaccination is a simple and non-invasive procedure, it provides a viable, easy and cost-effective strategy for disease prevention not only in the advanced countries but also in the developing countries. Therefore, transcutaneous immunization might be the best-accepted vaccination method by all patients. In this study, we challenge to apply our S/O nano dispersion technique to transcutaneous immunization in order to enhance the penetration of antigenic proteins and increase the antigen-specific and robust immune responses.

【Research Methods】

Figure 1 shows the transdermal immunization mechanism in this study. There are three important steps to construct an effective immunization system.

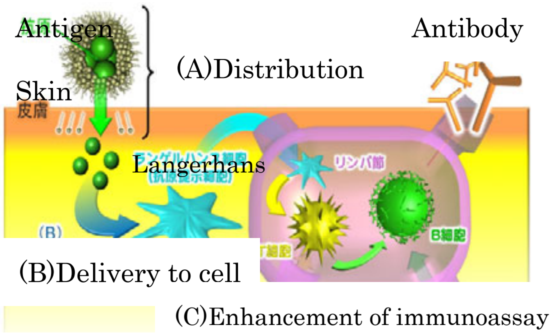

Figure 1 Immunization mechanism in this study

(A) Distribution of antigen to the skin
(B) Transfer of antigen to Langerhans cells
(C) Enhancement of immune assay

The surfactant-antigen complexes in which antigen proteins are coated with hydrophobic surfactant molecules can be dispersed in an oil of interest, and the nanodispersion of the surfactant -protein complex in the oil phase as a nano-order particle makes the proteins permeable into the skin without any physical enhancements or pre-treatments if a suitable oil with the properties of a chemical penetration enhancer is selected. An adjuvant also will be effective for enhancing the immunization in the step (3). In this study, we are focused on the development of transcutaneous cancer and pollen vaccines using S/O technology.

【Expected Research Achievements and Scientific Significance】

The transcutaneous immunization by S/O nanodispersion is able to enhance the antigen -specific antibody creation without any destruction or removal of the surface of skin. The vaccine formulation comprises the safe-to-use materials such as the edible sugar ester surfactant and penetration enhancer oil. These findings indicate that this oil-based transcutaneous approach has a great promise for constructing effective vaccination or immunotherapy. It will contribute the paradigm shift from medical care to prevention.

【Publications Relevant to the Project】

・ Y. Hirakawa, R. Wakabayashi, A. Naritomi, N. Kamiya, M. Goto, 'Transcutaneous immunization against cancer using solid-in-oil nanodispersions' *Med. Chem. Commun.*, 6, 1387-1392 (2015).
・ M. Kitaoka, N. Kamiya, M. Goto 'Transdermal Immunization using Solid-in-oil Nanodispersion with CpG Oligodeoxynucleotide Adjuvants', *Pharm. Res.*, 32(4), 1486-1492 (2015).

【Term of Project】 FY2016-2020

【Budget Allocation】 128,500 Thousand Yen

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Title of Project : All-round Micro-propulsion System for Multipurpose Utilization of Microsatellites

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Research Project Number : 16H06370 Researcher Number : 40361505
Research Area : Integrated Engineering
Keyword : Aerospace Engineering, Propulsion/Engine, Microsatellite, Electric Propulsion, Plasma

【Purpose and Background of the Research】

Recently, practical usages of microsatellites have progressed considerably worldwide. In 2015, 10% of risk money in USA was invested to new space business represented by microsatellites and NASA is planning to use them as pathfinders for innovative technologies in deep space explorations. One of the key technologies is micro-propulsions, propulsion systems for microsatellites. Increasing mission varieties are requiring various propulsive functions to a propulsion system. Moreover, microsatellites' rideshare launches and agile development adapting for them require ultra-green propulsion system which does not use any high pressure gas and toxic materials. Purposes of this research are realizing high-capability propulsion systems using ultra-green propellant for microsatellites.

【Research Methods】

The research consists of performance improvement of the ion thruster using water propellant, development of reaction control systems using green propellant, and collaborative development with microsatellite system.

Water has been regarded as an ideal propellant due to its safety, availability, and future procurement on the Moon and Mars. However, conventional ion thrusters have plasma sources significantly vulnerable for oxidization and they could not use water as its propellant. On the other hand, the ion thruster addressed here has plasma sources driven by microwave discharge which are tolerant for oxidization and usage of water.

Development of microsatellites has different features from conventional ones by strong interactions between components and considerably short development period. Hence their development style is different also from conventional ones. Key is a collaboration of propulsion system and satellite system from their initial phases of research and development. In this research, they are jointly conducted sharing all features of the propulsion and satellite system each other.

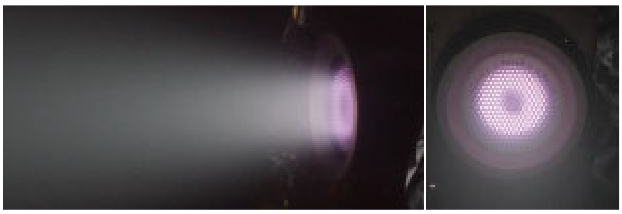

Figure 1 Ion thruster using water as the propellant

【Expected Research Achievements and Scientific Significance】

This research will generate micro-propulsion systems having various propulsive capabilities and high safety/handling-ability, which will expand the mission varieties by microsatellites. In particular, research of the ion thruster using water will provide effective tools understanding complicated molecular plasma which has wide applications in industry. Moreover, collaboration of a propulsion system with satellite system since their initial phase will suggest a new and effective style of microsatellite research and development.

【Publications Relevant to the Project】

- Koizumi, H., Kawahara, H., Yaginuma, K., Asakawa, J., Nakagawa, Y., Nakamura, Y., Kojima, S., Matsuguma, T., Funase, R., Nakatsuka, J., and Komurasaki, K., Initial Flight Operations of the Miniature Propulsion System installed on Small Space Probe: PROCYON, Transactions of Japan Soc. for Aeronautical and Space Sci., Aerospace Technology Japan, 2016, to be published.
- Takao, Y., Hiramoto, K., Nakagawa, Y., Kasagi, Y., Koizumi, H., and Komurasaki, K., "Electron extraction mechanisms of a micro-ECR neutralizer," Japanese Journal of Applied Physics, Volume 55, Number 7S2, 2016

【Term of Project】 FY2016-2020

【Budget Allocation】 128,800 Thousand Yen

【Homepage Address and Other Contact Information】

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