Title of Project : Creation and Development of Nanoscale Laboratory

Yasujiro Murata
(Kyoto University, Institute for Chemical Research, Professor)

Research Project Number : 17H06119 Researcher Number : 40314273
Research Area : Organic Chemistry
Keyword : Nanocarbon

【Purpose and Background of the Research】

Organic reactions are usually conducted in a vessel made of glasses or metals, by mixing substrate and reagent molecules in liquid solvents. There is a huge number of molecules, as many as the Avogadro constant, in such a reaction system. Therefore, a substrate molecule, for example, encounters other molecules and collides with them including solvent molecules, reagent molecules, and another substrate molecules, with interaction each other. One of the major purpose of organic chemistry is directed to a desired reaction to take place under such complicated conditions.

However, an interaction with one molecule to another is not always well understood because experimental studies are usually done by observing averaged molecular phenomena. Although gas-phase conditions are sometimes selected for studies on single molecular systems, high-vacuum conditions (10^{-10} Torr, 22.4 mL) even contain ca. 600 million molecules, rendering evaluation of pure molecular interaction rather difficult.

This research project aims to create a variety of nono-sized flasks and put one or two distinct chemical species into them in order to create basic science of the isolated materials. It will realize completely isolated single molecules and make it possible to study them under ambient conditions in solution. For the purpose, we need to construct suitable-sized and inert space which is completely isolated from outer condititons, i.e., the Nanospace Laboratory.

【Research Methods】

As shown in Figure 1, fullerenes, spherical clusters of carbon, have hollow space inside the carbon cages, which is suitable for accommodation of small molecules. Although several methods have been so far known for production of endohedral fullerenes encapsulating metal ions or atoms of rare gases, no general method is available for selective encapsulation of a variety of chemical species as well as for desired fullerene cages. In this project, we are going to synthesize endohedral fullerenes encapsulating various chemical species by "molecular surgery", which includes construction of an opening on the fullerene cage, insertion of a small molecule through it, and the following restoration of the opening by the technique of organic chemistry.

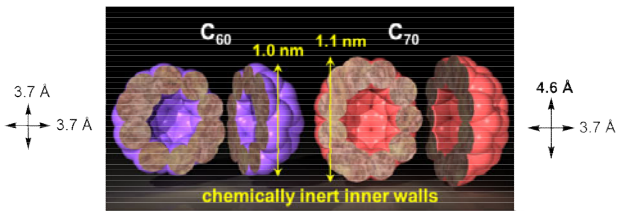


Figure 1 Structures of fullerene C_{60} and C_{70}

We expect encapsulation of a single molecule without any intermolecular interaction, a small molecule having an electronic or magnetic dipole, highly reactive chemical species, metal atoms, and several chemical species with combination of them. We need to develop rational synthetic routes for suitable openings (size, functional groups, and reality for restoration) and to realize the encapsulation for the Nanoscale Laboratory.

【Expected Research Achievements and Scientific Significance】

Taking advantage of completely isolated space, we expect that novel chemical species could be generated and that their properties should be unveiled. New properties of the isolated species that is different from those of bulk materials as well as unknown chemical species will provide great contribution toward new material science.

【Publications Relevant to the Project】

Endofullerenes: A New Family of Carbon Clusters, Edited by Akasaka, T. and Nagase, S., Springer Netherlands (2002).

【Term of Project】 FY2017-2021

【Budget Allocation】 160,100 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.scl.kyoto-u.ac.jp/~kouzou/

Title of Project : Interconversion of Quantum States Between Photon and Electron Spin Using Electrically Controlled Quantum Dots

Akira Oiwa
(Osaka University, The Institute of Scientific and Industrial Research, Professor)

Research Project Number : 17H06120 Researcher Number : 10321902
Research Area : Semiconductor Quantum Physics
Keyword : Electron spin, Photon, Quantum State Conversion, Quantum dot, Lateral p-n junction

【Purpose and Background of the Research】

Quantum communication provides a secure communication method. Quantum repeaters (QRs) is an indispensable technology for long distance quantum communications and are actively studied in various quantum systems. This project aims to establish the interconversion of quantum states between electron spins in electrically controlled GaAs quantum dots (QDs) and photon polarization transmitting information. Quantum state conversion from photons to electron spins and entanglement conversion from photon pairs to distant electron spin pairs will be demonstrated. The light-spin conversion in group IV devices will be developed toward a quantum memory for QRs. Moreover, we will develop single photon emitters by combining a lateral p-n junction with an electrically controlled QD to realize quantum state conversion from electron spins to photons.

【Research Methods】

1. Quantum state conversion from single photons to single electron spins using electrically controlled QDs

Quantum state conversion from single photons to single electron spins will be achieved by realizing measurement bases rotations of the single photoelectron spin. Moreover, the conversion of entanglement from photon pairs to electron spin pairs can be performed. The evaluation and improvement of the conversion efficiencies are crucial.

In addition, we elucidate the elemental processes of the conversion from polarized light to electron spin and the influence of indirect transition in Ge quantum structures using spin valve effect.

2. Quantum state conversion from electron spins to photons in lateral p-n junctions with a QD

We realize the electroluminescence from lateral p-n junctions. Then, a QD is fabricated in the lateral p-n junction. First, we will observe single photon emission by injecting single electrons from the QD. In the next step, angular momentum conversion is demonstrated by confirming the correspondence between spin direction generated in a QD and incident circularly polarization. Finally, we tackle the quantum state conversion by developing the correlation measurement and by designing the band structure for an optical transition allowing the quantum state conversion.

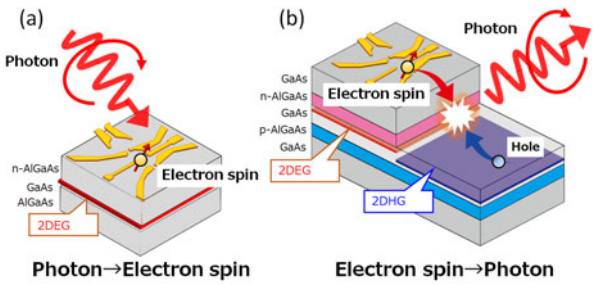


Figure 1 Schematic illustrations of quantum state conversions from photon to electron spin (a), and electron spin to photon (b).

【Expected Research Achievements and Scientific Significance】

Quantum state conversion from photons to electron spins in QDs and entanglement conversion from photon pairs to distant electron spin pairs will contribute greatly to realize QRs and to investigate the novel phenomena related to non-local entanglement in solids. On-demand quantum light sources emitting photons from spin states will create novel technologies for quantum information processing.

【Publications Relevant to the Project】

・Conversion from single photon to single electron spin using electrically controllable quantum dots, A. Oiwa *et al.*, J. Phys. Soc. Jpn. 86, 011008 (2017).
・Non-destructive Measurement of Single Photo-electrons by Inter-dot Tunneling in a Double Quantum Dot, T. Fujita *et al.*, Phys. Rev. Lett. 110, 226803 (2013).

【Term of Project】 FY2017-2021

【Budget Allocation】 166,100 Thousand Yen

【Homepage Address and Other Contact Information】

http:// www.sanken.osaka-u.ac.jp/labs/qse/
oiwa@sanken.osaka-u.ac.jp

Title of Project : Realization of nano-dynamics imaging of protein molecules in extremely soft membrane environments

Toshio Ando
(Kanazawa University, Bio-AFM Frontier Research Center, Specially-Appointed Professor)

Research Project Number : 17H06121 Researcher Number : 50184320
Research Area : Nano-Biosciences
Keyword : Single-molecule imaging, Nano-measurements

【Purpose and Background of the Research】

High-speed AFM (HS-AFM) that I developed enabled directly observing protein molecules in action. Following our pioneering imaging studies, various laboratories have been filming proteins in action using HS-AFM, enabling new discoveries that would be unable with conventional techniques. Nevertheless, HS-AFM imaging of membrane proteins working in extremely soft membranes, such as ion channels and translocons translocating polypeptides across membranes, has been infeasible. This is due to large deformation of the membranes caused by tip-contact, prohibiting high resolution imaging. Although this can be avoided by placing membrane fragments on a substrate, concentration gradients of ions and molecules across the membrane cannot be formed and polypeptides translocation across the membrane is hampered. In this study we will develop techniques that enable high resolution imaging of dynamic processes of proteins in soft membrane environments.

【Research Methods】

We will develop (i) a technique to suspend membrane protein-containing membranes at small areas, across which concentration gradients of ions and molecules can be formed, and (ii) high resolution scanning ion conductance microscopy (SICM), while further expanding our previous studies for high-speed and low-noise performances of SICM. SICM uses an electrolyte-filled glass pipette as a probe and relies on an ion current flowing between an electrode inside a pipette and another in an external bath solution (Fig. 1). The ion current passing through the small opening of the pipette is sensitive to the tip-sample surface separation. Hence, SICM can capture topographic images without tip-sample contact. To gain high resolution, the pipette tip has to be brought to the sample by a distance of the tip opening. However, the wall surrounding the opening is thick, and hence, an object right under the wall cannot be detected sensitively, leading to tip-sample contact. We will develop a technique to minimize the wall thickness and a technique to use carbon nanotubes as a probe for SICM. The innovative power of these techniques will be demonstrated by dynamic imaging of purified proteins and membrane proteins embedded in the outer and inner membranes of mitochondria.

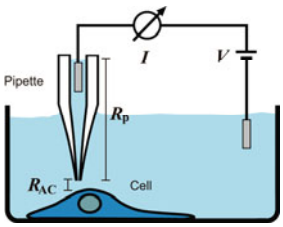


Fig.1 Schematic of SICM

【Expected Research Achievements and Scientific Significance】

SICM with high-speed, high-resolution and non-contact imaging capabilities will be materialized. This will make it possible to observe dynamic action of protein molecules working in extremely soft membranes. Moreover, imaging of suspended protein molecules will also become possible. Therefore, protein molecules in higher order structures, such as demembranated myofibrils, will be able to be observed. Future high-speed/high-resolution SICM has the potential to visualize the interior of live cells.

【Publications Relevant to the Project】

-T. Ando, T. Uchihashi, and S. Scheuring, Filming bio-molecular processes by high-speed atomic force microscopy (2014) *Chem. Rev.* **114**, 3120-3188.
-C.-C. Chen, Y. Zhou, and L. A. Baker, Scanning ion conductance microscopy (2012) *Annu. Rev. Anal. Chem.* **5**, 207-228.
-J. Geng *et al.*, Stochastic transport through carbon nanotubes in lipid bilayers and live cell membranes (2014) *Nature* **514**, 612-615.

【Term of Project】 FY2017-2021

【Budget Allocation】 126,400 Thousand Yen

【Homepage Address and Other Contact Information】

http://biophys.w3.kanazawa-u.ac.jp/index.htm

Title of Project : Direct visualization of molecular recognition forces by high-resolution atomic force microscopy and spectroscopy

Hirofumi Yamada
(Kyoto University, Graduate School of Engineering, Professor)

Research Project Number : 17H06122 Researcher Number : 40283626
Research Area : Nano/Micro science, Nanobioscience
Keyword : Single-molecule force spectroscopy, Atomic force microscopy

【Purpose and Background of the Research】

Three-dimensional (3D) force mapping based on frequency modulation atomic force microscopy (FM-AFM) is a powerful technique, capable of directly visualizing hydration structures and charge distribution in solution. The method is also applied to mapping of recognition forces between biological molecules. However, the detection probability of binding forces is often low because the effective interaction time in the measurements is not sufficiently long, which means that essential improvements of the method are required.

In this project we further develop 3D force mapping method not only by the precise control of the AFM probe motion but also by the real-time analysis of the response signal, which allows us to visualize 3D molecular recognition forces and other several forces originating from hydration structures and/or charge density of the molecules.

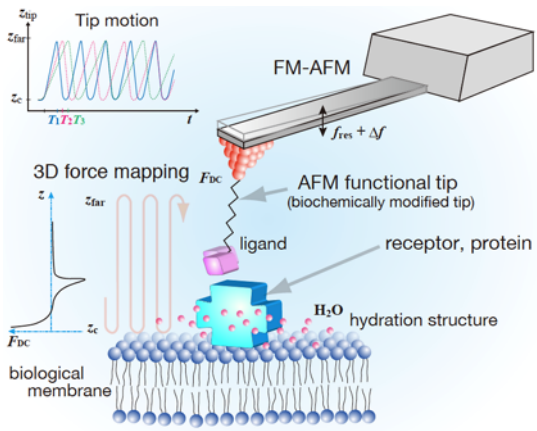


Fig. 1 3D molecular recognition force mapping

【Research Methods】

(1) Advanced 3D force mapping

Molecular binding forces are quantitatively detected in 3D force mapping by varying the interaction time of the probe tip in the vicinity of a target molecule. To minimize measurement disturbance possibly caused by the tip vibration in FM-AFM the natural oscillation driven by the thermal noise is utilized.

(2) Visualization of molecular recognition forces

Antibody-antigen binding: Oligomer formation of various IgG antibody molecules and the formation mechanism are investigated at the molecular level.

DNA-protein complex: DNA-protein complexes formed in the initial stage of eukaryotic DNA replication process are visualized and a series of the whole initial process is clarified.

(3) Visualization of hydration structures

Hydration shells/structures in the proximity of biological molecules having complex spatial structures are visualized by precise control of the probe tip. The relationship between hydration strictures and bio-functions in various protein molecules including ion channels is clarified.

【Expected Research Achievements and Scientific Significance】

This project is expected to make a significant contribution directly to the molecularly-targeted therapy. In engineering applications it is directly connected to development of biomaterials such as biocompatible materials and biosensors. In addition it is expected to produce a huge spinoff effect in both industrial and social life aspects.

【Publications Relevant to the Project】

・S. Ido *et al*. "Immunoactive two-dimensional self-assembly of monoclonal antibodies in aqueous solution revealed by atomic force microscopy", *Nature Materials*, **13**, 264-270 (2014).
・K. Umeda *et al*. "Molecular-scale quantitative charge density measurement of biological molecule by frequency modulation atomic force microscopy in aqueous solutions", *Nanotechnology*, **26**, 285103 (2015).

【Term of Project】 FY2017-2021

【Budget Allocation】 141,900 Thousand Yen

【Homepage Address and Other Contact Information】

http://piezo.kuee.kyoto-u.ac.jp/
h-yamada@kuee.kyoto-u.ac.jp

Title of Project : Giant strain effect of charge transport in organic single-crystal semiconductors and flexible mechano-electronics

Junichi Takeya
(The University of Tokyo, Graduate School of Frontier Science, Professor)

Research Project Number : 17H06123 Researcher Number : 20371289
Research Area : Applied materials
Keyword : Organic/Molecular electronics

【Purpose and Background of the Research】

Since organic semiconductors can constitute sensor devices on low cost plastic films, they are attracting attention as promising materials for next generation semiconductors, which are required in large quantities in the upcoming IoT society.
We have found transistors fabricated from single crystalline organic ultra thin films exhibit gigantic strain effects that mobility increases by 70% from 10 cm 2 / Vs by applying a slight force with fingers.
The mechanism of huge response is unknown, understanding of micro mechanisms and development of even better material design technology are urgently required. This study aims to elucidate the effect that strain contributes to electron transfer and electron scattering through elaborate physical property studies and elucidate the huge mechano - electronic response mechanism in flexible organic semiconductors.

【Research Methods】

In order to elucidate the whole phenomenon of the huge distortion response phenomenon of the flexible single crystal organic semiconductor crystal, we are working on "development of molecular layer single crystal organic semiconductor / polymer composite material" and "elucidation of structural properties and study of electronic properties of distortion effect" .

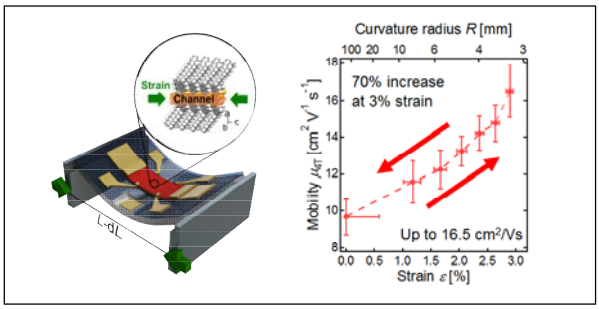


Figure 1 Strained organic semiconductor and strain / mobility characteristics

【Expected Research Achievements and Scientific Significance】

This research aims at "elucidation of a practical structure looking at device construction", and it is expected that ultrahigh - sensitivity strain sensor elements and high - efficiency vibration power generation elements can be realized so far. This ultra-sensitive sensor generates new structure deterioration diagnosis technology and new automatic production technology, and high efficiency power generation element leads to energy harvest by vibration power generation. Devices that combine these elements and printed LSIs create an industrial base of mechano-electronics, greatly advancing the IoT society, encouraging social change by constructing an autonomous network society, and impacting the foundation of innovation in the advanced information society.

【Publications Relevant to the Project】

・Takayoshi Kubo, Roger Häusermann, Junto Tsurumi, Junshi Soeda, Yugo Okada, Yu Yamashita, Norihisa Akamatsu, Atsushi Shishido, Chikahiko Mitsui, Toshihiro Okamoto, Susumu Yanagisawa, Hiroyuki Matsui & Jun Takeya, “Suppressing molecular vibrations in organic semiconductors by inducing strain” Nature Communications 7, 11156 (2016).
・K. Sakai, Y. Okada, S. Kitaoka, J. Tsurumi, Y. Ohishi, A. Fujiwara, K. Takimiya, and J. Takeya, “Anomalous pressure effect in heteroacene organic field-effect transistors”, Phys. Rev. Lett. 110, 096603 (2013).

【Term of Project】 FY2017-2021

【Budget Allocation】 163,300 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.organicel.k.u-tokyo.ac.jp/

Title of Project : New development of nonlinear photoelectronics based on terahertz strong field physics

Koichiro Tanaka
(Kyoto University, Graduate School of Science, Professor)

Research Project Number : 17H06124 Researcher Number : 90212034
Research Area : Optical Physics / Quantum Optics
Keyword : Nonlinear Optics, Strong Optical Field Physics, High-Harmonics Generation

【Purpose and Background of the Research】

Photoelectronics in a high frequency region exceeding 300 GHz is a leading research area where application development to the next generation high speed communication, nondestructive inspection, security, etc. is expected. There is a strong demand for new terahertz technology and science that support the basis of light sources and detectors.

In order to advance the photo electronics in the terahertz region dramatically, we study nonlinear optical effects in the mid-infrared ~ terahertz region using low-dimensional electronic material systems. In particular, we try to generate high-order harmonics for high-quality thin films of materials with Dirac electron systems such as graphene and single-layer two-dimensional materials such as MoS_2. We compare the results in material systems with different band dispersion and investigate whether nonlinear optical response can be explained by cooperation and competition between intraband process and interband process. We also elucidates the physical mechanism from the viewpoint of high intensity field physics.

【Research Methods】

To achieve the objectives, we will execute the following three research:

1. Optimization of high-order harmonics generation by clarifying the physical mechanism:

Experiments such as polarization dependence and crystal angle dependence of harmonic generation are systematically performed over a wide frequency range from the terahertz region to the infrared region, giving rise to the mechanism of the nonlinear optical effect. This will lead to the effective design guidelines for nonlinear optical devices.

2. Development of low dimensional materials and devices suitable for nonlinear optics:

We control defect density and Fermi surface in graphene and metal carbon nanotube and its device structure and optimize material system suitable for nonlinear optics in terahertz region.

3. Optimization of terahertz electromagnetic field by using metal structure and metal point contact:

We optimize the spatial electromagnetic field distribution in the nonlinear optical material by metal structures in order to effectively realize the nonlinear optical effect even for weak terahertz light. In addition, we consider the system of photo-induced STM as a nonlinear optical element with a metal point contact and search for novel nonlinear optical phenomena.

【Expected Research Achievements and Scientific Significance】

The main feature of this research is to pursue new theoretical basis of nonlinear optical phenomena caused by interaction between strong terahertz electric field and matter. We place the matter system in an extremely non-equilibrium state by applying a strong electric field of light that has not been searched so far. As a result, it is expected that new quantum effects. The theory that is ultimately constructed is directly linked to the development of future terahertz photonics and is also important from the viewpoint of securing the advantage of science and technology in our country.

【Publications Relevant to the Project】

・N. Yoshikawa, T. Tamaya, and K. Tanaka, "High-harmonic generation in graphene enhanced by elliptically polarized light excitation", Science 356, 736-738 (2017).
・T. Tamaya, A. Ishikawa, T. Ogawa, and K. Tanaka, "Diabatic Mechanisms of Higher-Order Harmonic Generation in Solid-State Materials under High-Intensity Electric Fields", Phys. Rev. Lett. 116, 016601 (2016).
・T. Kampfrath, K. Tanaka and K. A. Nelson, "Resonant and nonresonant control over matter and light by intense terahertz transients", Nature Photonics 7,680–690 (2013).

【Term of Project】 FY2017-2021

【Budget Allocation】 162,300 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.hikari.scphys.kyoto-u.ac.jp/jp/
kochan@scphys.kyoto-u.ac.jp

Title of Project : Spectral control of near-field thermal radiation for highly efficient thermo-photovoltaic power generation

Susumu Noda
(Kyoto University, Graduate School of Engineering, Professor)

Research Project Number : 17H06125 Researcher Number : 10208358
Research Area : Photonics
Keyword : Photonic crystal

【Purpose and Background of the Research】

Thermal radiation from heated objects to free space generally exhibits a broad spectrum and its peak intensity is limited to that of a blackbody at the same temperature. To overcome these limitations, in this project, we investigate the spectral control of thermal radiation using photonic crystals and near-field effects, and demonstrate narrowband near-field thermal radiation beyond the blackbody limit for highly efficient thermo-photovoltaic (T-PV) power generation.

【Research Methods】

Recently, we proposed a novel strategy for thermal emission control by simultaneously manipulating photonic states with photonic crystals and material absorption, and experimentally demonstrated highly efficient narrowband thermal emission to free space. In this project, we combine the above strategy and a near-field enhancement effect of thermal emission to realize frequency-selective thermal radiation beyond the blackbody limit between thermal emitters and PV cells placed in close proximity to each other. Specific research topics in the project are listed below:

(I) Theoretical study on the control of near-field thermal radiation spectra using photonic crystals: We will elucidate the role of photonic crystals (photonic bandgap, band folding, low group velocity effect, etc.) in the control of near-field thermal radiation spectra by developing a new simulation method based on the fluctuation-dissipation theorem and rigorous coupled wave analysis, and design the near-field TPV system shown in Fig. 1.

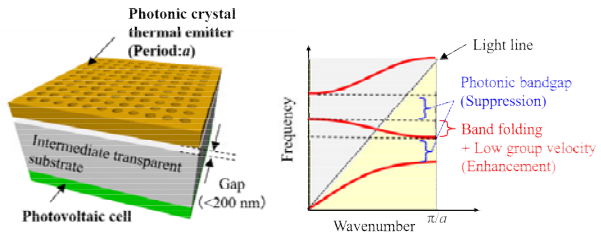


Figure 1. Thermal radiation control using photonic crystals and near-field effects.

(II) Experimental realization of near-field coupling between emitters and PV cells: By using semiconductor nano-processing technologies including wafer bonding, we will develop a method to realize close positioning (<200 nm) of photonic crystal thermal emitters and PV cells including the intermediate transparent substrate.

(III) Demonstration of narrowband near-field thermal radiation for T-PV applications: Using the system developed in (II), we will experimentally demonstrate near-field enhancement of thermal radiation as well as reveal the effect of photonic crystals. Furthermore, we will perform the experiment of T-PV and quantitatively evaluate the efficiency of energy transfer.

【Expected Research Achievements and Scientific Significance】

We believe that our research will provide a new systematic theory for the control of thermal radiation using photonic crystals and near-field effects. We also believe that the experimental technologies developed in this project will contribute to the realization of fundamental technologies for highly efficient T-PV power generation systems.

【Publications Relevant to the Project】

・T. Asano, M. Suemitsu, K. Hashimoto, M. D. Zoysa, T. Shibahara, T. Tsutsumi, and S. Noda, “”Near-infrared-to-visible highly selective thermal emitters based on an intrinsic semiconductor,” **Science Advances**, vol. 2, e1600499 (2016).
・T. Inoue, T. Asano, and S. Noda, “Near-field thermal radiation transfer between semiconductors based on thickness control and introduction of photonic crystals,” **Physical Review B**, vol. 95, 125307 (2017).

【Term of Project】 FY2017-2021

【Budget Allocation】 154,900 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.qoe.kuee.kyoto-u.ac.jp
snoda@kuee.kyoto-u.ac.jp

Title of Project : Transmission Muon Microscope by muon microbeam, realizing 3-D Imaging

Yasuhiro Miyake
(High Energy Accelerator Research Organization, Institute of Materials and Structure Science, Professor)

Research Project Number : 17H06126 Researcher Number : 80209882
Research Area : Quantum Beam
Keyword : Muon, Ultra slow muon, Laser, Microscopy, Quantum interference, wave

【Purpose and Background of the Research】

When a surface muon (4 MeV) is incident on a tungsten foil (silica aerogel), muonium (bound state of a muon and an electron, which is like a light isotope of H) evaporates into vacuum with a yield of around 4% (7%). By cooling muonium by 7-8 orders from 4 MeV to 0.2 eV (0.03 eV) combined with the application of the laser resonant ionization method (1p-2p-unbound), ultra slow muon (USM) can be generated. Then reacceleration and focusing of USM helps to achieve muon as coherent wave. The essence of this research is to create a high intensity muon microbeam with excellent time and spatial resolution by using supercooling and reacceleration to demonstrate the wave-particle duality of muon. It will also provide a novel insight (3D image) to materials research [Fig. 1].

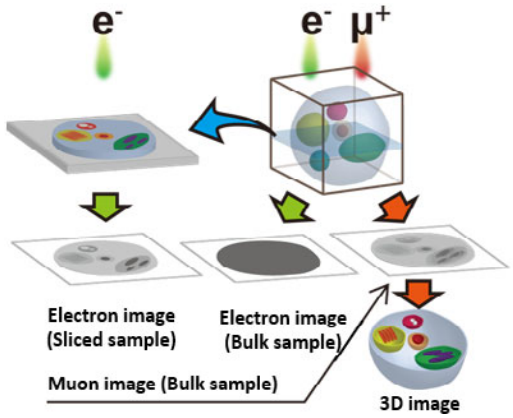


Fig. 1. 3D imaging of a 10 μm thick sample. Advantages of transmission muon microscope versus electron microscope.

【Research Methods】

To establish transmission muon microscope, the following 3 major research topics will be proceeded;
(A) Reacceleration of muon: USM will be accelerated up to 300 keV by induction acceleration to demonstrates the wave nature of the muon, and finally reaccelerated up to 10 MeV to get muon microbeam.
(B) Superconducting objective lens: It will be developed and used to focus muon which has 200 times heavier mass than electron.
(C) Transmission imaging: Development of normal focusing/projection lens and muon image detector for imaging of thick sample, such as alive cell or solar cell.

【Expected Research Achievements and Scientific Significance】

(1) Direct proof of quantum coherency of 2nd generation lepton: To demonstrate the muon as wave, a single crystal thin film of gold sample will be used to observe a muon diffraction image. A gold grating (408 pm) with diffraction angles 0.66 and 0.38 mrad for the acceleration voltages of 100 and 300 keV, respectively, will show diffraction patterns at a distance of 1m on a two dimensional image sensor SOI detector (14 μm resolution) compatible with vacuum. It will be a historical achievement to prove the quantum coherency exhibited by muon as a 2nd generation lepton in the standard model.
(2) Microscopic imaging of materials: Thick samples (> μm) will be visualized by using the transmission capability of the transmission muon microscope. The quantum interference of muon can be achieved by phase contrast method, and the electromagnetic field distribution inside the sample will be visualized using a phase plate made of carbon thin film (Aharonov-Bohm effect). The number of muons required to observe an image with a resolution of 256 x 256 pixels with a dynamic range of 8 bits is 256^3, and the time required to acquire one image in U-Line is several ten minutes to several hours.

【Publications Relevant to the Project】

・**"Ultra Slow Muon Project at J-PARC MUSE"** , Y. Miyake et al., JPS Conf. Proc. 2, (2014)010101
・**"Ultra Slow Muon Microscopy by Laser Resonant Ionization at J-PARC, MUSE"**, Y. Miyake, et al., Hyperfine Interactions 216 (2013) 79-83

【Term of Project】 FY2017-2021

【Budget Allocation】 159,300 Thousand Yen

【Homepage Address and Other Contact Information】

http://slowmuon.kek.jp/MuonMicroscopy.html

Title of Project : Algebraic Geometry and Integrable Systems - Deepning of Theory and New Developments in Mathematics and Mathematical Physics -

Masa-Hiko Saito
(Kobe University, Graduate School of Science, Professor)

Research Project Number : 17H06127 Researcher Number : 80183044
Research Area : Mathematical and physical sciences, Mathematics, Algebra
Keyword : Algebraic Geometry, Integrable Systems, Differential Geometry, Moduli Theory, Mirror Symmetry

【Purpose and Background of the Research】

From our construction of moduli spaces of stable parabolic connections with regular singularities over a nonsingular algebraic curve and detailed analysis of Riemann-Hilbert correspondences, one can give a rigorous proof of the geometric Painlevé property of isomonodromic diff. equations. At this point, one can also deal with the construction of moduli space of connections with irregular singularities and their Stokes Phenomenon. Moreover we are interested in mathematical foundations of mirror symmetry, WKB analysis and topological recursion of Eynard-Orantan. We would like to understand the relation between asymptotic analysis of connections and numerical invariants. From the view point of higher dimensional birational geometry, it is interesting to understand the detailed geometric structure of good model of moduli spaces of connections and Higgs bundles.

From these backgrounds, our research objectives can be listed below.

1. Study of the geometry of Riemann-Hilbert correspondences (Irregular singularity)
2. Study of the minimal model theory in the birational geometry and its applications to phase spaces and geometric Langlands conjecture.
3. Study of quantum invariants and their correlation functions and mathematical understanding of mirror symmetry.

【Research Methods】

Project members in Kobe will work together with other related researchers from the various fields like differential equations, integrable systems, birational geometry, differential geometry, moduli theory, mirror symmetry, representation theory, derived category and mathematical physics. According to the research purposes, we encourage each project member to promote each individual research and collaborations with other members. In order to share newly obtained results and new problems to be solved, we will organize workshops and research conferences. Keeping in touch with related overseas researchers, we will update the research project and obtain fruitful collaboration with them. Maintaining the home page of the project, we deliver the research information. Employing young PD researchers, we will promote the researches in next generations.

【Expected Research Achievements and Scientific Significance】

We establish the geometric of Riemann-Hilbert correspondence of connections with irregular singularities. This will promote a unified understanding of the symmetry of the integrable system and the theory of asymptotic expansion. In addition, geometric Langlands conjecture will be solved in some special cases. With these, it is expected that the integral system and algebraic geometry will merge, and we will establish the fundamental theory to understand superstring theory and mirror symmetry.

【Publications Relevant to the Project】

[1] F. Loray, M .-H. Saito, “Lagrangian fibrations in duality on moduli spaces of rank 2 logarithmic connections over the projective line”, IMRN, no. 4, 995–1043, (2015).
[2] M.-a. Inaba, M.-H. Saito, “Moduli of unramified irregular singular parabolic connections on a smooth projective curve”. Kyoto J. Math., 53, no. 2, 433–482, (2013).
[3] New developments in algebraic geometry, integrable systems and mirror symmetry (RIMS, Kyoto, 2008)”, Edited by M.-H. Saito, S. Hosno, K . Yoshioka, ASPM, 59, MSJ, (2010).

【Term of Project】 FY2017-2021

【Budget Allocation】 92,000 Thousand Yen

【Homepage Address and Other Contact Information】

http://www2.kobe-u.ac.jp/~mhsaito/ftop.html

Title of Project : Innovative Research of Geometric Topology and Singularities of Differentiable Mappings

Osamu Saeki
(Kyushu University, Institute of Mathematics for Industry, Professor)

Research Project Number : 17H06128 Researcher Number : 30201510
Research Area : Differential Topology
Keyword : Singularity, Low-dimensional Topology

【Purpose and Background of the Research】

Differential Topology, born in mid-20th century, gave a great shock to Mathematics community with Milnor's discovery of exotic differentiable structures, where singularities of functions played an important role. Thom proposed Catastrophe Theory based on Singularity Theory, exhibiting its applications to various fields. Later, strong analytic techniques were introduced in Topology, although they are not very constructive. With recent maturity of analytic ideas, importance of Geometric Topology, which is based on concrete constructions, is increasing. Under such circumstances, our project aims to reform Singularity Theory with concrete and constructive ideas of Geometric Topology, and to innovate formulations, concepts and techniques. We also open up a new road in Geometric Topology from singularity theoretical viewpoints, and solve important problems. We thereby establish a new research field, "Next-generation Catastrophe Theory", and give evolution to Topology.

【Research Methods】

We effectively use singular fibers (established by leader Saeki), singular geometric structures, mapping class groups (member Endo's contribution is essential). We use "charts" which visualize braid groups and monodromies (invented by member Kamada) in order to unify various invariants that have not been understood geometrically. Using characteristic classes and homotopy theory (members Ohmoto and Iwase's contribution is essential), we systematically study the elimination problem of singularities. We use real singularity theory techniques to attack the 4-dimensional smooth Poincaré conjecture (member Ishikawa's contribution is essential). Based on these methods, the members of the project conduct individual as well as joint researches by frequently discussing with each other. We also hold seminars and conferences in order to activate the relevant fields.

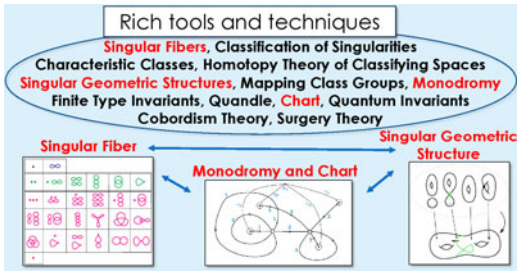


Figure 1 Research Methods

【Expected Research Achievements and Scientific Significance】

We get new contributions to crucial problems in Differential Topology. We open up new applications of Singularity Theory to other disciplines by using concrete and constructive ideas, and create a new research field. Developments in related fields in Mathematics are accelerated, where the versatility of Singularity Theory plays important roles. By activating Catastrophe Theory, we aim to solve problems in industry, propose new methods in other disciplines in science, and we thereby spread our results to other fields.

Figure 2 Research Outcomes

【Publications Relevant to the Project】

- R.A. dos Santos, M.A.B. Hohlenwerger, O. Saeki and T.O. Souza, New examples of Neuwirth-Stallings pairs and non-trivial real Milnor fibrations, Ann. Inst. Fourier (Grenoble) 66 (2016), 83-104.
- Saeki, Topology of singular fibers of differentiable maps, Lecture Notes in Math., Vol.1854, Springer-Verlag, 2004.

【Term of Project】 FY2017-2021

【Budget Allocation】 62,800 Thousand Yen

【Homepage Address and Other Contact Information】

http://imi.kyushu-u.ac.jp/~saeki/

Title of Project : Establishing processes of galaxy structure revealed by a Subaru tomographic adaptive optics

Masayuki Akiyama
(Tohoku University, Astronomical Institute, Professor)

Research Project Number : 17H06129 Researcher Number : 50425401
Research Area : Astronomy
Keyword : Optical near-infrared astronomy, applied optics

【Purpose and Background of the Research】

How have been the structures of the galaxies with bulge and thin disk in the present-day universe established? Recent observations of the galaxies in the early universe reveal that young galaxies have surprisingly different structures than the present-day galaxies: turbulent gas disk with large velocity dispersion and compact central region, which has 3 orders of magnitude higher stellar number density than seen in the present-day galaxies. The purpose of this research is to observationally reveal establishment processes of the structure of galaxies seen today by observing distributions and dynamical motions of stars inside distant galaxies.

【Research Methods】

The spatial distribution of stars inside distant galaxies will be revealed by high spatial resolution imaging in the near infrared. Such observation can be achieved by installing a newly developed fiber-laser light source to the current Subaru telescope 188 element adaptive optics system. The observation will be conducted with the infrared camera and spectrograph (IRCS) on the Subaru telescope.

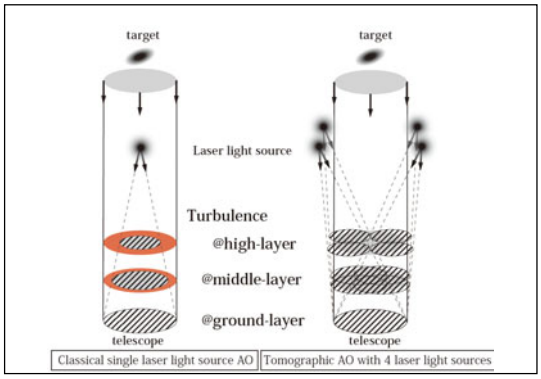


Figure. 1

On the other hand, stellar dynamical structure of the galaxies is revealed by visible redshifted absorption lines of distant galaxies seen in the visible wavelength. We achieve such observation by introducing a tomographic adaptive optics system. In the current AO system with a single laser light source, the performance of the AO is limited by the fact that the light source is at a finite distance and its light passes through a conical region as shown in figure 1. Introducing 4 laser light sources, we will cover the cylindrical light path of the astronomical targets at infinity. The measured wavefronts will be analyzed by a tomographic estimation method. With this tomographic adaptive optics system, we can achieve good AO correction in the visible wavelength range where laser AO systems have not been effective. The high spatial resolution integral field spectroscopy will be conducted with visible integral field spectrograph, 3DII.

【Expected Research Achievements and Scientific Significance】

High spatial observations in the visible and near-infrared provide us with the crucial information to understand the stellar distribution and dynamics inside distant galaxies.

AO system with laser light source is not operational in the visible wavelength all over the world, and this laser tomography AO system will open a new window to conduct a high-resolution observation.

【Publications Relevant to the Project】

"Multi time-step wavefront reconstruction for tomographic adaptive-optics systems", Ono, Y., Akiyama, M., Oya, S., et al., Journal of Optical Society of America, A., 2016, 33, 726

【Term of Project】 FY2017-2021

【Budget Allocation】 161,300 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.astr.tohoku.ac.jp/~akiyama/index_Res_TMTinst.html
akiyama@astr.tohoku.ac.jp

Title of Project : Study of cosmic star-formation history based on an unbiased survey of millimeter- and submillimeter-wave emission-line galaxies

Kotaro Kohno
(The University of Tokyo, Graduate School of Science, Professor)

Research Project Number : 17H06130 Researcher Number : 80321587
Research Area : Astronomy
Keyword : Mm/submm waves, cosmic star formation history, emission-line galaxies, superconductors

【Purpose and Background of the Research】

The history of star formation over time (i.e., redshift or z) is closely related to the evolution of the universe, and hence is one of the key subjects in astronomy. In this study we will tackle major unresolved problems of it, including the precise physical mechanism that governs the variation of star formation activities, by conducting an extensive survey of emission-line galaxies at mm and submm waves. Specifically, we will (1) survey star-forming galaxies at z = 4-8 with the [CII] 158 μm line, which is the brightest line in the far-infrared band, to measure the [CII] luminosity functions and star- formation rate densities (SFRD) at the early epoch, and (2) conduct an unbiased survey of relatively low-J CO lines, which are a tracer of the molecular gas, to constrain the CO luminosity functions and then detect the variation of molecular gas mass density at z = 0-2.

【Research Methods】

To achieve the goals, we will develop DESHIMA, a mm/submm-wave imaging spectrograph covering from 210 to 360 GHz instantaneously (about 13 times wider than the single tuning of ALMA) by exploiting the state-of-the-art superconducting technology. DESHIMA equipped with a few 10s of spatial pixels will enable us to conduct ultra-wide-band spectroscopy over a field of view comparable with, or wider than, that of ALMA. We plan to install this instrument on the LMT 50 m telescope, which is one of the world largest mm-wave single-dish telescopes, and to conduct extensive surveys of emission-line galaxies.

【Expected Research Achievements and Scientific Significance】

This program will produce the first astronomical observational results of spectroscopy for a wide bandwidth of 150 GHz. It will be a showcase of the unique and new technology, i.e., on-chip super-conducting spectrograph, proposed by a Japanese scientist.

To determine the SFRD based on the observations of the galaxies that emit the [CII] 158 μm line has the following two major advantages over conventional dust-continuum surveys. First, it immediately gives their spectroscopic redshifts. Second, it enables us to make a systematic search for a new class of star-forming galaxies that have bright emission lines with suppressed dust continuum emission. They would be good targets for ALMA follow-up observations and would no doubt lead to the significant scientific outcome from Japan.

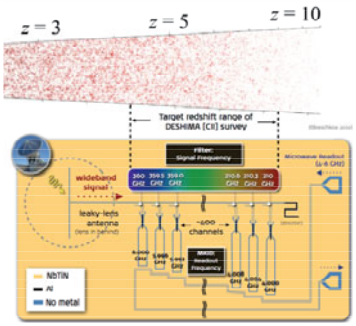


Figure 1 DESHIMA, an on-chip spectrograph based on super-conducting resonators, for z=4-8 [CII] lines.

【Publications Relevant to the Project】

・Yamaguchi, Y., Tamura, Y., Kohno, K., et al., "SXDF-ALMA 2 arcmin^2 deep survey: Resolving and characterizing the infrared extragalactic background light down to 0.5 mJy", Publ. Astron. Soc. Japan, 68, id. 82, 15 pp. (2016)
・Endo, A., et al., "Design of an Integrated Filterbank for DESHIMA: A submillimeter Imaging Spectrograph Based on Super-conducting Resonators", J. Low Temp. Phys., 167, 341-346 (2012)

【Term of Project】 FY2017-2021

【Budget Allocation】 163,700 Thousand Yen

【Homepage Address and Other Contact Information】

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

Title of Project：Study of the Extreme Universe with the CTA Large Size Telescopes

Masahiro Teshima
(The University of Tokyo, Institute for Cosmic Ray Research, Professor)

Research Project Number：17H06131　Researcher Number：40197778
Research Area：Cosmic Ray Physics, High Energy Astrophysics
Keyword：Cosmic Rays, Gamma Rays, Black Holes, Super Nova Remnants, Dark Matter

【Purpose and Background of the Research】

The study of the high-energy Universe has been developed for the past few decades with ground-based Cherenkov telescopes and been established as an energy frontier in astrophysics. Further significant development is expected with the next generation telescopes CTA. CTA Japan is now constructing four Large Size Telescopes at La Palma, Spain, within the framework of an international collaboration. In this project, we start to produce scientific results using in the early stage of the CTA project these four Large Size Telescopes. Major research topics are 1) The first observation and study of Gamma Ray Bursts above 10GeV, 2) Study of the high-energy process around Active Galactic Nuclei, and Super Massive Black Holes, 3) Indirect Dark Matter Search with high energy gamma rays from Spheroidal Dwarf Galaxies and the Galactic Center.

【Research Methods】

In the last decades, the gamma ray observation technique with imaging atmospheric Cherenkov telescopes has been established as an important new window in astrophysics. At present, more than 200 galactic and extragalactic sources are observed.

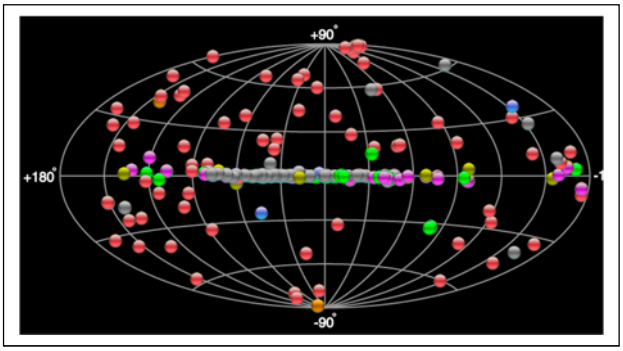


Figure 1: >100GeV Gamma Ray Sources in the galactic coordinate. Galactic sources are concentrated on the galactic plane and Active Galactic Nuclei are seen at high latitude.

We are planning to construct and operate the four large size telescopes, one by one, within three years. The array of four large size telescopes will be completed in FY2019 and will expand the visible Universe with high energy gamma rays up to a redshift of z <4. It will bring us extremely important insights into AGNs and GRBs. Furthermore, the search for the dark matter in the dwarf spheroidal galaxies and the Galactic Center is another important subject.

Figure 2: Artist view of the array of CTA Large Size Telescopes. Construction and operation will be realized one by one, and full operation will start in FY 2019.

【Expected Research Achievements and Scientific Significance】

This project will significantly advance the understanding of the high-energy Universe. It will also offer an international research environment to young scientists and make them global leaders in this field.

【Publications Relevant to the Project】

・Introducing the CTA Concept, CTA Consortium, Astropart. Phys. 43 (2013) 3-18.
・Black hole lightning due to particle acceleration at subhorizon scales, MAGIC Collaboration, Science, 346 (2014) 1080-1084.
・Detection of very high energy gamma-ray emission from the gravitationally-lensed blazar QSO B0218+357, MAGIC Collaboration, Astron. Astrophys. 595 (2016) A68.

【Term of Project】FY2017-2021

【Budget Allocation】157,100 Thousand Yen

【Homepage Address and Ohter Contact Information】

http://www.cta-observatory.jp
mteshima@icrr.u-tokyo.ac.jp

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

Science and Engineering (Mathematical and Physical Sciences)

Title of Project : Cosmic gamma-ray observation by balloon borne emulsion telescope to study unsolved issues

Shigeki Aoki
(Kobe University, Graduate School of Human Development and Environment, Professor)

Research Project Number : 17H06132 Researcher Number : 80211689
Research Area : Particle, Nuclear, Cosmic ray, Astro physics
Keyword : Gamma-ray, Nuclear Emulsion

【Purpose and Background of the Research】

Gamma-ray is the most energetic light which gives us direct information from high energy phenomena in the Universe. Gamma-ray astronomy has remarkably developed through the use of the Large Area Telescope (LAT) of NASA's Fermi Gamma-ray Space Telescope launched in 2008. Fermi-LAT reconstructs the incident angle of the gamma-ray detecting tracks of electron positron pair converted by the gamma-ray with semi-conductor detectors. On the other hand, the angular resolution is inadequate to compare the spatial information with the result observed in other wavelength bands. And it is hard to detect polarization which is informative to discuss its production mechanism.

In this project, we shall realize a gamma-ray telescope using nuclear emulsion films whose principle is the same as that of silver halide photograph. The emulsion telescope can improve angular resolution of a gamma-ray with much finer tracking of the electron and the positron. Moreover, it is sensitive to polarization of the gamma-ray.

【Research Methods】

The emulsion film can record the tracks of electron and positron converted from the gamma-ray as shown in figure 1. The emulsion telescope consists of a converter to tell the gamma-ray angle, a time-stamper to tell the timing of the gamma-ray incident and an attitude monitor to tell the orientation of the telescope relative to the celestial sphere.

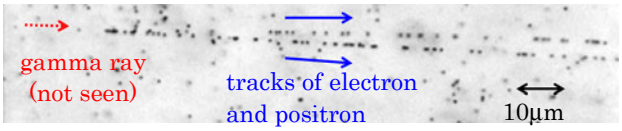


Figure 1 electron positron pair in emulsion film

The converter is made of a stack of emulsion films which is a tracking detector of the electron and the positron as well as a medium for gamma-ray conversion. All the tracks are read out by the fully automated scanning microscope system named Hyper Track Selector (HTS) shown in figure 2 (left).

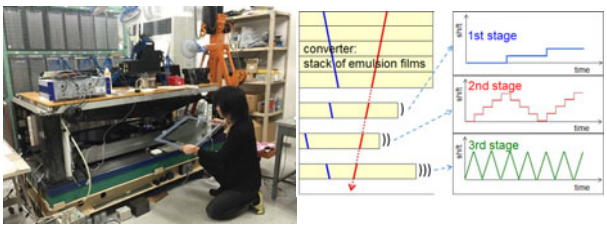


Figure 2 (left) Hyper Track Selector (0.5 m²/h)
(right) multi stage shifter for time-stamper

Tracks recorded in the emulsion film basically have time ambiguity during the period from its production to its development process. The time information of each gamma-ray is necessary since the celestial sphere rotates and the orientation of the telescope changes due to the rotation and swing of the gondola of the telescope. Several films located under the converter are intentionally shifted back and forth in the individual period. The combination of each shift enables us to get the time information. (figure 2 (right))

【Expected Research Achievements and Scientific Significance】

We shall start scientific observation realizing a gamma-ray telescope with 10m² aperture area (the world's largest) in this project in order to study unsolved issues of the cosmic gamma-ray.

【Publications Relevant to the Project】

"GRAINE 2015, a balloon-borne emulsion γ–ray telescope experiment in Australia", S. Takahashi et al., PTEP, Vol.2016, 073F01
"GRAINE project: The first balloon-borne, emulsion gamma-ray telescope experiment", S. Takahashi et al., PTEP, Vol.2015, 043H01

【Term of Project】 FY2017-2021

【Budget Allocation】 153,900 Thousand Yen

【Homepage Address and Other Contact Information】

http://neweb.h.kobe-u.ac.jp/labo/aoki/
aoki@kobe-u.ac.jp

Title of Project : Calibration Standard and High-Precision Data Analysis toward the Observational Era of Gravitational Waves

Nobuyuki Kanda
(Osaka City University, Graduate School of Science, Professor)

Research Project Number : 17H06133 Researcher Number : 50251484
Research Area : Mathematical and Physical Sciences
Keyword : Gravitational Wave, Relativity, Data Analysis, Laser Interferometer, Astrophysics

【Purpose and Background of the Research】

In 2015, the US experiment LIGO finally achieved the first gravitational wave detection. It is supposed that the source is a coalescence of black hole binary of about 30 solar mass, and has attracted great interest on physics, astrophysics and astronomy. Expecting LIGO and Virgo (in Europe) update plans and KAGRA project in Japan, the "gravitational wave observational era" with more frequent event observation will be started in the near future.

However, there is a systematic error of several to 10% in the current observation. Further, more highly accurate analysis is strongly desired.

In this research, we proceed with a collaboration of hardware and data analysis, (1) global standard of calibration, (2) high fidelity reproduction of time series gravitational wave signal *h(t)*, and (3) research on physics that be possible by high precision data analysis.

【Research Methods】

In this research, calibration, reproduction of signal, and high precision data analysis are main items.

The photon calibrator is a method to excite the displacement of the mirror by the radiation pressure of the laser light. It has already been introduced in LIGO and is also under construction in KAGRA. We will introduce an integrating sphere for an accurately measurement of the laser power, and will measure in LIGO, KAGRA, respectively. By establishing the calibration standard for the international observation network, we are aiming at a systematic error of 1% or less.

We will develop high-fidelity *h(t)* reconstruction software. We will also develop more accurate analysis, and clarify whether new science can be expected by improving calibration precision.

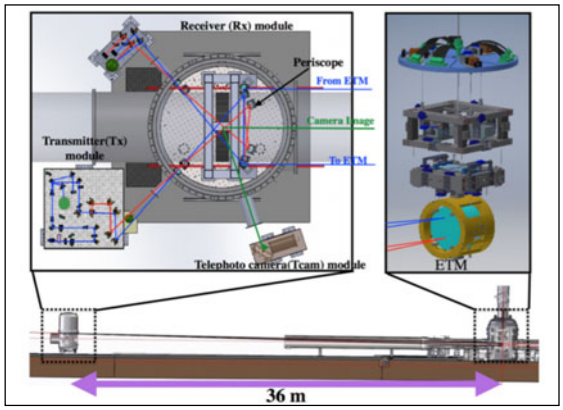


Figure 1. KAGRA Photon calibrator

【Expected Research Achievements and Scientific Significance】

The current amplitude error propagates an error of about 15% for the compact binary existence rate. This research may reduce this error about 3%. By suppressing the error of the observed waveform about 1%, the influence of the systematic error can be suppressed to less than the statistical error in the analysis with an order of 100 events.

In the second half of this research, KAGRA operation with a low temperature mirror is scheduled. Our research will be adopted on KAGRA.

【Publications Relevant to the Project】

・「初観測された重力波が開いた宇宙への新しい窓」, 神田展行、雑誌パリティ, (“New window for the universe opened by the first gravitational wave observation”, Nobuyuki Kanda, Parity, Maruzen), Vol. 31, No. 10, 14-18, (2016)

・"The detection rate of inspiral and quasi-normal modes of Population III binary black holes which can confirm or refute the general relativity in the strong gravity region", Tomoya Kinugawa, Akinobu Miyamoto, Nobuyuki Kanda, Takashi Nakamura, Mon. Not. Roy. Astron. Soc. 456 (2016) no.1, 1093-1114

【Term of Project】 FY2017-2021

【Budget Allocation】 139,600 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.gw.hep.osaka-cu.ac.jp/
kanda@sci.osaka-cu.ac.jp

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

Science and Engineering (Mathematical and Physical Sciences)

Title of Project : Quest for the origin of the Big-Bang and measurements of sum of the neutrino masses by using the world's largest CMB telescope array

Osamu Tajima
(Kyoto University, Graduate School of Science, Associate Professor)

Research Project Number : 17H06134 Researcher Number : 80391704
Research Area : Cosmology and high energy physics
Keyword : Cosmology experiment, Cosmic Microwave Background radiation

【Purpose and Background of the Research】

Cosmic Inflation is the modern cosmology which describes the origin of the Big-Bang in the early stage of the universe. Many cosmological observations support this theory. The last piece to prove this theory is the detection of the primordial gravitational waves (PGW). As shown in Figure 1, PGW generate characteristic imprints in the polarization patterns of the cosmic microwave background radiation (CMB). These odd-parity patterns are called "B-modes", and it particular degree-scale B-modes are considered to be the best probe of PGW. The sub-degree scale B-modes can also probe the weak lensing effect caused by galactic clusters. Because neutrinos are unique massive particles that are not localized within galaxies, the weak lensing effect is sensitive to the sum of neutrino masses (Σm_ν). Therefore, precise measurements of the B-modes can potentially detect PGW and constrain Σm_ν (see Figure 1 and 2). We will pursue these two main research targets with the world's largest next generation CMB telescope array experiment, ``Simons Observatory" (SO).

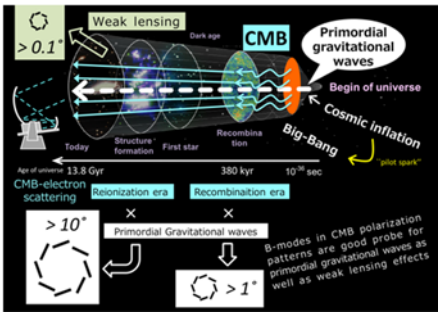


Figure 1 B-modes are probes of the primordial gravitational waves and weak lensing effect.

【Research Methods】

We will develop one of the SO telescopes, and conduct scientific observation in the international collaboration. In order to successfully perform large angular scale observations of the CMB polarization, we must simultaneously achieve high mitigation of atmospheric fluctuation effects, high sensitivity, and high statistics. The combination of Japan and USA technologies, e.g. superconducting detectors and patent cooling technologies, will be the key for success of the project. In FY2017, we plan to fix specifications of our telescope. We will then continue the development our instruments and target to start observations in FY2020. We will evaluate the performance of our experiment based on the initial data set and will confirm our scientific prospects.

【Expected Research Achievements and Scientific Significance】

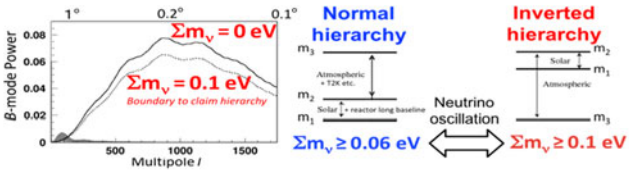


Figure 2 Measurements of Σm_ν potentially determine mass hierarchy of neutrino.

The world's largest CMB telescope array will produce the most precise CMB polarization data to date. This measurement can potentially prove cosmic inflation which provides explanations to unsolved subjects in cosmology, e.g. the flatness of the universe, the horizon problem, and the absence of the monopole. Detection of PWG via B-mode observations can show that the energy scale of the inflationary potential corresponds to the energy scale of the grand unified theory in the particle physics at 10^{16} GeV. Moreover, the existence of PWG is evidence for the quantization of gravity in the early stage of the universe. Measurements of Σm_ν potentially determine the mass hierarchy of neutrinos.

【Publications Relevant to the Project】

QUIET Collaboration, ApJ, **760**, 145, 1 – 10 (2013).
POLARBEAR Collaboration, ApJ, **794**, 2, 171 – 191 (2014).

【Term of Project】 FY2017-2021

【Budget Allocation】 161,100 Thousand Yen

【Homepage Address and Other Contact Information】

https://simonsobservatory.org/

Title of Project : Study on the charged lepton flavor mixing using the high-intensity pulsed muon beam

Satoshi Mihara
(High Energy Accelerator Research Organization, Institute of Particle and Nuclear Studies, Professor)

Research Project Number : 17H06135 Researcher Number : 80292837
Research Area : Physics
Keyword : Particle Physics Experiment, Quantum Beam

【Purpose and Background of the Research】

The Charged Lepton Flavor Violation (cLFV) is strictly forbidden in the Standard Model even with neutrino oscillation implemented. However, if new physics at TeV scale exists, cLFV process(es) can be observed in experiments. Therefore, cLFV process is thought to be a clue to investigate the higher energy scale than the LHC experiment (Figure 1).

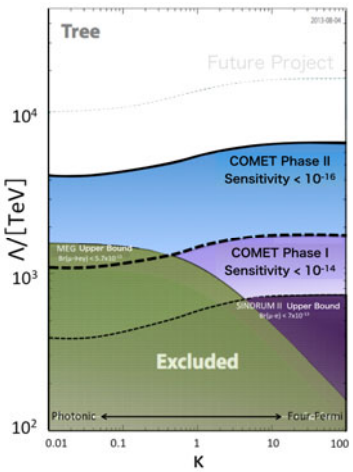


Figure 1 COMET experiment energy reach. The horizontal axis is for the parameter describing elementary processes.

At the moment several new cLFV experiments are in preparation in the world. Among these, this research project intends to optimize the high-intensity pulsed muon beam to realize the COMET experiment with a μ-e conversion search sensitivity of 10^{-16} as early as possible. We believe that this will provide great progress in muon flavor physics and contribute to realize the world's top-class experiment in Japan.

【Research Methods】

We develop a pulsed muon beam necessary to realize the target sensitivity of the COMET experiment (Phase I: 10^{-14}, Phase II 10^{-16}). For this purpose, we develop a LYSO calorimeter detector in addition to the straw-tube tracker for momentum measurement being constructed in our institute, and integrate them to "StrEcal Detector" (Figure 2 left). Based on the result obtained with this new detector, optimization of the beam collimator system will also made along with development of a new proton target producing pions/muons.

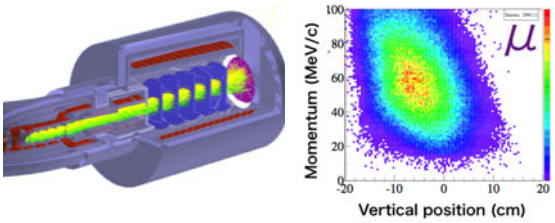


Figure 2 StrEcal detector (left) and simulated beam phase-space distribution (right)

【Expected Research Achievements and Scientific Significance】

The muon beam is the essential part of the μ-e conversion search experiment. Usual muon beam lines available in the world have momentum spread of an order of a few % while the COMET needs several tens MeV spread to maximize the beam intensity. A dedicated detector system is necessary for optimizing such beam. In this research project, we will collaborate with the COMET experiment group and J-PARC facility group to establish the world's best sensitivity in the cLFV search with the new detector system.

【Publications Relevant to the Project】

"Charged Lepton investigating new Physics", S. Mihara, JPS Journal, Vol. 70, 10 (2015)
S. Mihara et al., Annual Review of Nuclear and Particle Science, 63:1 (2013) 531-552

【Term of Project】 FY2017-2021

【Budget Allocation】 152,000 Thousand Yen

【Homepage Address and Other Contact Information】

http://comet.kek.jp/kiban-s

Title of Project : DC Electric Field and Current: Novel Control Parameters for Strongly Correlated Electron Systems

Yoshiteru Maeno
(Kyoto University, Graduate School of Science, Professor)

Research Project Number : 17H06136 Researcher Number : 80181600
Research Area : Mathematical and physical sciences
Keyword : Strongly correlated system

【Purpose and Background of the Research】

As control parameters of the Mott insulating state characteristic of strongly correlated electron systems, element substitution and pressure have been widely used; novel phenomena such as high-temperature superconductivity, colossal magnetoresistance and spin-triplet superconductivity have been found.

The purpose of this research is to establish the effectiveness of the DC electric field and current as novel control parameters of strongly correlated electron systems. We study new phenomena emerging in the non-equilibrium steady state mainly under the DC current, and deepen the understanding of these phenomena as well as of their physical mechanism.

【Research Methods】

As the main target material, we choose the 4d-electron ruthenium oxide Ca_2RuO_4 and aim to clarify the mechanism of its insulator/metal transition induced by DC electric field, as well as unusual magnetism induced by DC current that we recently discovered. Furthermore, we will clarify the details of the current-induced phenomena in the related system $Ca_3Ru_2O_7$.

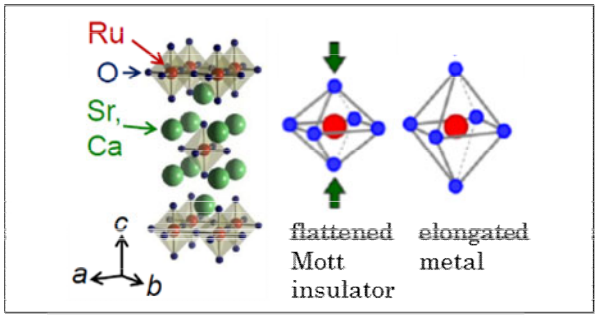


Figure 1 Crystal structure of Ca_2RuO_4

In addition, among 3d and 5d electron oxides, we select Mott insulators with relatively small energy gap and clarify the effect of DC electric field and current. In this project, we also establish experimental techniques of photoemission spectroscopy under electric current, and reveal the variations of electronic states under the non-equilibrium steady conditions. We also extend international collaborations to develop theoretical models, to examine phonon instabilities and to study local dynamics by scanning probes.

【Expected Research Achievements and Scientific Significance】

The ability to change the conductivity and magnetism remarkably by just switching on and off the DC current is a breakthrough phenomenon utilizing the nature of many-body effects in strongly correlated electron systems. This approach opens up a possibility to induce electronic states never accessible with conventional control parameters: in addition to unusual magnetism, other phenomena such as unconventional superconductivity may emerge. Thus, the outcome of this project may well provide a strong impact in the basic knowledge of modern condensed matter physics and also a suggestive direction for future device application.

【Publications Relevant to the Project】

・"Electric-field-induced metal maintained by current of the Mott insulator Ca_2RuO_4",
F. Nakamura, M. Sakaki, Y. Yamanaka, S. Tamaru, T. Suzuki, Y. Maeno,
Sci. Rep. **3**, 2536 (1-6) (2013).
・"Current-induced strong diamagnetism in the Mott insulator Ca_2RuO_4",
C. Sow, S. Yonezawa, S. Kitamura, T. Oka, K. Kuroki, F. Nakamura, Y. Maeno,
arXiv: 1610.02222 (2016).

【Term of Project】 FY2017-2021

【Budget Allocation】 159,000 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.ss.scphys.kyoto-u.ac.jp/kibanS_h29-33/index.html

Title of Project : Frustration-induced spin textures

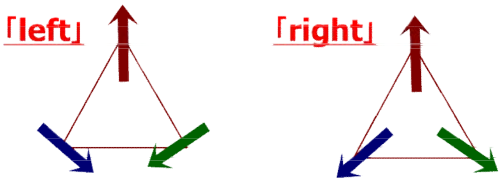
Hikaru Kawamura
(Osaka University, Graduate School of Science, Professor)

Research Project Number : 17H06137 Researcher Number : 30153018
Research Area : Mathematical and Physical Sciences
Keyword : Magnetism, Frustration, Spin texture, Z_2 vortex, Skyrmion

【Purpose and Background of the Research】

In physical science, "frustration" means the situation where several optimizing conditions compete with each other and cannot be satisfied simultaneously. "Frustrated systems" then often find difficulty in settling down in obvious stable states and exhibit enhanced fluctuations, leading to novel orders, exotic thermodynamic states and gigantic responses, *etc.*

Our research project targets magnets. Microscopically, magnets consist of a huge number of atomic-scale micromagnets called "spins". Usually, two spins tend to align in the same direction (ferromagnet) or the opposite direction (antiferromagnet). Meanwhile, anti-ferromagnetic spins located on a triangle are not allowed to take mutually antiparallel directions. In such "frustrated magnets", spins often cant taking "curved" structures. A consequence of it is the emergence of the "right-circular" and "left-circular" states: see the figure. Such "right



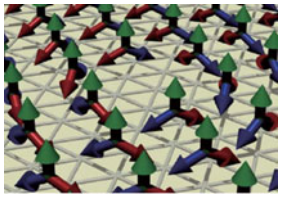
vs. left" degrees of freedom is called "chirality". In frustrated magnets, these two chiral states have exactly the same energy.

Curved spin structures induced by frustration has a lot of variety. In the present project, we take up two examples: "Z_2 vortex" and "skyrmion". Both are topologically stable nano-scale "spin textures", containing chiral degrees of freedom. Z_2 vortex, as demonstrated in the figure, was found theoretically more than 30 years ago by the project leader. Skyrmions attract much current interest, while such skyrmions are "antisymmetric" in that the right and the left are energetically inequivalent, while the skyrmion of our target is "symmetric", and is expected to show properties distinct from the standard skyrmions.

In this project, via the close collaboration between theorists and experimentalist, we wish to clarify novel phases and dynamics driven by frustration-induced spin textures in frustrated magnets, which contain rich internal degrees of freedom associated with the chirality.

【Research Methods】

Based on theoretical predictions by the project leader, we perform elastic and inelastic neutron scattering and resonant X-ray scattering experiments in zero and high fields. By comparing with the spin-dynamics simulations on localized sin models and with the bulk measurements, we establish the existence of the Z_2 vortex and the symmetric skyrmion for a series of triangular magnets. Preparing new candidate materials including metals, and performing transport measurements, we unravel the novel properties arising from frustration-induced spin textures.



【Expected Research Achievements and Scientific Significance】

Deepening of our fundamental understanding of topological aspects of statistical physics and condensed matter physics. Providing a possible clue toward future spintronics technologies.

【Publications Relevant to the Project】

・H. Kawamura, "Spin and Magnetism --- Essence of Modern Physics" Science-sya, 2016 (in Japanese).
・T. Okubo, S. Chung and H. Kawamura, Phys. Rev. Letters, **108**, 017206-(1-5) (2012).

【Term of Project】 FY2017-2021

【Budget Allocation】 165,300 Thousand Yen

【Homepage Address and Other Contact Information】

http:// thmat8.ess.sci.osaka-u.ac.jp/fstex/

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

Science and Engineering (Mathematical and Physical Sciences)

Title of Project : Variety and universality of bulk-edge correspondence in topological phases: From solid state physics to transdisciplinary concepts

Yasuhiro Hatsugai
(University of Tsukuba, Division of Physics, Professor)

Research Project Number : 17H06138 Researcher Number : 80218495
Research Area : Mathematical and Physical Sciences
Keyword : Bulk-edge correspondence, topological phases, cold atoms, ARPES, photonic crystals

【Purpose and Background of the Research】

Many of the topological phases do not possess characteristic bulk observables which are experimentally accessible. Non-trivial feature of the phase is the existence of generic "edge states" that are localized near the system boundaries or impurities. This relation is the "bulk-edge correspondence" that has been successfully applied for various systems not only for solid state physics.

Based on the previous successful project by 3 groups of theoretical physics, cold atoms and ARPES experiments working together to establish "universality of the bulk-edge correspondence", we extend the project to include groups of photonic crystals and mathematicians in the new project.

We further pursuit universality of the bulk-edge correspondence in various phases not only for quantum world, that is, some of them are classical. We also try to establish transdisciplinary concepts putting a focus on the bulk-edge correspondence in collaboration with people in wide area such as mathematics and engineering.

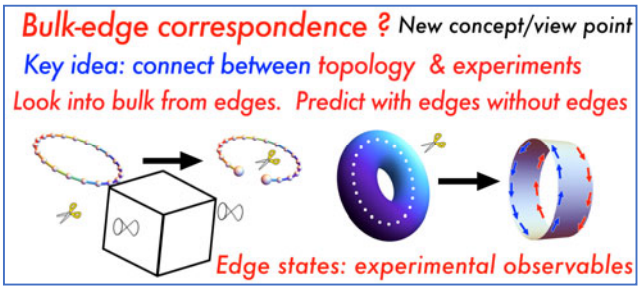


Figure 1: Bulk-edge correspondence

【Research Methods】

Theoreticians and experimentalists in condensed matter physics, cold atoms and photonics as well as mathematicians are working together sharing a common interest for the bulk-edge correspondence. Through the brainstorming discussion, we try to reach a breakthrough in some of the concrete problems. Based on the new results in each field, further developments are expected with close and informal communication between the groups. To achieve the goal, we regularly organize informal meetings among the group members including young scientists and students. To make the project international and encourage international collaboration, several international workshops will be organized as the important project activities.

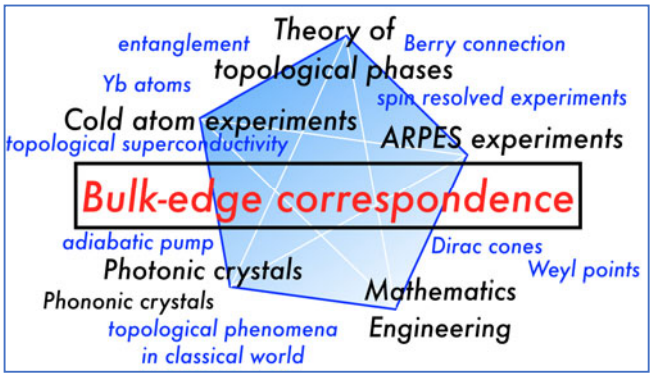


Figure 2: Scheme of the project

【Expected Research Achievements and Scientific Significance】

Since the project members of the project possess unique technique and are well-established in each field, informal communication between them putting a focus on the single interest-shared topic "bulk-edge correspondence" will be certainly productive. We also expect "unexpected" achievements based on the close collaboration over different areas. Our final long-term goal is to establish transdisciplinary sciences based on the bulk-edge correspondence. The present project paves a way to this ultimate goal.

【Publications Relevant to the Project】

・Y.Hatsugai, "Chern number and edge states in the integer quantum Hall effect", Phys. Rev. Lett. **71**, 3697-3700 (1993)
・Y.Hatsugai, "Edge states in the integer quantum Hall effect and the Riemann surface of the Bloch function", Phys. Rev. B **48**, 11851-11862 (1993)

【Term of Project】 FY2017-2021

【Budget Allocation】 157,800 Thousand Yen

【Homepage Address and Other Contact Information】

http://rhodia.ph.tsukuba.ac.jp/kaken-s-e.html
hatsugai @rhodia.ph.tsukuba.ac.jp

Title of Project : Analysis of cloud microphysics and vertical velocity by synergy use of next generation space-borne active sensors

Hajime Okamoto
(Kyushu University, Research Institute for Applied Mechanics, Professor)

Research Project Number : 17H06139 Researcher Number : 10333783
Research Area : Atmospheric physics
Keyword : Meteorology, Earth observation, Remote sensing, Climate change

【Purpose and Background of the Research】

Cloud microphysics control Earth's radiation budget and the hydrological cycles. Comparisons of simulated cloud microphysics by general circulation models show large discrepancies among the models. Clouds are the major contributor (70%) to the total uncertainties in climate predictions. Cloud radar onboard CloudSat satellite and lidar onboard CALIPSO have started cloud and aerosol observation since 2006. ADM-Aeolus with Doppler lidar and EarthCARE with Doppler cloud radar and high spectral resolution lidar (HSRL) will be lunched after 2018. Retrieval of Vertical motion, cloud microphysics, mass fluxes of cloud/ precipitation, vertical profiles of horizontal wind velocity are expected from them, though the retrieval methods have not yet been established.

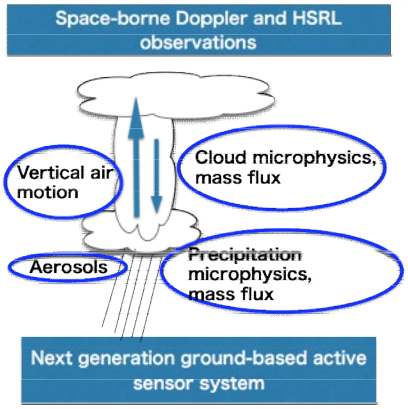
Main objectives of this project are to perform global analysis of cloud microphysics, mass flux, vertical air motion and their interactions, effect of horizontal wind shear on cloud formation.

【Research Methods】

We develop a next-generation-ground-based observation system including a multiple-scattering Doppler lidar and a multiple scattering multi-wavelength (355nm, 532nm and 1064nm) HSRL lidar systems that are based on the multi-field-of-view multiple-scattering polarization idar (MFMSPL) technique, which can overcome the observational limitation of existing ground-based conventional lidars. Cloud particle types, cloud and aerosol microphysics, as well as vertical air motion inside clouds will be retrieved. The next-generation system will be adopted to develop algorithms for EarthCARE and ADM-Aeolus satellites. These will further provide global analyses of cloud microphysics, mass fluxes of cloud/precipitations and vertical air-motion within 10km-horizontal scale and the effect of wind shear of horizontal wind velocity on cloud formation.

【Expected Research Achievements and Scientific Significance】

The next generation system is able to bridge the existing scale-gap between the ground-based and space-borne lidars and will be used to develop and improve algorithms for the satellites. Synergy use of Doppler cloud radar and the multiple-scattering Doppler lidar will provide dual Doppler information of clouds and simultaneous retrievals of particle fall velocity and vertical air-motion. The system gives the opportunity to evaluate and improve the cloud parameterization.



【Publications Relevant to the Project】

・H. Okamoto, K. Sato, Y, Hagihara, Global analysis of ice microphysics from CloudSat and CALIPSO: incorporation of specular reflection in lidar signals, J. Geophys. Res., 115, D22209 1-20, 2010.
・H. Okamoto, K. Sato, T. Nishizawa, N. Sugimoto et al., Development of a multiple-field-of-view multiple-scattering polarization lidar: comparison with cloud radar, Opt. Express, 24, 26, 30053-30067, 2016.

【Term of Project】 FY2017-2021

【Budget Allocation】 147,900 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.riam.kyushu-u.ac.jp/gfd/okamoto.html
okamoto@riam.kyushu-u.ac.jp

Title of Project : Analyses and Verification of Particle Acceleration and Scattering by Electromagnetic Cyclotron Waves in Space Plasmas

Yoshiharu Omura
(Kyoto University, Research Institute for Sustainable Humanosphere, Professor)

Research Project Number : 17H06140 Researcher Number : 50177002
Research Area : Earth and Planetary Science
Keyword : Waves in space plasma, Earth's magnetosphere

【Purpose and Background of the Research】

There exist various kinds of electromagnetic waves in space plasmas. Among them, electromagnetic cyclotron waves resonate with energetic electrons with their transverse wave fields forming helical structures along the magnetic field. When energetic electrons of 10-30 keV are injected into the inner magnetosphere at times of geomagnetic disturbances, they generate chorus emissions with rising-tone frequency as shown in Figure 1. A fraction of resonant electrons are effectively accelerated to MeV energy through nonlinear trapping by the excited chorus waves. It is understood that the accelerated relativistic electrons form the outer radiation belt. We verify the acceleration mechanism through analysis of wave and particle data obtained by multiple spacecraft. We also try to test the applicability of the nonlinear acceleration process to different regions in space. Based on the acquired insights, we develop new instruments for observation of wave-particle interaction in space plasmas. The short title of this project is PCWAVE (Particle and Cyclotron Wave Analyses and VErification).

【Research Methods】

We perform a series of test particle simulations of electron trajectories under wave models based on wave and particle observation by Arase spacecraft in the radiation belts. We also analyze data from MMS spacecraft in the magnetic reconnection regions of the Earth's magnetosphere. While miniaturization of the plasma wave instruments has been performed by forming integrated circuits on semiconductor, a critical issue of the particle instruments is how to ensure the detection area for particle fluxes with the miniaturized parts. We will solve the issue by forming multi-layer structures of the parts.

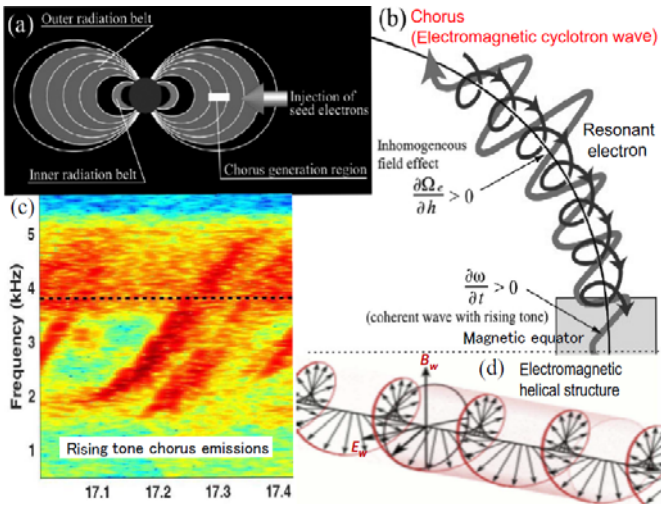


Figure 1 Chorus waves

【Expected Research Achievements and Scientific Significance】

Fundamental energy conversion processes through nonlinear wave-particle interactions in different regions of space plasmas will be clarified. Very small and light instruments for observation of wave-particle interactions will be developed, enabling us to propose new missions for space exploration with multiple small spacecraft.

【Publications Relevant to the Project】

・Omura, Y., Y. Miyashita, M. Yoshikawa et al., Formation process of relativistic electron flux through interaction with chorus emissions in the Earth's inner magnetosphere, J. Geophys. Res. Space Physics, 120, 9545-9562, 2015.
・Foster, J. C., P. J. Erickson, Y. Omura, D. N. Baker, C. A. Kletzing, and S. G. Claudepierre, Van Allen Probes observations of prompt MeV radiation belt electron acceleration in nonlinear interactions with VLF chorus, J. Geophys. Res. Space Physics, 122, 324-339, 2017.

【Term of Project】 FY2017-2021

【Budget Allocation】 133,700 Thousand Yen

【Homepage Address and Other Contact Information】

http://pcwave.rish.kyoto-u.ac.jp/
omura@rish.kyoto-u.ac.jp

Title of Project : Visualizing ultrafast dynamics of molecular structure with femtosecond X-ray solution scattering

Shin-ichi Adachi
(High Energy Accelerator Research Organization, Institute of Materials Structure Science, Professor)

Research Project Number : 17H06141 Researcher Number : 60260220
Research Area : Synchrotron Radiation Science, Physical Chemistry
Keyword : Ultrafast Dynamics, Structure Science

【Purpose and Background of the Research】

One of the fundamental goals in physical chemistry is to describe how a chemical reaction proceeds from reactants to products via intermediates, if they exist, at the atomic and molecular levels. In particular, solution-phase reaction dynamics are of much interest since many chemical and biologically relevant reactions occur in solution. Time-resolved X-ray solution scattering provides direct information of the transient molecular structures, because scattering signals are sensitive to all chemical species present in the sample and can be compared with the theoretical scattering signal calculated from 3-D atomic coordinates of the chemical species involved. In this project, we capture ultrafast structural dynamics of molecules by time-resolved X-ray solution scattering technique with femtosecond X-ray pulses.

【Research Methods】

The major limitation of time-resolved X-ray solution scattering was the limited temporal resolution from the duration of the available X-ray pulses, which is ~100 picoseconds from synchrotron storage rings. However, the limitation of the X-ray pulse width has been improved into the femtosecond regime with the advent of X-ray free electron lasers (XFELs). We applied time-resolved X-ray solution scattering technique to Au-Au bond formation reaction of $Au(CN)_2^-$ oligomers in liquid phase by using both synchrotron storage ring and XFEL facilities, and successfully elucidated the ultrafast structural dynamics of the Au-Au bond formation process at the atomic level (Fig. 1).

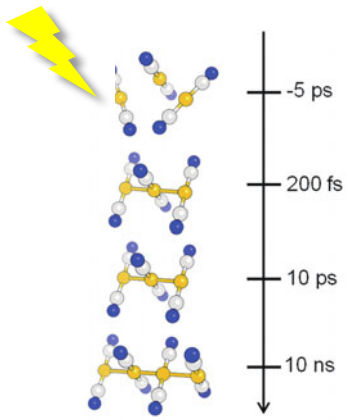


Fig. 1 Ultrafast structural dynamics of Au-Au bond formation of $Au(CN)_2^-$ oligomers.

【Expected Research Achievements and Scientific Significance】

Based on the previous work, this project is aiming to directly detect ultrafast vibrational motion of molecules by femtosecond time-resolved X-ray solution scattering technique. This experimental technique will hopefully open a new research field of fundamental chemistry as "ultrafast molecular structure science in the liquid phase".

【Publications Relevant to the Project】

"Direct observation of bond formation in solution with femtosecond X-ray scattering"
Kim, Kim, Nozawa, Sato, Ihee, & Adachi *et al.*
Nature, 518, 385-389 (2015).

"Synchrotron-Based Time-Resolved X-ray Solution Scattering (Liquidography)"
S. Adachi, J. Kim, & H. Ihee
Advances in Lasers and Electro Optics, Nelson Costa and Adolfo Cartaxo Ed., (2010) ISBN: 978-953-307-088-9, INTECH.

【Term of Project】 FY2017-2021

【Budget Allocation】 154,400 Thousand Yen

【Homepage Address and Other Contact Information】

http://www2.kek.jp/imss/pf/
shinichi.adachi@kek.jp

Title of Project : New Frontier of Substrate-Controlled Chemical Reaction

Hisashi Yamamoto
(Chubu University, Molecular Catalyst Research Center, Professor)

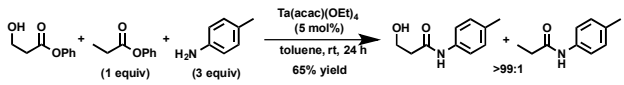
Research Project Number : 17H06142 Researcher Number : 20026298
Research Area : Basic Chemistry, Organic Chemistry
Keyword : Substrate Controlled Chemical Reaction

【Purpose and Background of the Research】

Unlike reagent controlled reactions which played significant role in organic synthesis in the past, substrate controlled reactions are relatively newer approach. Nevertheless, since its discovery the latter has become an indispensible tool in modern organic synthesis. In these reactions, an electron donor polar substituent in the substrate, namely a "directing group", actively facilitates the transient interplay between the achiral substrate and the chiral catalyst via nonbonding interaction, in such a fashion that the incoming group attacks from a particular regio-position with enantiotopic face. Thus the region- and stereochemical outcome of an organic reaction is largely dependent on the nature of the substrate.

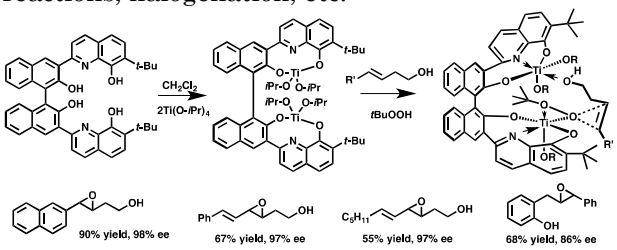
【Research Methods】

In 2016, we observed that the transformation of ester to amide is able to proceed efficiently using a new tantalum catalyst. Substrate having a β-OH group is selectively transformed to amide even in the presence of an equimolar amount of structurally related ester lacking β-OH group. This result indicates that the reaction should proceed *via* the formation of metal hydroxyl ester as the transition state (*J. Am. Chem. Soc.* 2016).



Using our new Ta catalyst system, we have tested the possible transformation of serine methyl ester or threonine methyl ester to the corresponding dipeptides. As expected, the desired dipeptides are prepared in high yields. After the reaction, the Boc protecting group can be removed without any problems.

The new Ti-complex developed in our group acts as a bimetallic catalyst for regio- and enantioselective epoxidation, sulfoxidation, and amine oxide synthesis. The selective binding abilities of the ligand with metal ions in the bimetallic catalyst-scaffold bear a resemblance to biological enzymatic systems. We are planning to prepare various ligands with not only 8-hydroxyl quinolone as the metal folding site but also orthophenanthroline, dipyridyl, and various heterocyclic sub-unites. Hence, the new ligand system will offer numerous opportunities for various transformations, including epoxidation, sulfoxide synthesis, C-H activation, Diels-Alder reactions, halogenation, etc.



【Expected Research Achievements and Scientific Significance】

Enzyme reaction is one of the long-standing targets for organic synthesis. Unfortunately, however, organic transformation is still much less selective compare to the biological processes. I believe substrate controlled reaction will be able to make a breakthrough for this situation. The concept of this project hopefully may provide one possibility for this future problem.

【Publications Relevant to the Project】

Tsuji,H.;Yamamoto,H. 、 Hydroxy-Directed Amidation of Carboxylic Acid Esters Using a Tantalum Alkoxide Catalyst、J. Am. Chem. Soc.、138、14218-14221、2016
Bhadra,S.;Akakura,M.;Yamamoto,H.、Design of a New Bimetallic Catalyst for Asymmetric Epoxidation and Sulfoxidation、J. Am. Chem. Soc.、137、15612-15615、2015

【Term of Project】 FY2017-2021

【Budget Allocation】 159,200 Thousand Yen

【Homepage Address and Other Contact Information】

https://www3.chubu.ac.jp/catalyst/member/hisashi_yamamoto/

Title of Project : Development of Carbon Dioxide Fixation Reactions

Nobuharu Iwasawa
(Tokyo Institute of Technology, Faculty of Science, Professor)

Research Project Number : 17H06143　Researcher Number : 40168563
Research Area : Organic Chemistry
Keyword : Synthetic Organic Chemistry

【Purpose and Background of the Research】

Development of useful methods to utilize carbon dioxide as a one-carbon source is of paramount importance not only from the standpoint of basic science to realize efficient activation of non-reactive molecules, but also from the standpoint of solving the problem of carbon resources facing our society. In this study, based on the research carried out in our group to realize transition metal-catalyzed carbon dioxide fixation reactions, various new approaches will be examined to realize more general and efficient catalytic reactions, and furthermore, conceptually new methods for carbon dioxide fixation reactions will be explored.

【Research Methods】

The basic approach to realize this goal is the development of newly-designed transition metal complexes, which would utilize novel metal-metal interactions to enable efficient catalytic introduction of carbon dioxide into organic molecules. Utilization of solar energy is another important approach, which will also be investigated extensively. For specific examples, various pincer-type complexes containing metal-metal bonds will be prepared for exploration of efficient hydrocarboxylation reactions of unsaturated hydrocarbons and direct C-H carboxylation reactions of various simple hydrocarbons. Novel metallalactone formation and its application to catalytic synthesis of α,β-unsaturated carboxylic acids will also be studied. Combination of photoredox and carboxylation catalysts to realize metallic reductant-free carboxylation reactions and utilization of photo-excited states as reactive species for carboxylation reactions are also important approaches of this research. New methods for activation of carbon dioxide utilizing cooperative interaction between various transition metal complexes will also be investigated.

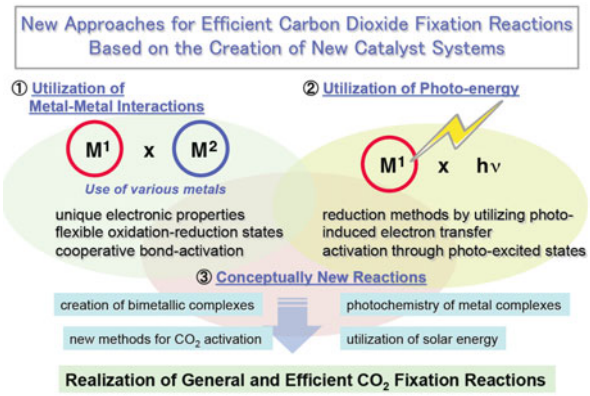


Figure 1 Purpose and Research Methods

【Expected Research Achievements and Scientific Significance】

Development of this research will enable highly useful and efficient atom-economical carbon dioxide fixation reactions, which employ easily available hydrocarbons as starting material. Furthermore, new concepts will be established for novel transition metal catalysis utilizing metal-metal interactions, cooperation of multiple transition metal complexes for developing conceptually new reactions, and utilization of solar energy for CO_2 transformation. This research would also afford new possibilities towards the problem of carbon resources facing our society.

【Publications Relevant to the Project】

・Mechanistic Study of the Rhodium-Catalyzed Carboxylation of Simple Aromatic Compounds with Carbon Dioxide, T. Suga, T. Saitou, J. Takaya and N. Iwasawa, *Chem. Sci.*, **8**, 1454-1462 (2017).
・Construction of a Visible Light-Driven Hydrocarboxylation Cycle of Alkenes by the Combined Use of Rh(I) and Photoredox Catalysts, K. Murata, N. Numasawa, K. Shimomaki, J. Takaya, N. Iwasawa, *Chem. Commun.*, **53**, 3098-3101 (2017).

【Term of Project】 FY2017-2021

【Budget Allocation】 161,300 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.chemistry.titech.ac.jp/~iwasawa/index.html
niwasawa@chem.titech.ac.jp

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

Science and Engineering (Chemistry)

Title of Project : Utilizing the Sacrificial Bonding Principle to Create Soft-Hard Composites with Toughness that Surpasses Metals and Novel Functions

Jian Ping Gong
(Hokkaido University, Faculty of Advanced Life Science, Professor)

Research Project Number : 17H06144 Researcher Number : 20250417
Research Area : Polymer Science
Keyword : Composite, Polymeric Materials, Soft Matter, Gel, High Toughness

【Purpose and Background of the Research】

Our group has proposed a "sacrificial bonding (s-bond) principle" for toughening gels and elastomers, which has enabled the production of unique materials such as double network hydrogels, which contain 90% water but are mechanically comparable to robust industrial rubbers. However, many materials which require high strength rely on stiff reinforcements, resulting in materials like fiber-reinforced plastics (FRP) which are strong and light-weight materials. Recently, we have observed that soft/hard composites whose soft phase is composed of tough, soft materials based on the s-bond principle possess extremely high toughness (tougher than metal) due to the synergetic combination of the two phases. Based on this preliminary result, in this project we will adopt the s-bond principle to soft/hard composites to create a new field of composite materials whose toughness dramatically exceeds that of conventional tough hard materials such as metals and FRPs. Through these studies, we will attempt to establish a scientific model to understand and optimize toughening of soft/hard composite materials.

【Research Methods】

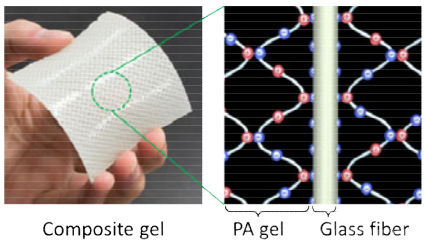


Figure 1. An example of a tough soft/hard composite whose soft phase works as s-bonds.

Our research plan is to fabricate tough soft/hard composites through the following two methods: 1. combining specially-designed, s-bond containing soft phases with conventional hard materials such as glass fibers and metal; 2. combining specially-designed hard phases working as s-bonds with compliant soft phases. Examples of both approaches are shown in Figures 1 and 2.

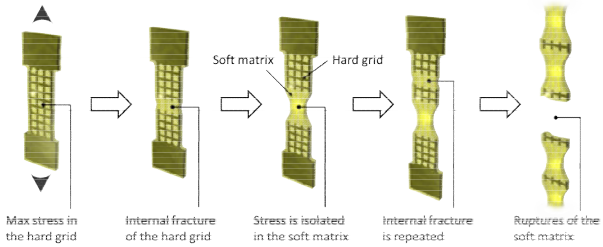


Figure 2. A design of a tough soft/hard composite whose hard phase works as s-bonds.

The effect of sacrificial bonds on the mechanical properties of the composites will be investigated by measuring the energy dissipation during deformation and fracture.

【Expected Research Achievements and Scientific Significance】

Previous research on conventional hard/hard composites has concentrated on their mechanical properties at small strain, such as modulus. In contrast, in this project we will focus on energy dissipation upon large deformation, which plays an important role for toughening of soft materials. This study will lead to a general understanding of soft/hard composites, which may possess properties which greatly surpass current structural materials.

【Publications Relevant to the Project】

Y. Huang, D. R. King, T. L. Sun, T. Nonoyama, T. Kurokawa, T. Nakajima, J. P. Gong, *Adv. Funct. Mater.*, 27(9), 1605350 (2017).

D. R. King, T. L. Sun, Y. Huang, T. Kurokawa, T. Nonoyama, A. J. Crosby, J. P. Gong, *Mater. Horiz.*, 2(6), 584-591 (2015).

【Term of Project】 FY2017-2021

【Budget Allocation】 157,000 Thousand Yen

【Homepage Address and Other Contact Information】

http://altair.sci.hokudai.ac.jp/g2/index.html
gong@sci.hokudai.ac.jp

Title of Project : Creation of superionic conductors

Ryoji Kanno
(Tokyo Institute of Technology, School of Materials and Chemical Technology, Professor)

Research Project Number : 17H06145 Researcher Number : 90135426
Research Area : Solid State Ionics, Solid State Chemistry
Keyword : Superionic conductors, Electrochemical devices, Neutron, Synchrotron X-ray

【Purpose and Background of the Research】

Superionic conductors are the materials showing fast ionic diffusion in the solids. These materials are expected to be used as solid electrolytes in the electrochemical devices and enable the development of novel energy devices such as lithium / sodium batteries with extremely high energy density and power characteristics (Fig. 1).
These materials also provide the oxygen / proton systems with high efficiency power system. On the other hand, novel conducting species such as hydride ion expands novel research fields and energy devices.
In the present study, the key materials which show superionic conductivity will be searched and developed for the energy devices in the future. Especially, the current research focuses on the lithium or hydride ion conductors.
1. Material system to exploit: (i) Bulk material search with wide composition range and (ii) Interfacial design of nano-region of the electrochemical system, which shows superionic conduction.
2. Purpose: Development of the methods for new materials search: (i) Conventional synthesis technique by element substitutions, (ii) Systematic synthesis based on phase diagram, and (iii) Computational chemistry.

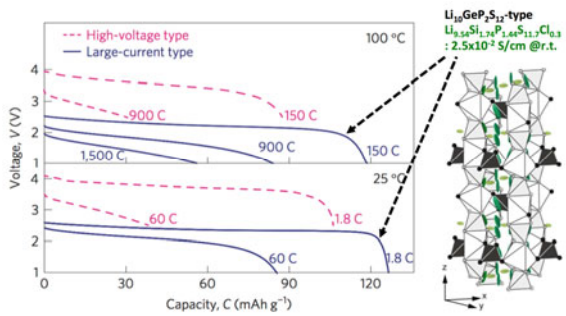


Figure 1 Performances of all solid-state battery using Li superionic conductor, $Li_{9.51}Si_{1.74}P_{1.44}S_{11.7}Cl_{0.3}$.

【Research Methods】

Bulk superionic conductors: Conventional sintering technique and high-pressure synthesis for creating phase diagrams and new materials.
Development of nano interface: Creating a hetero-interface for fast ionic diffusion by single crystal film synthesis under vacuum.
Construction of systematic synthesis method: Introducing computational chemistry method.
Characterization, device construction, and establishment of material search direction: physical property evaluation, evaluation of device characteristics.

【Expected Research Achievements and Scientific Significance】

New materials: Material development based on our new synthesis strategy could provide new energy storage and conversion devices which strongly impact on our society.
Material search method: While the conventional synthesis methods were efficient for the materials search, new methodology is necessary for the developments of materials for the next generation. By combining the conventional technique and new computational chemistry, new methodology for the materials search will be looked for. New superionic conductors will be developed.
Ionic conduction at nano interface: Systematic investigation of the nano region for the ideal hetero-interface is important for designing electrochemical interface in the devices.
Development of ion conduction species: Hydride ion conductor is a new superionic conducting system and may lead to new science in solid-state chemistry and energy chemistry fields.

【Publications Relevant to the Project】

・*Nat Mater*, **10**, 682-686 (2011).
・*Nature Energy*, **1**, 16030 (2016).
・*Science*, **351**, 1314-1317 (2016).

【Term of Project】 FY2017-2020

【Budget Allocation】 129,500 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.kanno.echem.titech.ac.jp

Title of Project : Creation and development of high-order nano-space structures through innovative control of stress field

Yang Ju
(Nagoya University, Graduate School of Engineering, Professor)

Research Project Number : 17H06146 Researcher Number : 60312609
Research Area : Mechanics of Materials, Nanomaterial Engineering
Keyword : Nanomaterial and fabrication process, Nanostructure, Mechanics of nanomaterials

【Purpose and Background of the Research】

This research will establish a radical manufacturing method for high-quality metallic and semiconductive nanospace structures that are highly ordered and highly dense by explaining the diffusion phenomenon of atoms in stress fields. High degrees of control for shapes, dimensions, and spatial positions of nanospace structures will be achieved to realize a low-resistance and high-transmittance transparent conductive film, and a low-cost high-conversion-efficiency solar hydrogen manufacturing device.

【Research Methods】

The diffusion velocity of metallic atoms and the formation velocity of surface oxidation films will be investigated in detail. The control of the atomic arrangements and molecular formations during the growth process will make it possible to control shapes, dimensions, and positions of the ultra-high-quality, highly ordered metallic and semiconductive nanostructures. The mechanisms for the formation of various nanostructures will be systematically explained by expounding on the effects of the stress gradients arising from the thermal expansion of materials and the volumetric expansion due to the oxidation film on the atomic diffusion rate. Furthermore, the effects of the temperature, humidity, and catalyst on the formation rate of the material surface oxidation film, along with the effects of the stress concentrations, crystalline structure, and atomic density on the formation of nanostructures, will also be examined. The formation of a transparent conductive film with a low-resistance that offers a high-transmittance, and a solar hydrogen manufacturing device at a low cost that offers an ultra-high-conversion efficiency will also be carried out.

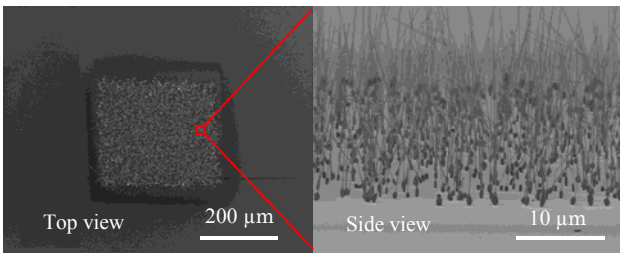


Fig.1 High density Al nanowires

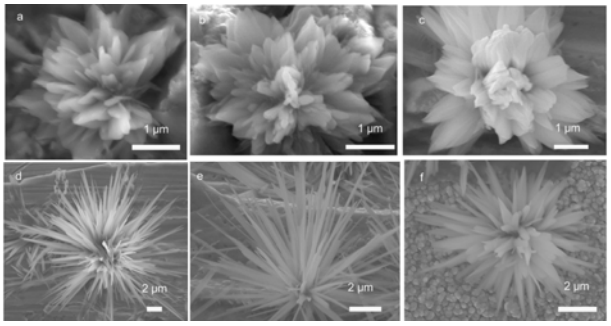


Fig.2 Different structured Cu_2O nanoflowers

【Expected Research Achievements and Scientific Significance】

It will be possible to develop devices which will, in turn, resolve the current issues of transparent conductive film manufacturing cost and solar hydrogen decomposition efficiency in a single sweep, bringing about significant contributions to society.

【Publications Relevant to the Project】

・L. Hu, Y. Ju, M. Chen, A. Hosoi, S. Arai, Growth of Cu_2O Flower/Grass-like Nano Architectures and their Photovoltaic Effects, Applied Surface Science, 305, 710-715, 2014.
・Chen Y. Yue, and Y. Ju, Growth of Metal and Metal Oxide Nanowires Driven by the Stress-induced Migration, Journal of Applied Physics, 111, 104305-1-6, 2012.

【Term of Project】 FY2017-2021

【Budget Allocation】 161,000 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.mech.nagoya-u.ac.jp/ju/index_E.html

Title of Project : Realization of Sustainable Green Society Through 99.9% Class Efficiency Electric Power Conversion

Atsuo Kawamura
(Yokohama National University, Faculty of Engineering, Professor)

Research Project Number : 17H06147　Researcher Number : 80186139
Research Area : Electrical and Electronic Engineering
Keyword : Power conversion, Power electronics, High efficiency inverter

【Purpose and Background of the Research】

One of fundamental key technologies for realization of sustainable industrial society is ultra-high efficiency electric power conversion technology, which enables the super energy saving and increases the more use of renewable energy.

The goal of this project is that it will be experimentally proved that a 5 kw 99.9 % efficiency class inverter can be realized, and using it almost free allocation of distributed energy generators can be realized in the power distribution system.

In the 1st stage, realization of 99.9% class efficiency single-phase inverter will be challenged, and in the 2nd stage, three-phase inverter will be realized at 99.9% class efficiency. Third, it will be experimentally proved that using the above inverter a rapid energy control of PV system is possible. Forth, using this result, it will be verified that super high efficient energy control between the electric vehicle battery and the solar power system is possible. In the final stage, a new concept for the electric power distribution system will be proposed based on the obtained new knowledge.

【Research Methods】

To realize an ultra-efficient flexible energy flow in the low voltage electric energy distribution system, this project is divided into five subtasks, in which five different targets are clearly defined. One of the key targets is the realization of 99.9 % class efficiency inverter, which is made of two parts. One is a high efficient chopper circuit based on the principle of partial power conversion, and the other is turning-up circuit as shown in Fig. 1. The former aims at the reduction of switching loss and the latter targets the conduction loss reduction.

【Expected Research Achievements and Scientific Significance】

The renewable energy has inherent fluctuation within a short period, and a special care is required for the stable operation and voltage regulation of an electric power system. A few kW inverter with 99.9% class efficiency can solve this problem if a rapid energy flow control is realized in the low voltage power distribution system. This technology can be widely applicable for any power conversion field, and one typical example is targeted for a proposal of new power distribution system including renewable energy, which will be one of the basic technologies for the sustainable industrial society.

【Publications Relevant to the Project】

(1) K. Aoyama, N. Motoi, Y. Tsuruta, A. Kawamura, "High Efficient Energy Conversion System for the Decrease in the Battery Terminal Voltage of Electric Vehicles", IEEJ Journal of Industry Applications, Vol.5, No.1, pp.12-19, 2016
(2) Y. Hosoyamada, M.Takeda, T.Nozaki, A.Kawamura, "High Efficiency Series Chopper Power Train for Electric Vehicles Using a Motor Test Bench", IEEJ Journal of Industry Applications, Vol.4, No.4, pp.460-468, 2015

【Term of Project】 FY2017-2021

【Budget Allocation】 138,000 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.kawalab.dnj.ynu.ac.jp/

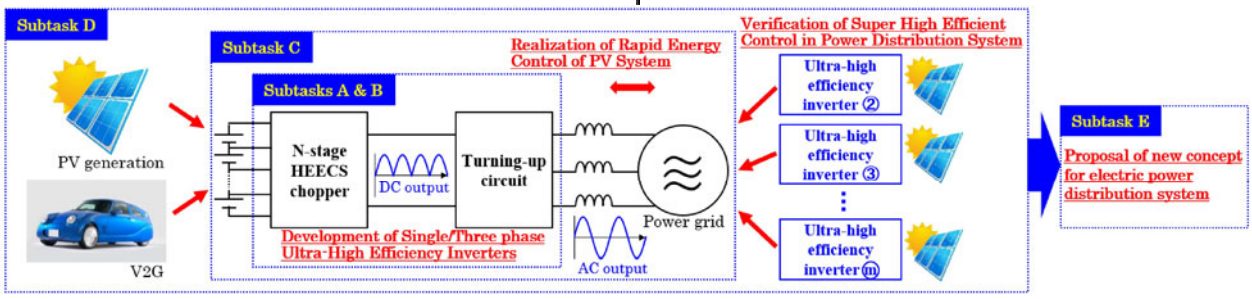


Figure 1　Proposed system configuration and research subtasks

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

Science and Engineering (Engineering)

Title of Project : Precise structure control of 3-dimensional integration CMOS using high mobility materials through layer transfer

Shinichi Takagi
(The University of Tokyo, School of Engineering, Professor)

Research Project Number : 17H06148 Researcher Number : 30372402
Research Area : Electric and Electronic Material Engineering
Keyword : MOSFET, Germanium, III-V compound semiconductors

【Purpose and Background of the Research】

The physical limitations of miniaturization of CMOS used in LSI have recently more evident, leading to the difficulty in satisfying both increase in transistor numbers and improvement in performance. From this viewpoint, 3-dimensional stacked CMOS has started to be examined to increase the number of CMOS without losing the performance. In this study, we establish following science and technologies needed for realizing 3D stacked CMOS using high mobility channel materials, which is promising as a future scaled CMOS, (1) channel formation by layer transfer (2) SD formation and 3D connectivity technology (3) MOS interface control. A typical example of the CMOS structures is shown in Fig. 1. We pursue for methodology of precisely controlling the structure down to nm order, resulting in realizing performance of 3D stacked CMOS and clarifying the direction for future generation scaled CMOS.

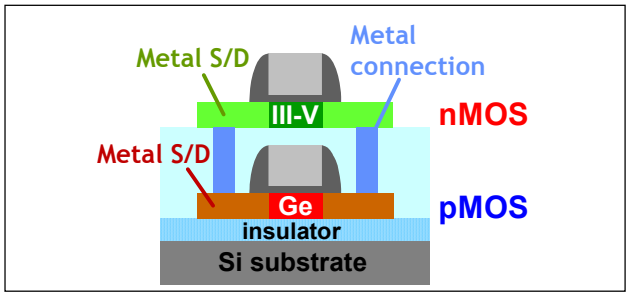


Fig.1 example of stacked CMOS structure

【Research Methods】

(1) Channel formation by layer transfer

We realize ultrathin and flat GOI/III-V-OI films with high crystal quality by using smart cut, shown in Fig. 2, epitaxial lift-off and so on. In addition, we clarify the electronic properties of ultrathin semiconductor channels.

(2) Low temperature source/drain (S/D) formation and 3D connectivity

We pursue for metal S/D materials and the formation process appropriate for the ultrathin Ge/III-V channels with high controllability at low temperature.

(3) High quality MOS interface formation

We establish MOS interface control technologies for minimizing GOI/III-V-OI MOS interface defects.

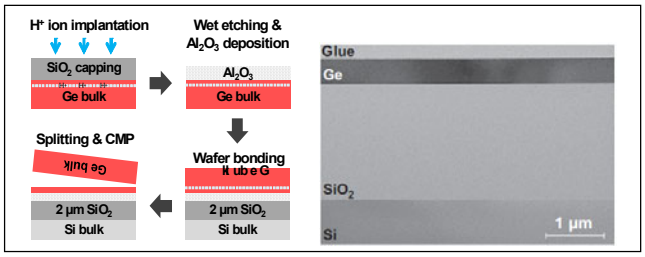


Fig. 2 GOI formation method by smart cut and example of fabricated GOI structure

【Expected Research Achievements and Scientific Significance】

・Establish formation and control technologies for realizing 3D integrated III-V/Ge CMOS with understanding the basic physics

・Clarify interface physics underlying nm-size contacts at hetero-material interfaces

・Develop the transfer technologies of different materials and expand the applications

・Esbatlish comprehensive understanding of the III-V/Ge CMOS technologies from fandamental science to device design and manufacturing.

【Publications Relevant to the Project】

・S. Takagi et al., "III-V/Ge Channel MOS Device Technologies in Nano CMOS era", Jpn. J. Appl. Phys., vol. 54, 06FA01 (2015)

・T. Irisawa, T. Maeda et al., "Demonstration of Ultimate CMOS based on 3D Stacked InGaAs-OI/SGOI Wire Channel MOSFETs with Independent Back Gate", 2014 Symposium on VLSI Technology, 146 (2014)

【Term of Project】 FY2017-2021

【Budget Allocation】 158,900 Thousand Yen

【Homepage Address and Other Contact Information】

http: // www.mosfet.k.u-tokyo.ac.jp/

Title of Project : Evaluation of Drug Response by Elastic Multipoint Electrode Array Using Cardiomyocyte Sheet

Takao Someya
(The University of Tokyo, School of Engineering, Professor)

Research Project Number : 17H06149 Researcher Number : 90292755
Research Area : Electrical and electronics engineering
Keyword : Electronic device and integrated circuit

【Purpose and Background of the Research】

In recent years, stretchable electronics has attracted much attention because it is expected that stretchy and soft electronic materials can improve significantly compatibility with living organisms. Recently, the authors succeeded in realizing high performance organic devices on ultrathin polymer film with a thickness of 1 micrometer. Ultrathin films can be attached to follow complicated surface shapes like living bodies. Indeed, this device was attached to a complex surface of a living body surface such as animal's heart, lungs, and skin, and biological information was monitored. In this research, we aim to apply stretchable electronics to the evaluation of drug reaction.

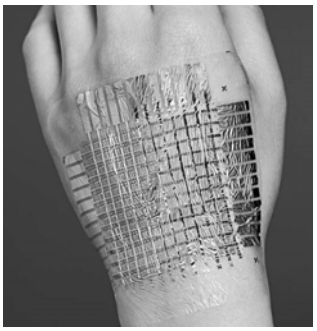


Figure 1: An organic device

【Research Methods】

We have established techniques for producing highly stretchable electronic components on various soft materials such as ultrathin polymer films, rubber sheets, fabrics and so on. In this research, we improve the durability of stretchable devices while maintaining softness.

We evaluate durability of the devices quantitatively while maintaining softness. In particular, we will consider not only the materials themselves but also improve the durability from the viewpoint of the manufacturing process. After that, electrical measurements on myocardial cells are advanced, and the quality of biomedical signals is increased.

【Expected Research Achievements and Scientific Significance】

In this research, we will deepen understanding of science of biointerface where living body and stretchable electronics contact. In the biointerface whose compatibility with the living body is markedly improved by softness, it is expected that the biological signal can be measured stably over a long period of time. By promoting research based on this high stability and reliability as a strength, a biointerface has established a method for highly efficiently converting biological signals by various media such as electrons, ions, chemical substances into electric signals of electronics, Great development is expected for electronics and its application to drug response evaluation.

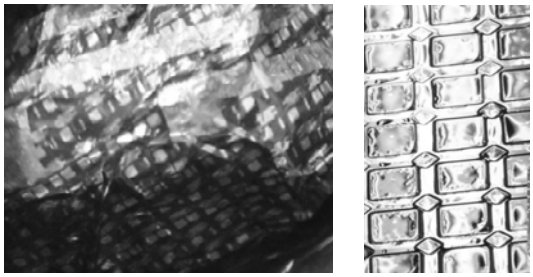


Figure 2: An organic device attached on a rat's heart

【Publications Relevant to the Project】

・Sungwon Lee, Takao Someya, et al., Nature Nanotechnology, vol. 11, pp.472–478 (2016).
・Martin Kaltenbrunner, Takao Someya, et al., Nature, vol. 499, pp.458-463 (2013).

【Term of Project】 FY2017-2021

【Budget Allocation】 157,100 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.ntech.t.u-tokyo.ac.jp/
someya-sec@ee.t.u-tokyo.ac.jp

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

Science and Engineering (Engineering)

Title of Project : Source of various behaviors of living things that understands from zombification of insects

Koichi Osuka
(Osaka University, Graduate School of Engineering, Professor)

Research Project Number : 17H06150 Researcher Number : 50191937
Research Area : Control Engineering, Biology
Keyword : Various Behaviors, Zombification, Implicit Control, Control Structure, Brain-Body-Field

【Purpose and Background of the Research】

Living things show sufficiently high adaptive behavior even if it is a species that has only a tiny central nervous system. Such behavior is thought to be generated from the interaction of the brain, the body, and the environment, but the mechanism of its emergence remains unclear. In order to understand this essence, it is necessary to pay attention to a minimalistic set of interactions of the brain, the body, and the environment, and to extract the control structure underlying it.

Therefore, in this study, we propose a novel methodology to observe the behavior after stepwise inhibiting (zombification) the upper brain function of the animal alive. Based on the control structure identified by this study, we develop a robot adaptable to the real world with a dramatically simple control scheme.

【Research Methods】

We got inspiration from the hunting behavior of Ampulex compressa and came up with a novel methodology to "zombie" without killing the crickets. It is a method to pharmacologically inhibit the brain function of crickets. If such a "zombie cricket" can be realized, it will be possible to reach the smallest cranial nervous system for the first time. And at that time we gained confidence that "a source to create diverse gaits" will come to light.

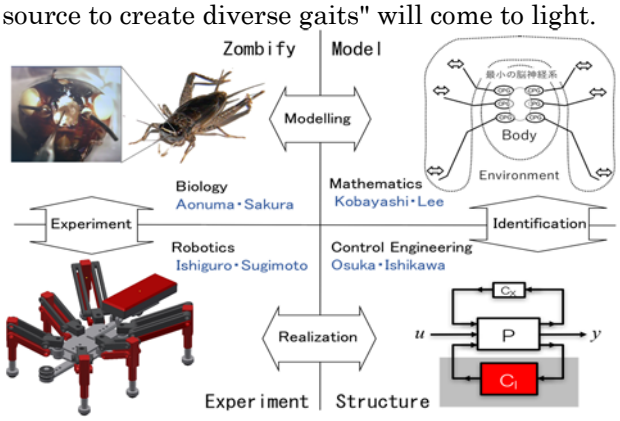


Fig.1 Research procedure

Therefore, as shown in Fig. 1, by combining biology, mathematical science, control engineering and robot engineering, we carry out research by the following procedure.

Theme1: We establish a new method called "Zombification". Here, by properly administering a properly formulated drug to the appropriate part of the brain nerve system, the act of inhibiting the function of that part is called "Zombification".

Theme 2: "Zombie cricket" which gradually strips cranial brain system level is walked in various places by external stimulation. Then, we obtain a mathematical model of the situation, and identify the control structure generating the transformation of the gait. This is the "source of behavior" that we are seeking in this research.

Theme 3: Prove the validity of this research by prototyping a demonstration robot that realizes the identified "source".

【Expected Research Achievements and Scientific Significance】

The success of this trial will gain a major step towards elucidation of the mechanism of development of intellectual behavior shown by living things with simple brain nervous system only.

【Publications Relevant to the Project】

K.Osuka, etc.,al.: Implicit Control Law Embedded in Control System Solves Problem of Adaptive Function!?, J. of the Robotics Society of Japan,Vol.28,No.4,pp.491-502 (2012)

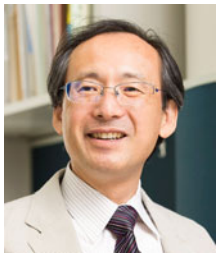
K.Osuka, etc.,al. :Development of Implicit Controlled Centipede Robot (i-CentiPot), Proc. of SICE Symposium on Decentralized Autonomous Systems, pp.18-23(2017)

【Term of Project】 FY2017-2021

【Budget Allocation】 136,800 Thousand Yen

【Homepage Address and Other Contact Information】

http://www-dsc.mech.eng.osaka-u.ac.jp/



Title of Project : Field survey on Impact of living environments on brain, cardiovascular, respiratory and locomotive system, and co-benefit evaluation of disease and long-term care prevention

Toshiharu Ikaga
(Keio University, Faculty of Science and Technology, Professor)

Research Project Number : 17H06151 Researcher Number : 30302631
Research Area : Built environment engineering, Public health
Keyword : Housing insulation, Healthy life expectancy, Cohort study, Intervention study, Co-benefit

【Purpose and Background of the Research】

The influence on health by housing is summarized in many papers including WHO report, such as influence on overall health and mental health by cold, respiratory illness due to air quality or dampness. Housing and health studies are particularly advanced in United Kingdom and New Zealand. Besides, The chapter 9: Building of IPCC/AR5/WG3 report suggested visualization of co-benefits of residents' health and workplace productivity are effective for promoting low carbon buildings.

【Research Methods】

Outline of the research method is shown in Fig.1.

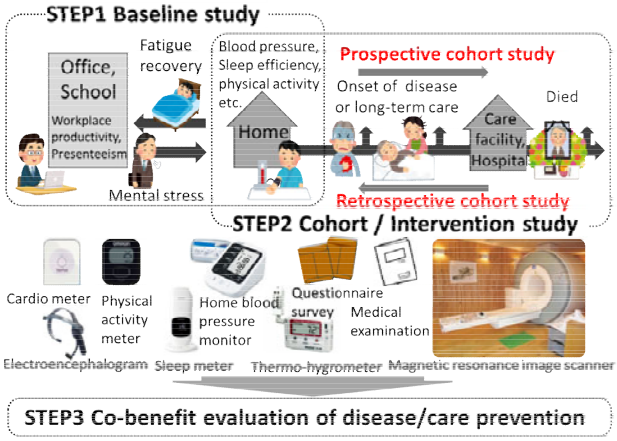


Figure 1. Outline of the research method

STEP1 Baseline study

The research team has conducted a baseline survey on the influence of various living environments on health indicators of residents of a wide range of age ranges from infants to the elderly, with good relationships with the national government, local governments, companies and residents carry out.

STEP2 Cohort / Intervention study

Cohort studies several years after STEP 1 and intervention studies before and after new construction and renovation will be conducted.

STEP3 Co-benefits of disease/care prevention

Combining the research results of STEP 2 with official statistical data, co-benefits of diseases/ care prevention for each household and future forecasts for each national and local governments.

Table1. Architectural and medical research team

1	Keio University	Prof. Toshiharu Ikaga	Architectural and Urban Environmental Engineering	Dr.,Eng.
2		Assoc. Prof. Yasue Mitsukura	Brain Engineering	
3		Assoc. Prof. Yuko Oguma	Exercise Epidemiology	Dr., Medicine
4	Tokyo Metropolitan University	Prof. Emeritus Tanji Hoshi	Public Health	
5		Prof. Fumiko Ito	Urban Planning	Dr., Eng.
6	Jichi Medical University	Prof. Kazuomi Kario	Cardiovascular Medicine	Dr., Medicine
7		Assoc. Prof. Satoshi Hoshide		
8	University of Occupational and Environmental Health	Assoc. Prof. Yoshihisa Fujino	Public Health	
9		Lecturer Tatsuhiko Kubo		
10	Kanazawa University	Prof. Hiroyuki Nakamura		
11	Toho University	Prof. Fjiko Fukushima	Midwifery	
12	Tokyo Dental College	Prof. Masaru Suzuki	Emergency Medicine	
13	National Institute of Health Sciences	Dr. Maiko Watanabe	Health Microbiology	Dr., Science
14	University of Kitakyusyu	Prof. Yasuyuki Shiraishi	Architectural and Urban Environmental Engineering	Dr., Eng.
15		Lecturer Shintaro Ando		
16	Hosei University	Lecturer Shun Kawakubo		

【Expected Research Achievements and Scientific Significance】

In this research, architectural studies and medical experts shown in Table 1 cooperate with national government, local governments, companies and residents to measure living environment in daily life and health data. Results of this research are useful not only for individuals but also for policy makers.

【Publications Relevant to the Project】

-Evaluation of Investment in Residential Thermal Insulation, Considering Non-Energy Benefits delivered by Health, Journal of Environmental Engineering, Architectural institute of Japan, Vol. 76, No. 666, 2011
-Lower Physical Performance in Colder Seasons and Colder Houses: Evidence from a Field Study on Older People Living in the Community, Int. J. Environ. Res. Public Health, 2017

【Term of Project】 FY2017-2021

【Budget Allocation】 159,700 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.ikaga.sd.keio.ac.jp/index-en.php
ikaga@sd.keio.ac.jp

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

Science and Engineering (Engineering)

Title of Project : Spin-dependent conduction mechanism of half-metallic Heusler alloys and applications to practical devices

Kazuhiro Hono
(National Institute for Materials Science, Research Center for Magnetic and Spintronic Materials, Fellow)

Research Project Number : 17H06152 Researcher Number : 60229151
Research Area : Metallic materials
Keyword : Spintronics, Half metal, Heusler alloy, CPP-GMR

【Purpose and Background of the Research】

Spintronics is the field of science and technology to develop devices for data storage and memory for the IoT society, such as non-volatile magnetic random access memories (MRAM) and high-sensitive magnetic sensors. We have been working on the half-metallicity of Co-based Heusler alloys for spintronics applications. By employing new alloys, we have successively renewed the world record of the magnetoresistance (MR) ratio of current-perpendicular-to-plane giant magnetoresistance (CPP-GMR) devices, which consist of two ferromagnetic (FM) layers separated by a non-magnetic (NM) spacer layer. A large MR ratio of 285% at 10 K was recently achieved; however, it drops to 82% at room temperature. The purpose of this study is to understand the underlying mechanism of the large temperature degradation MR at room temperature and to develop practical devices with large MR ratio at room temperature through the investigation of the structure and the electronic state of Heusler alloys.

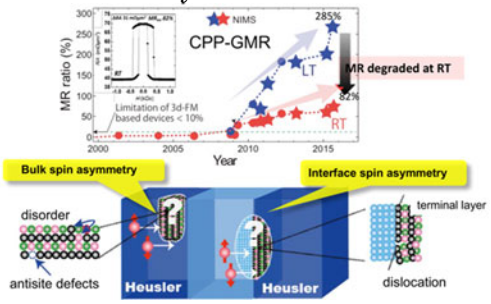


Fig. 1 Trend of CPP-GMR and two spin asymmetries to be considered as underlying mechanism.

【Research Methods】

First, we prepare thin films of Heusler alloys and evaluate the spin polarization from the measurement of the anisotropic magnetoresistance. We also prepare CPP-GMR devices and examine the MR properties. Electronic states of the Heusler alloys and its variation at FM/NM interfaces are s examined by pin resolved photo electron spectroscopy (PES). Magnetic moment of the atoms at FM/NM interfaces are examined by x-ray magnetic circular dichroism (XMCD). The degree of chemical order is investigated by abnormal dispersion XRD using synchrotron radiation for resolving species with similar atomic numbers. Aberration corrected scanning transmission electron microscopy (STEM) is utilized to observe the local nano structure at the interfaces. In addition, first principles calculations are used to expect the structural and electronic properties.

On the basis of the experimental and theoretical investigations, new materials and processes is developed and evaluated for improving the MR properties at room temperature and realizing ultrahigh sensitive magnetic sensors.

【Expected Research Achievements and Scientific Significance】

A distinguishing feature of this study is to combine various research methods such as sample preparation, characterizations and theoretical investigations for resolving scientific and technological issues for realizing half-metallicity at room temperature. It would lead to ultimate performance in not only CPP-GMR sensors but also other spintronic devices such as tunnel magnetoresistance (TMR).

【Publications Relevant to the Project】

・J. W. Jung *et al.*, *Enhancement of magnetoresistance by inserting thin NiAl layers at the interfaces in $Co_2FeGa_{0.5}Ge_{0.5}$/Ag/$Co_2FeGa_{0.5}Ge_{0.5}$ current-perpendicular-to-plane pseudo spin valves*, Appl. Phys. Lett. 108, 10408 (2016).
・Y. Sakuraba *et al.*, *Quantitative analysis of anisotropic magnetoresistance in Co_2MnZ and Co_2FeZ epitaxial thin films: A facile way to investigate spin-polarization in half-metallic Heusler compounds*, Appl. Phys. Lett. 104, 172407 (2014).

【Term of Project】 FY2017-2021

【Budget Allocation】 162,400 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.nims.go.jp/mmu/index.html
kazuhiro.hono@nims.go.jp

Title of Project : New evolution of materials concept and application of electrides

Hideo Hosono
(Tokyo Institute of Technology, Institute for Innovative Research, Professor)

Research Project Number : 17H06153 Researcher Number : 30157028
Research Area : Inorganic Materials･Materials Property
Keyword : Novel Inorganic Materials, Electrides

【Purpose and Background of the Research】

Electride is a compound in which electrons serve as anions and may be regarded as the crystal of solvated electrons. First electride materials were synthesized by dissolving alkali metal into crown ether solutions in 1983. Although these organic electrides attracted attention as an exotic material as cited in university textbooks of inorganic chemistry, their property research remained almost uncultivated due primarily to extremely high sensitivity to heat and oxidation. We realized the first RT-stable electride C12A7:e in 2003 by replacing O^{2-} ions as counter anions in $12CaO \cdot 7Al_2O_3$(C12A7) with electrons, and found several unique properties such as insulator-metal-superconductor transition and very small work function. Subsequently, we found 2-dimensional electride, Ca_2N, in which anionic electrons are sandwiched by cationic $[Ca_2N]^+$ slabs. These works stimulated the condensed matter community, leading to rapid growth of research on electride materials worldwide, recently. However, electride research so far has been restricted to anion deficient-type crystalline materials.

Our objective in the project is to cultivate new area of electride materials and their applications based on the recent findings of new crystalline and amorphous electrides.

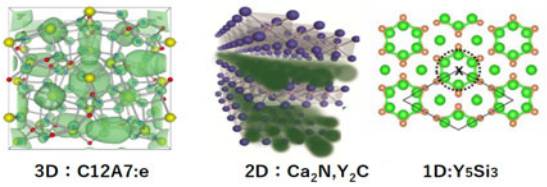


Fig.1. New electrides reported by our group

【Research Methods】

Focused fundamentals : Focuses are low dimensional electride materials in electron deficient type, neutral electrides and surface electride materials. Material systems for exploration expand to intermetallic compounds.

Applications: Thin film fabrication is examined for electric device applications. In particular, amorphous C12A7:e thin films are focused as an electron-injection layer in the inverted OLEDs which are difficult to fabricate the devices with a good performance.

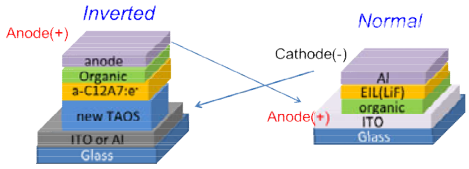


Figure 2. Inverted OLED

【Expected Research Achievements and Scientific Significance】

It is expected that materials concept for electrides is expanded and opportunity of applications based on the intrinsic nature is rather increased. Since amorphous electride is a novel class of amorphous semiconductors, research on this subject would open a new frontier. In device application, inverted OLEDs with performance comparable/superior to the normal type would be realized. We expect the good catalytic activity for new electride materials.

【Publications Relevant to the Project】

・H.Hosono et al. Superconductivity in room-temperature stable electride and high-pressure phases of alkali metals; Phil. Trans. R. Soc. A373, 20140450-62(2015).
・E. Johnsona, P.V. Sushko, Y.Tomota, and H.Hosono: Electron anions and the glass transition temperature; Proc. Natl. Acad. Sci. USA, 113, 10007-10012(2016).

【Term of Project】 FY2017-2021

【Budget Allocation】 134,600 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.msl.titech.ac.jp/~hosono/

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

Science and Engineering (Engineering)

Title of Project : Research and development on artificial production of next generation of Rare-Earth Free Magnets with $L1_0$ phase similar to Cosmic magnet

Akihiro Makino
(Tohoku University, New Industry Creation Hatchery Center, Professor)

Research Project Number : 17H06154　Researcher Number : 30315642
Research Area : Engineering
Keyword : Energy Materials

【Purpose and Background of the Research】

High performance rare earth based magnet (Nd-Fe-B) developed domestically about 30 years ago resulted in the production of small sized and high efficiency motors for next generation of automobiles (HV, PHV, EV, FCV), home appliances, and industrial machineries. These magnets contribute significantly in saving energy, and led the world to grow in a sustainable manner. Further improvements in the performance of rare earth based magnets have reached the limit. Additionally, economic advantages are disappearing due to expiration of basic patents. Above all, the major obstacle is in the sustainable supply of rare earth elements, and it is predicted to be serious in future. Shortage in supply can hamper the growth of economy, industries and energy saving technologies in our country. Therefore, demand for a new low cost and high performance magnetic material, that can replace rare earth magnets is intense. In the current scenario, a trace amount of hard magnetic $L1_0$ FeNi phase discovered in meteorites (which were formed over billions of years) is of huge interest. This is because of magnetic performance similar to rare earth, but the artificial production of this phase is extremely difficult.

This project dares to create a chemically ordered $L1_0$ FeNi phase artificially. The aim is to develop a next generation of completely rare earth free magnet.

【Research Methods】

Our focus is on achieving a fast atomic diffusion at lower temperatures that is observed during nanocrystallization of amorphous phase. By nanocrystallizing an FeNi-based amorphous alloy, we have obtained $L1_0$ FeNi phase with ordering parameter ~ 0.8 and volume fraction ~ 10%. In this project, first of all, we will grasp the fundamental physical properties of this artificially prepared $L1_0$ FeNi phase, and clarify its potential as a hard magnetic material for next generation of magnets. Therefore, we aim at grasping the optimum alloy composition by exploring different FeNi-based amorphous systems and optimizing the nanocrystallization process. This is to increase the volume fraction of ordered phase in the currently obtained sample, and measure the intrinsic physical properties of $L1_0$ ordered phase alone. Subsequently, we will grasp the basic physical properties in detail by thermal analysis using differential scanning calorimeter (DSC), magnetic properties by vibrating sample magnetometer (VSM), structural properties by high resolution electron microscopy observation, micromagnetics simulation, etc.. After it, we will extract and resolve the issues related to production and industrialization of FeNi based magnets.

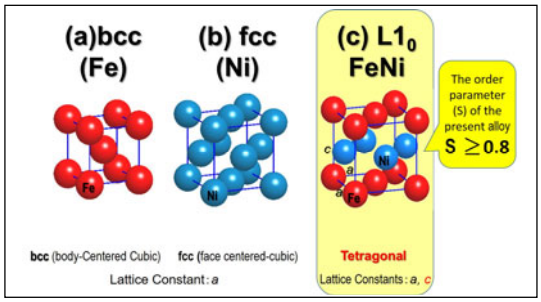


Figure 1　Representative phases in Fe-Ni binary system and their atomic arrangements

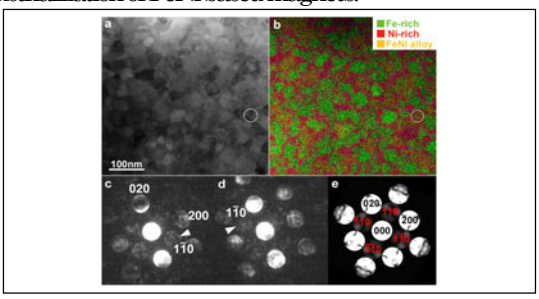


Figure 2 TEM observations on artificially produced $L1_0$ FeNi phase.

【Expected Research Achievements and Scientific Significance】

We resolve the risks of rare earth supply, secure Japan's future technological superiority based on energy saving technologies and contribute to the maintenance of international competitiveness in our country. It revives the stagnating field of hard magnetic materials, and it is expected to open the door to new "super equilibrium" in material science through non-equilibrium.

【Publications Relevant to the Project】

・An Artificially Produced Rare-Earth Free Cosmic Magnet. [Scientific Reports,5,(2015),16627-1-16627-7]
Makino A., Sharma P., Sato K., Takeuchi A., Zhang Y., Takenaka K.
・Crystallization induced ordering of hard magnetic $L1_0$ phase in melt-spun FeNi-based ribbons. [AIP Advances,6(5),(2016),055218-1-055218-9]
Sato K., Sharma P., Zhang Y., Takenaka K., Makino A.

【Term of Project】 FY2017-2021

【Budget Allocation】 156,600Thousand Yen

【Homepage Address and Other Contact Information】

http://nanom.imr.tohoku.ac.jp/
nanom@imr.tohoku.ac.jp

Title of Project : Modeling of solidification dynamics supported by 3D time-resolved in-situ observations

Hideyuki Yasuda
(Kyoto University, Graduate School of Science and Engineering, Professor)

Research Project Number : 17H06155 Researcher Number : 60239762
Research Area : Materials Science, Solidification Processing
Keyword : Melting/Solidification, Casting, Crystal growth/Fabrication

【Purpose and Background of the Research】

The control of solidification structures and the reduction of solidification defects are critical issues for improving the materials properties. Difficulties with observing solidification phenomena *in-situ* for metallic alloys, particularly those with high melting temperatures, have led to ambiguities in under-standing the solidification process. Recently, our group has developed 2D time-resolved *in-situ* observation techniques (using transmission images) at SPring-8 addressing some of these ambiguities. Further advances are possible with 3D time-resolved *in-situ* observation (4D-CT) and these will assist in the development and verification of quantitative models.

In this project, 4D-CT techniques for observing solidification will be developed using X-ray imaging techniques developed by our group and using the advanced photon source at SPring-8. 4D-CT is applied to observe solidification phenomena. Fundamentals and previously unobtainable knowledge relating to the solidification process and the formation of casting defects will be obtained using these methods.

【Research Methods】

[A] Development of 4D-CT

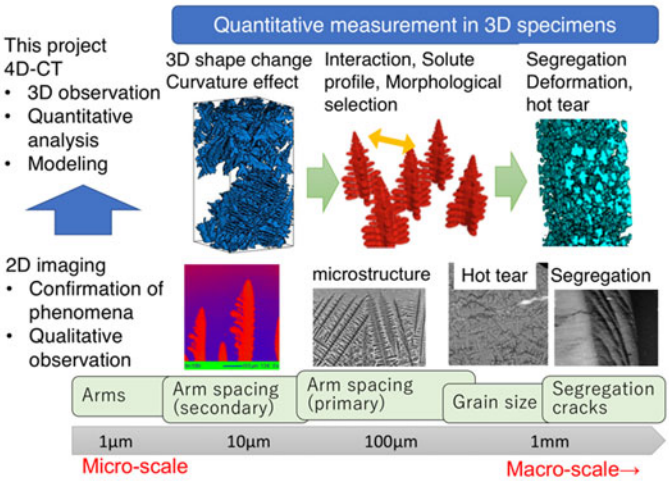
A 4D-CT technique will be developed for observing the evolution of solidification structure in metallic alloys. Expected spatial resolutions are 10μm for fast CT (period: 2s) and 1μm for high resolution CT (10s), respectively.

[B] 3D time-resolved in-situ observation

4D-CT observations will be performed for solidification of metallic alloys. For example, observation of 3D configuration and crystallographic orientation of solid grains in the semisolid state will help in understanding semisolid deformation, which is valuable for predicting casting defects.

[C] Quantitative modeling and simulation

Solidification models considering curvature effects and the configuration of solid grains will be constructed for predicting solidification structure and defects. In addition, computational materials science will be used for understanding experimental results.



【Expected Research Achievements and Scientific Significance】

New knowledge for understanding the solidification process will be obtained by the 4D-CT observations. The knowledge will contribute to the development of reliable models, which will be validated by the observations. The models will allow a greater degree of microstructure control during typical commercial solidification processes.

【Publications Relevant to the Project】

・M.A.A. Mohd Salleh, C. M. Gourlay, J. W. Xian, S. Belyakov, H. Yasuda, S. McDonald, K. Nogita, Sci Rep, 7 (2017) 40010.
・K. Yamane, H. Yasuda, A. Sugiyama, T. Nagira, M. Yoshiya, K. Morishita, K. Uesugi, A. Takeuchi, Y. Suzuki, Metall Mater Trans A, 46A (2015) 4937.
・T. Nagira et al, Metall Mater Trans A, 45A (2014) 1415.

【Term of Project】 FY2017-2021

【Budget Allocation】 130,200 Thousand Yen

【Homepage Address and Other Contact Information】

http://cast.mtl.kyoto-u.ac.jp
yasuda.hideyuki.6s@kyoto-u.ac.jp

Title of Project : The Theory of Microwave-induced Nonequilibrium State and its Application to the Manipulation of Solid/Interfacial Chemical Reactions

Yuji Wada
(Tokyo Institute of Technology, School of Materials and Chemical Technology, Professor)

Research Project Number : 17H06156 Researcher Number : 40182985
Research Area : Process/Chemical engineering, Catalyst/Resource chemical process
Keyword : Microwaves, Control of catalytic reactions, Nonequilibrium reaction field, Microwave special effects

【Purpose and Background of the Research】

Microwaves induce mobile excitation of electrons, ions, molecular structures, and crystal lattices, giving rise to "nonequilibrium states" which cannot be achieved by conventional heating processes. These "non-equilibrium states" occurring at local solid surfaces in a short time lead to not only enhancement of chemical reactions but also selective heating of specific substances (Fig. 1).

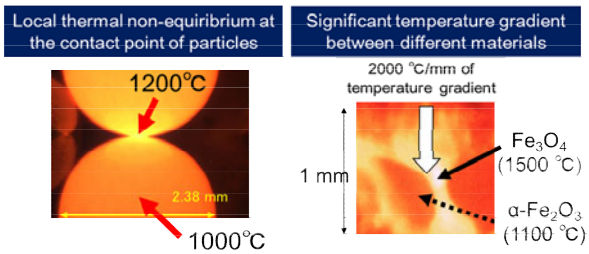


Fig. 1, Local thermal non-equilibrium generated under microwave irradiation

We will establish in situ observation methods of short-lived and local non-equilibrium states occurring at surfaces and/or bulk of substances for understanding the theory of specific enhancement of chemical reactions. Our targets are 1) to reveal the mechanism of non-equilibrium states leading to the manipulation of catalytic reactions under microwaves, 2) to reveal specific enhancement and lowering the temperatures in reduction of metal oxides under microwaves leading to a novel smelting technology of metal, 3) to establish a synthetic method of non-equilibrium phase (new compounds, supersaturated solid solutions), 4) creation of new ferroelectric, ferromagnetic, photo-electric, or photo-magnetic materials which are never synthesized by conventional reactions.

【Research Methods】

The joint research group of Wada lab (Tokyo Tech) and Takizawa lab (Tohoku Univ.) will challenge *in situ* observations of "non-equilibrium states" induced by microwaves and apply them to manipulation of chemical reactions.

Target 1: To understand the mechanisms of non-equilibrium states by *in situ* observation: 1) To design and create *in situ* observation systems, 2) To establish a simulation method of electromagnetic and heat transfer for analyzing heterogeneous temperature distribution, 3) To create a measuring system of absorption capacity of microwaves at microscopic local area.

Target 2 by Tokyo Tech group: To create novel catalytic systems using microwaves.

Target 3 by Tohoku Univ. group: To create novel materials using microwaves.

【Expected Research Achievements and Scientific Significance】

Researches on manipulation of chemical reactions based on thermodynamics and kinetics including catalysts etc. have matured, but we need to challenge chemical activation of stable compounds such as methane and carbon dioxide which requires a novel approach. In addition, we need new materials which can be made using "non-equilibrium state" induced by microwaves. The present study will provide a new generation technology in manipulation of chemical reactions.

【Publications Relevant to the Project】

・T. Ano, F. Kishimoto, R. Sasaki, S. Tsubaki, M. M. Maitani, E. Suzuki, Y. Wada, *In situ* temperature measurements of reaction spaces under microwaves using photoluminescent probes, *Phys. Chem. Chem. Phys.*, 18, 13173-13179, (2016).
・D. Nagao, J. Fukushima, Y. Hayashi and H. Takizawa, Synthesis of homologous compounds $Fe_2O_3(ZnO)_m$ (m = 6, 8, 34) by various selective microwave heating conditions, *Ceram. Int.*, 41, 14021-14028, (2015).

【Term of Project】 FY2017-2021

【Budget Allocation】 160,200 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.apc.titech.ac.jp/~ywada/wada/
yuji-w(at)apc.titech.ac.jp

Title of Project : Integrated platform for mammalian cell-based cell and bioprocess engineering

Takeshi Omasa
(Osaka University, Graduate School of Engineering, Professor)

Research Project Number : 17H06157 Researcher Number : 00252586
Research Area : Process engineering, Biochemical engineering
Keyword : Biopharmaceutical, mammalian cell engineering

【Purpose and Background of the Research】

Mammalian cell lines are important host cells for the industrial production of pharmaceutical proteins owing to their capacity for correct folding, assembly and post-translational modification. In particular, Chinese hamster ovary (CHO) cells are the most dependable host cells for the industrial production of therapeutic proteins, such as therapeutic antibodies. Growing demand for therapeutic proteins is promoting the development of technologies to increase the productivity and output quality of CHO expression systems. Ideally, a CHO expression system should exceed g/L levels of production, whilst minimizing cell culture costs. To achieve this, the cultivation of CHO cells requires optimization. In this proposal, we focus on the genomic instability of CHO cells and analyze the instability/heterogeneity of the CHO chromosomes (genome). In particular, we aim to: (1) construct a genomic cell engineering system, (2) analyze the log-term and/or continuous bioprocess involved, and (3) construct an integrated platform for CHO cell-based cell and cell culture engineering.

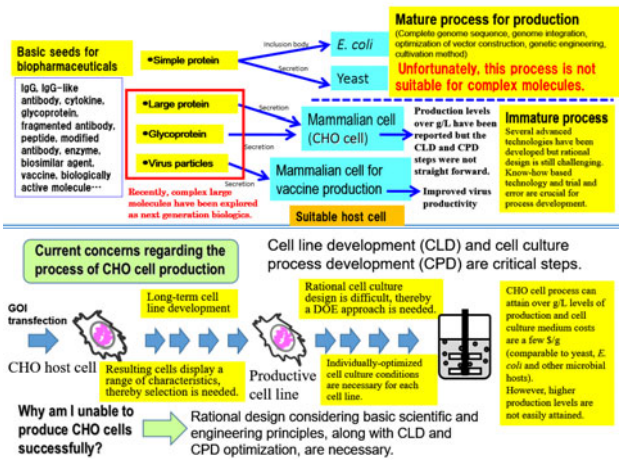


Figure 1 CHO bioprocess for biopharmaceutical production

【Research Methods】

The methodology applied in this study can be divided into three sections: (1) cell engineering using target-integration into CHO chromosomes to establish genome-scale cell engineering, (2) construction of an advanced bioprocess on the basis of stability and heterogeneity analysis of the CHO cell genome under log-term and/or continuous operation, and (3) integration between cell engineering and the advanced bioprocess to construct platform technology for CHO cell-based cell and cell culture engineering.

【Expected Research Achievements and Scientific Significance】

The genome sequence of CHO cells has been published; however, the instability of the CHO genome means that these sequence data are not always accurate or applicable. Therefore, to construct an integrated platform, we developed a strategy of advanced cell and bioprocess engineering, as illustrated in Figure 1.

【Publications Relevant to the Project】

Noriko Yamano, Mai Takahashi, Seyed Mohammad Ali Haghparast, Masayoshi Onitsuka, Toshitaka Kumamoto, Jana Frank, and Takeshi Omasa "Increased recombinant protein production owing to expanded opportunities for vector integration in high chromosome number Chinese hamster ovary cells" Journal of Bioscience and Bioengineering, **122**(2):226-231 (2016).

Yihua Cao, Shuichi Kimura, Takayuki Itoi, Kohsuke Honda, Hisao Ohtake, and Takeshi Omasa "Construction of BAC-based physical map and analysis of chromosome rearrangement in Chinese hamster ovary cell lines" Biotechnology and Bioengineering, **109**(6):1357-1367 (2012).

【Term of Project】 FY2017-2021

【Budget Allocation】 118,400 Thousand Yen

【Homepage Address and Other Contact Information】

http://www-bio.mls.eng.osaka-u.ac.jp/
omasa@bio.eng.osaka-u.ac.jp

Title of Project : Development of platform for ultra high-throughput screening of novel bioactive compound producers

Haruko Takeyama
(Waseda University, Faculty of Science and Engineering, Professor)

Research Project Number : 17H06158 Researcher Number : 60262234
Research Area : Biofunction, Bioprocess
Keyword : Raman spectrometry, Database, Bioactive compound, Single-cell analysis, Microbe

【Purpose and Background of the Research】

The studies for screening of lead compounds (bioactive compounds) from microbes have a long history. So far, over 20000 kinds of bioactive compounds have been discovered from environmental microbes. If we can identify the potential producers and obtain the biosynthetic gene clusters for the production of bioactive compounds, we can achieve to acquiring the lead compounds and apply them for production of new drugs. To achieve this, we need a new platform for ultra-high-throughput screening of bioactive compound producers from various microbes and obtaining biosynthetic gene sequences from uncultivable strains.

【Research Methods】

In this study, we aimed to construct the Raman spectrum database of microbial secondary metabolite from libraries of microbes isolated from soil and the ocean. The Raman spectroscopy can reveal the molecular structure of target molecule non-invasively, so that cells producing metabolites can be identified at the single-cell level. Furthermore, in order to screen bioactive compound producers from environmental microbes, we will acquire Raman spectrum of single cells based on microfluidic platform. For uncultivable microbes, we will also obtain genome information from single cells. For this purpose, we will improve high throughput cell-handling technology using microfluidic device and informatics analysis method for analyze their genomic features. We will proceed with the functional analysis of the obtained novel bioactive compound gene clusters and establish this technique as world leading reading technology in the field of drug discovery lead compound screening (Fig. 1).

【Expected Research Achievements and Scientific Significance】

The *in vivo* Raman signal database which constructed in this research is expected to be useful tool in various research fields including drug discovery and industrial production of biochemical compounds. In addition, the single-cell genomics platform will make effective use of unused resources such as uncultivable microbes. This ultra-high-throughput screening platform would be a fundamental technology indispensable for exploring lead compounds in future drug discovery research and its applications.

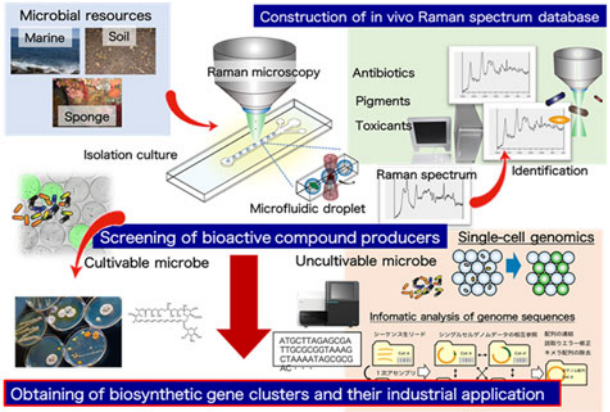


Fig. 1 Platform for screening of bioactive compound producers

【Publications Relevant to the Project】

・Miyaoka R, et al. 2014. In situ detection of antibiotics Amphotericin B produced in *Streptomyces nodosus* using Raman microspectroscopy. Marine Drugs. 12(5), 2827-2839
・Wilson MC, et al. 2014. An environmental bacterial taxon with a large and distinct metabolic repertoire. Nature 12959. 506(7486):58-62

【Term of Project】 FY2017-2021

【Budget Allocation】 157,700 Thousand Yen

【Homepage Address and Other Contact Information】

http:// www.f.waseda.jp/haruko-takeyama/
haruko-takeyama@waseda.jp

Title of Project : Study on Multi-photon gamma-ray coincidence tomography

Hiroyuki Takahashi
(The University of Tokyo, Institute of Engineering Innovation, Professor)

Research Project Number : 17H06159 Researcher Number : 70216753
Research Area : Nuclear Engineering
Keyword : Radiation Measurement, Nuclear Medicine, Imaging, Coincidence, Gamma ray

【Purpose and Background of the Research】

Conventional gamma-ray diagnostics methods such as PET and SPECT have some fundamental limitations in resolution and sensitivity, respectively. We propose a new concept of time/position correlation type tomography method based on electron-tracking type gamma camera which can identify incident gamma-ray direction. This tomography method utilizes the correlation between multiple photons and provides the radioactivity concentration in the body with high resolution, high sensitivity, and high signal to noise ratio. We will study basic characteristics of this revolutionary gamma-ray imaging approach and try to fabricate a hemisphere scanner and explore the new principle. We plan to demonstrate molecular imaging with the In-111 labelled peptide through the two photon emission nuclide detection scheme for establishing a new gamma-ray diagnostic technique for the multiple gamma photon emitting nuclide such as Sc-44.

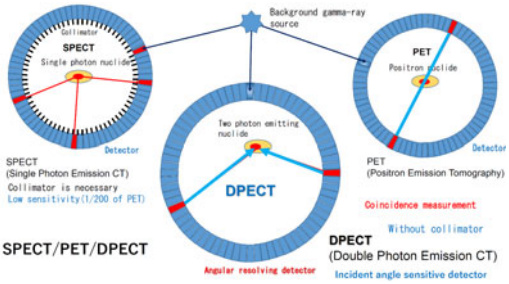


Figure 1 Comparison of SPECT/PET/DPECT

【Research Methods】

Gamma-ray imaging technique based on Time/Space correlation method will be proven and demonstrated. Pursuing its very high spatial resolution, sensitivity, and signal to noise ratio, This method is superior to others because the basic performance. The double photon emission computed tomography(DPECT: see Figure 1) is proposed here. We plan to make a hemisphere scanner which shows an event position without reconstruction methods. This research work is to develop a dedicated detector module, which consists of a semiconductor high resolution electron tracking detector and a high resolution scintillator pixel array. We also plan to fabricate a DPECT scanner using these modules arranged in a hemisphere geometry. Finally we will use an In-111 labelled peptide to show a mouse imaging as a demonstration of DPECT imaging scheme.

【Expected Research Achievements and Scientific Significance】

Establishment of a novel gamma-ray imaging principle and high-resolution molecular imaging beyond PET. PET requires 10^6 line of responses (LORs). Figure 2 shows two Compton camera images. Coincidence image is greatly improved.
Even one event provides one drug position in case if we use electron tracking method. This implies a very high sensitivity of molecular imaging, which can describe molecular interactions or antibody labelled tumor research.

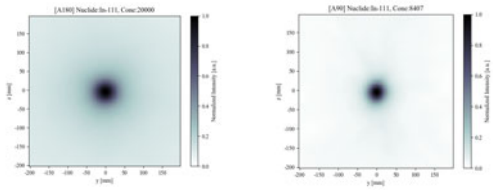


Figure 2 Two Compton camera images without coincidence (left) and with coincidence (right)

【Publications Relevant to the Project】

Y. Yoshihara, et al. Evaluation of double photon coincidence Compton imaging method with GEANT4 simulation, Nucl. Instr. and Meth. A, in press.

【Term of Project】 FY2017-2021

【Budget Allocation】 158,300 Thousand Yen

【Homepage Address and Other Contact Information】

http://sophie.q.t.u-tokyo.ac.jp/~mpect
leo@n.t.u-tokyo.ac.jp