

【Grant-in-Aid for Specially Promoted Research】
Science and Engineering (Mathematics/Physics)



Title of Project : Ultrahigh-pressure Material Science of the Central regions of the Earth and Planet

Eiji Ohtani
(Tohoku University, Graduate school of Science, Professor)

Research Area : High Pressure Earth Science

Keyword : Earth and Planetary Materials, Evolution of Earth, Core, Mineral Physics

【Purpose and Background of the Research】

The first objective is to generate pressure and temperature conditions that cover the center of the Earth.

The second objective is to clarify the nature of the various transitions occurring in the lower mantle and core. These transitions include spin crossovers and the post-perovskite transition in lower mantle minerals, and magnetic transitions in iron alloys at high pressures and temperatures.

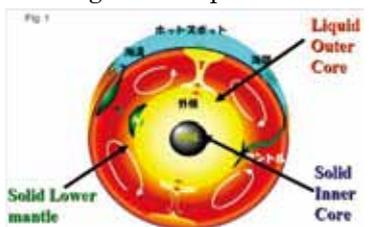
The third objective is to clarify the sound velocities of the lower mantle and core materials. A unique mineralogical model has not yet been proposed for the central region of the Earth because of a lack of reliable data on the sound velocity of the deep Earth's interior.

【Research Methods】

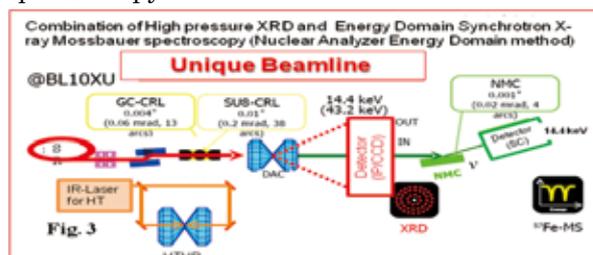
We will make simultaneous measurements of the compression and sound velocity of MgO and the B1 and B2 phases of NaCl to establish a primary pressure scale for core conditions.

We will also establish routine procedures for the generation of high temperatures exceeding 3000 K at core pressures, and we will perform in situ X-ray observations.

We will conduct X-ray Mossbauer spectroscopy using the nuclear analyzer energy domain method, together with the conventional X-ray powder diffraction method at high pressures and temperatures (Figure 3) to determine the valence states of the iron, the spin states of the iron in lower mantle silicates, and the magnetic properties of iron alloys in micro-samples under extreme conditions. We will also perform sound velocity measurements of the mantle and core forming minerals at high pressures and



temperatures using inelastic X-ray scattering (IXS) spectroscopy and Brillouin scattering spectroscopy.



【Expected Research Achievements and Scientific Significance】

Previous mineralogical models of the Earth's deep interior have been limited to the density model because of a lack of reliable data on the seismic velocities of the materials in the lower mantle and core.

Our goal is to present an advanced model of the lower mantle and core that can explain both the seismic velocities and the density observed in seismology. We can break through the current limit in our understanding of the Earth's deep interior with the results of this project.

【Publications Relevant to the Project】

- E. Ohtani, Melting relations and the equation of state of magmas at high pressure: application to geodynamics, Chemical Geology, Vol. 265, No. 3-4, 279-288, 2009.
- E. Ohtani, D. Andrault, P. D. Asimow, L. Stixrude, Y.Wang, Editors, Advances in high-pressure mineral physics: From the deep mantle to the core, Physics of the Earth and Planetary Interiors, 174, Issues 1-4, 2009.

【Term of Project】 FY2010-2014

【Budget Allocation】 371, 100 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.ganko.tohoku.ac.jp/bussei/newHP/busseihp/tokusuiHP_22-26/index_e.html

Grant-in-Aid for Specially Promoted Research

【Grant-in-Aid for Specially Promoted Research】
Science and Engineering (Mathematics/Physics)



Title of Project : New phase of Ocean Hemisphere Project: Imaging the normal oceanic mantle by advanced ocean bottom observations

Hisashi Utada
(The University of Tokyo, Earthquake Research Institute,
Professor)

Research Area : Earth and planetary science, Solid Earth and planetary physics

Keyword : Ocean bottom geophysical observations, oceanic mantle

【Purpose and Background of the Research】

The oceanic mantle is an important region to understand the Earth system, as more than 2/3 of the Earth surface is covered by oceanic area. In the ‘normal oceanic mantle’ between mid oceanic ridge and subduction zone in particular, there remain a couple of most fundamental questions in Earth science.

First question is the cause of asthenosphere, which is a soft (fluid) layer below oceanic plate (lithosphere). Plate tectonics is based on a concept that a rigid lithosphere moves over a weaker asthenosphere, and thus the precise knowledge of its fluidity is fundamental to understand how our planet works.

The presence of water is one of the properties characterizing the planet Earth. Second question is the amount of water in the mantle transition zone, which is essential to understand the Earth’s total water budget. The question may never be fully solved without the knowledge for the “normal oceanic mantle” that occupies the largest part of the entire mantle.

In the present project, we aim to solve these two fundamental problems from observational approach, by using advanced ocean bottom geophysical instruments that were originally developed by our group.

【Research Methods】

Physical conditions of the oceanic mantle in our concern will be investigated based on the structural images which are obtained by ocean bottom seismological and electromagnetic (EM) observations. The combination of seismological and EM parameters enables us accurate estimation of the conditions. We plan to deploy new seismometers and electrometers (see attached photos), as well as ordinary ocean bottom instruments which were also developed by ourselves, on the ‘normal ocean floor’ in the northwestern Pacific for 2-3 years.

Our new seismometer enables us to measure horizontal ground motions at a noise level comparable to that at land stations, which has so far been hard for ocean bottom instruments. Our new electrometer also

reduced the electric field noise significantly. Thus we are able to extract various kinds of information on the normal oceanic mantle by applying a wide variety of analysis methods.



【Expected Research Achievements and Scientific Significance】

The present project is expected to make two important contributions to the solid Earth science community in the world. One is made by providing clear scientific results to answer the two fundamental questions on the normal oceanic mantle as described above. The other can be made by thus displaying a new scientific approach to understand the mantle dynamics, which will introduce a new infrastructure and induce a new trend in Earth science.

【Publications Relevant to the Project】

- (1) Utada, H., et al., (2009) A joint interpretation of electromagnetic and seismic tomography models suggests the mantle transition zone below Europe is dry, *Earth Planet. Sci. Lett.*, **281**, 249-257.
- (2) Kawakatsu, H., et al., (2009), Seismic Evidence for Sharp Lithosphere-Asthenosphere Boundaries of Oceanic Plates, *Science*, **324**, 499-502.

【Term of Project】 FY2010-2014

【Budget Allocation】 429,600 Thousand Yen

【Homepage Address and Other Contact Information】

<http://www.eri.u-tokyo.ac.jp/yesman/>

【Grant-in-Aid for Specially Promoted Research】
Science and Engineering (Mathematics/Physics)



Title of Project : MEG Experiment – From Lepton Flavor Violation toward Grand Unified Theory

Toshinori Mori
(The University of Tokyo, International Center for Elementary Particle Physics, Professor)

Research Area : Physics, Particle/ Nuclear/ Cosmic ray/ Astrophysics

Keyword : Particle physics (experiment)

【Purpose and Background of the Research】

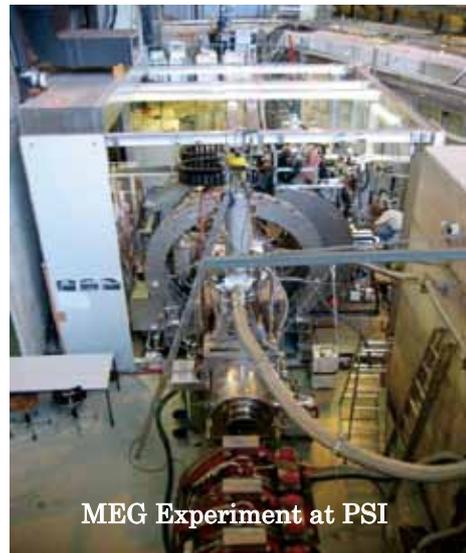
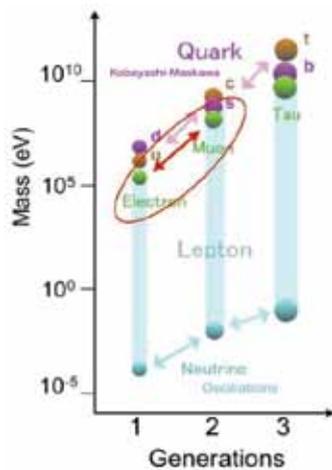
There are three generations of elementary particles which include heavier particles than those that compose ordinary matter (Figure). Transitions between quarks in different generations are well understood by the Kobayashi-Maskawa theory in the framework of the Standard Model (SM). Unexpected oscillations among neutrinos, discovered by Super-Kamiokande, have made it more important to understand flavor-violating transitions in the lepton sector. In fact, it was pointed out that transitions among charged leptons (electrons and muons), strictly forbidden by the SM, should occur at a measurable rate in Supersymmetric Grand Unified Theories (SUSY GUT), highly respected theories beyond the SM. The aim of this research project is to experimentally verify SUSY GUT by searching for $\mu \rightarrow e\gamma$ decays, muon's transition into an electron, which violates lepton flavor.

【Research Methods】

The MEG experiment with innovative and ingenious detectors to reach an unprecedentedly small branching ratio of 10^{-13} has been started at Paul Scherrer Institute (PSI), where good quality high intensity muon beam is available. In this research project, in collaboration with Switzerland, Italy, Russia and U.S., we operate the experiment and significantly improve the physics sensitivity to experimentally verify SUSY GUT. In parallel R&D to realize an ultimate experiment with much higher sensitivity will be carried out.

【Expected Research Achievements and Scientific Significance】

The discovery of $\mu \rightarrow e\gamma$ will immediately prove existence of new physics beyond the SM such as SUSY GUT, which could revolutionize particle physics. Results obtained here will be complementary to studies being carried out at LHC and are essential in reaching correct understanding of new physics beyond the SM.



MEG Experiment at PSI

【Publications Relevant to the Project】

- "A Limit for the $\mu \rightarrow e\gamma$ Decay from the MEG Experiment," MEG Collaboration (T. Mori, S. Mihara, W. Ootani, A. Baldini, et al.), Nucl. Phys. B 834 (2010) 1-12.
- "Charged Lepton Flavor Violation Experiment," W.J. Marciano, T. Mori, and J.M. Roney, Annu. Rev. Nucl. Part. Sci. 58 (2008) 315-341.

【Term of Project】 FY2010-2014

【Budget Allocation】 415, 200 Thousand Yen

【Homepage Address and Other Contact Information】

<http://www.icepp.s.u-tokyo.ac.jp/meg/>
<http://meg.icepp.s.u-tokyo.ac.jp/>

【Grant-in-Aid for Specially Promoted Research】
Science and Engineering (Mathematics/Physics)



Title of Project : Development of Exoplanet Researches with New IR Technologies

Motohide Tamura
(National Astronomical Observatory/NINS, Optical and Infrared Division, Associate Professor)

Research Area : Astronomy

Keyword : IR Astronomy, Exoplanet, Adaptive Optics, Infrared Detector, Wavelength Calibration

【Purpose and Background of the Research】

Since the first detection of exoplanets orbiting normal stars in 1995, more than 450 exoplanet candidates have been discovered mainly by indirect methods and many exciting discoveries have been made, but our understanding of planetary systems and their formation is far from complete. A census of companions to stars over a wide range of ages will provide important clues to the formation and evolution of stars, brown dwarfs, and planets. On the other hand, although the standard theory of planetary formation predicts existence of a number of Earth-like planets, they are basically yet uncovered. Therefore, in the rapidly growing exoplanet studies, the next two critical milestones are direct imaging and Earth-like planet detection.

【Research Methods】

In this research we will conduct a first large scale "direct imaging survey" with our newly developed high-contrast instrument for exoplanet systems similar to our solar system. The survey will explore the regions where the previous indirect methods such as the radial velocity or transit ones have been unable to observe (Figure 1).

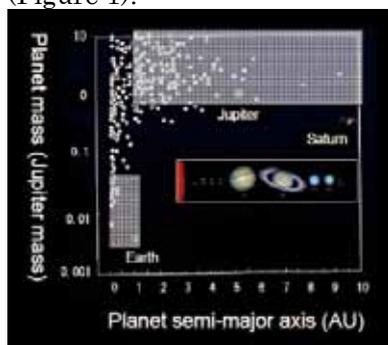


Figure 1 Planets inside and outside our Solar System as well as the parameter spaces to be explored in this research.

We will develop a high precision near-infrared radial velocity instrument with employing various new IR technologies such as

frequency-comb, IR arrays, gratings, and IR wavefront sensing.

【Expected Research Achievements and Scientific Significance】

We aim to detect many giant planets at a few to a few tens astronomical units (Figure 2) and derive their properties (luminosity, temperature, composition). With a comparison of the disk observations at the same regions, we can reveal the origin of the diversity of exoplanets and discuss if our Solar System is unique or not.

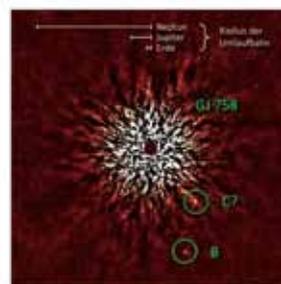


Figure 2 Direct imaging of an exoplanet.

We also aim for detecting down to one Earth-mass planet in habitable zones around low-mass stars by the IR radial velocity method (Figure 1). This will enable us to discuss the statistics of Earth-like planets and even the life in other worlds.

【Publications Relevant to the Project】

Watanabe, J. et al. eds, Nippon-Hyoron-sha, Modern Astronomy Vol.9, 2008.
Ida, S., Sato, B., Tamura, M., Suto, Y, Gijyutsu Hyoron-sha, Many Other Earths, 2008.

【Term of Project】 FY2010-2014

【Budget Allocation】 396, 900 Thousand Yen

【Homepage Address and Other Contact Information】

<http://optik2.mtk.nao.ac.jp/~hide/index.html>
motohide.tamura@nao.ac.jp

【Grant-in-Aid for Specially Promoted Research】 Science and Engineering (Chemistry)



Title of Project : Development of synthetic photo-functional molecules for medical applications

Tetsuo Nagano
(The University of Tokyo, Graduate School of Pharmaceutical Sciences, Professor)

Research Area : Chemistry related to living body

Keyword : Biofunctional chemistry, Biological recognition/Biofunctional chemistry

【Purpose and Background of the Research】

Despite the advance of medical sciences, it is still difficult to diagnose and cure diseases such as cancer and cardiovascular disorder, which are major causes of death in Japan. Molecular imaging technologies are attracting attention because they may provide not only mechanistic insight, but also noninvasive and accurate diagnosis of such diseases. With respect to chemistry, extensive research is being performed for the development of functional molecules, such as fluorescent probes and MRI contrast agents that can selectively visualize lesions.

Over the last decade, our group has focused on the development of photo-functional molecules. More than fifty compounds have been developed based on design strategies established by ourselves (Fig. 1), and 14 of them are now commercially available. In this research project, taking advantage of our world-leading experience in this field, we aim to develop novel photo-functional molecules for medical applications, including diagnosis and treatment.

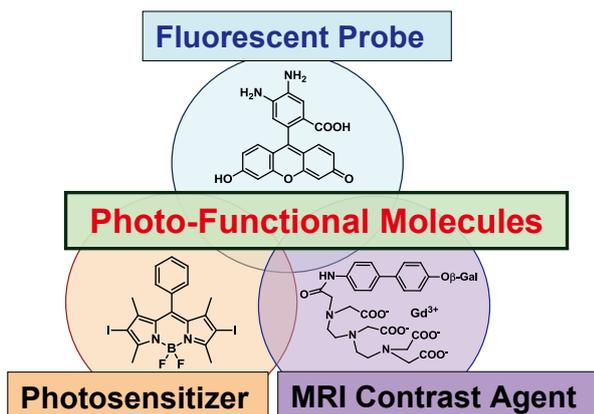


Fig. 1 Examples of photo-functional molecules developed by our group

【Research Methods】

To detect fluorescence emitted within the body, fluorescent probes that are excited at wavelengths in the near-infrared region (650-900 nm) are necessary. Therefore, we plan to develop novel long-wavelength fluorophores

that are compatible with a range of chemical modifications, and functionalize them by incorporating reactive moieties with specific targets. In addition, we will develop fluorescent probes and contrast agents that react with chemical species related to cancer and ischemia, and apply them for in vivo imaging. Probes for use in the screening of drug candidates and for blood tests will also be developed.

As to photosensitizers, we plan to develop molecules that produce reactive oxygen species only in the target lesions, thereby reducing the adverse effects of the current systems.

【Expected Research Achievements and Scientific Significance】

Using the novel probes, dynamic analysis of target molecules in vivo will be feasible, and this will be helpful to understand the mechanisms of diseases. Development of novel therapeutic agents is also expected.

【Publications Relevant to the Project】

- (1) "Development and Application of a Near-Infrared Fluorescence Probe for Oxidative Stress Based on Differential Reactivity of Linked Cyanine Dyes" D. Oushiki, H. Kojima, T. Terai, M. Arita, K. Hanaoka, Y. Urano and T. Nagano, *J. Am. Chem. Soc.*, **132**, 2795-2801 (2010).
- (2) "Design and Development of Enzymatically Activatable Photosensitizer Based on Unique Characteristics of Thiazole Orange" Y. Koide, Y. Urano, A. Yatsushige, K. Hanaoka, T. Terai and T. Nagano, *J. Am. Chem. Soc.*, **131**, 6058-6059 (2009).

【Term of Project】 FY2010-2014

【Budget Allocation】 419,200 Thousand Yen

【Homepage Address and Other Contact Information】

<http://www.f.u-tokyo.ac.jp/~tlong/Japanese/top.html>
tlong@mol.f.u-tokyo.ac.jp

【Grant-in-Aid for Specially Promoted Research】
Science and Engineering (Chemistry)



**Title of Project : Creation of genome manipulation technology
using super restriction enzyme**

Makoto Komiyama
(The University of Tokyo, Research Center for Advanced
Science and Technology, Professor)

Research Area : Chemistry related to living body

Keyword : Nucleic acid, Genome analysis, Biotechnology, Recombination

【Purpose and Background of the Research】

It is now well recognized that the genomes of higher animals and plants are never simple aggregates of many genes. Rather, these genes and their regulation factors are placed at predetermined sites in the genomes and communicate each other for precise regulation. Apparently, a method to manipulate genomes in a predetermined fashion is essential to understand biological functions of genomes and further employ them for our practical needs. However, there have been few tools to manipulate huge genomes, and accordingly there has been little information on the detailed functions of genome systems.

We already developed man-made tool (Artificial Restriction DNA Cutter; ARCUT) which cuts huge double-stranded DNA at desired site. The objectives of this project are to complete ARCUT-based method of genome manipulation, and also to clarify the functions of genome systems. The “genome manipulation technology”, which is constructed here, could alter the basic concepts of conventional biotechnology.

【Research Methods】

We will first establish the method to manipulate huge genomes using ARCUT. Then, this technology is used for precise analysis of the function of gene(s) in genomes. Specifically, we cut genomes at the target site, and clarify the communication of genes (and also with the regulation factors) in genomes. The following four approaches are attempted. (1) Alteration of a target gene to a desired gene through homologous recombination which is promoted by ARCUT-induced site-selective scission of genome, (2) silencing of a target gene also through homologous recombination, (3) segregation of a gene from other genes by cutting a predetermined site of genome by ARCUT, where the influence of this genome manipulation on biochemical properties (transcription efficiency, protein localization in cell, etc.) is quantitatively assessed, and (4) clipping of a portion of genomes by ARCUT, which is analyzed in detail in vitro by spectroscopic and other physicochemical means.

【Expected Research Achievements and Scientific Significance】

In the present project, the method of genome manipulation is provided for the first time. Undoubtedly, this method should dramatically accelerate the progresses of new biotechnology (e.g., drug discovery). In the current biotechnology, external genes are mostly introduced to cells by using vectors, where these genes should primarily work independently from each other. Thus, the mutual communications of genes and regulation cofactors cannot be appropriately evaluated. In extreme cases, the best gene for the therapy of a disease, for example, could be thrown away in the screening process, simply because of the lack of appropriate mutual communications with other genes and regulation cofactors in the cells. The present work provides straightforward solutions to these problems. Of course, the genome manipulation technique should be directly applicable to gene therapy which is one of the most challenging topics.

【Publications Relevant to the Project】

- [1] “Artificial restriction DNA cutter for site-selective scission of double-stranded DNA with tunable scission-site and specificity”, M. Komiyama, Y. Aiba, Y. Yamamoto, J. Sumaoka, *Nature Protoc.*, 3, 655-662 (2008).
- [2] “Homologous Recombination in Human Cells using Artificial Restriction DNA Cutter”, H. Katada, H. J. Chen, N. Shigi, M. Komiyama, *Chem. Commun.*, 6545-6547 (2009).

【Term of Project】 FY2010-2014

【Budget Allocation】 400,400 Thousand Yen

【Homepage Address and Other Contact Information】

<http://www.mkomi.rcast.u-tokyo.ac.jp/index.html>

**【Grant-in-Aid for Specially Promoted Research】
Science and Engineering (Chemistry)**



Title of Project : Synthesis and Nano-organization of Organic Semiconductors for Efficient Photoelectronic Conversion

Eiichi Nakamura
(The University of Tokyo, School of Science, Professor)

Research Area : Physical Organic Chemistry, Organic Synthesis, Organic Electronics

Keyword : π -Electronic System, Fullerene, Organic Semiconductor, Thin-film Structure, Organic Thin-film Photovoltaic Cells

【Purpose and Background of the Research】

Because of the infinite diversity of organic semiconductor molecules and the structures they form, the design of efficient organic thin-film solar cells consisting of various organic compounds with different functions is an exciting new challenge for the chemist. Because the efficient use of solar energy has an intimate connection with the survival of human beings, this is an important research topic in which chemists should play a positive role. Unlike the pharmaceutical and agricultural applications of organic chemistry, which have existed for a long time, its full-scale application to electronic technology is only just beginning.

Based on the new guideline in organic electronics, “finding functional molecules with new reactions,” this project aims to design and synthesize planar π -conjugated molecules with semiconductor properties and spherical fullerene derivatives to develop methods of controlling the structure of these molecular entities at the nanosize level, and successfully to achieve the production of efficient organic thin-film solar cells.

【Research Methods】

The “small molecule-based solution processable organic thin-film solar cells” in this research have many superior features compared with conventional organic thin-film solar cells in regard to various factors such as durability and diversity of material design. The following topics are addressed in this project: (1) finding organic semiconductor molecules and undertaking their molecular design and synthesis; (2) fabricating layered nanostructure devices; and (3) analyzing the nanostructure of these semiconductor materials (molecular-level analysis of aperiodic structures). By combining these topics, we hope to develop highly efficient, highly durable, new organic thin-film solar cells at low cost.

【Expected Research Achievements and Scientific Significance】

The “design of highly functional semiconductor molecules,” “full layering of molecular structures from nanoscale to macroscale,” and “molecular-level analysis of aperiodic structures,” which has never been seriously attempted in chemistry research until now, are key to this research, and are expected to lead to the opening up of new fields of basic science. If the organic solar cells developed in this research reach the level of practical utilization, they would make an invaluable contribution towards solution of the energy crisis.

【Publications Relevant to the Project】

- “Columnar Structure in Bulk Heterojunction in Solution-Processable Three-Layered p-i-n Organic Photovoltaic Devices Using Tetrabenzoporphyrin Precursor and Silylmethyl[60]fullerene”, Y. Matsuo, Y. Sato, T. Niinomi, I. Soga, H. Tanaka, E. Nakamura, *J. Am. Chem. Soc.*, **131**, 16048-16050 (2009).
- “Bis(carbazolyl)benzodifuran: A High-mobility Ambipolar Material for Homojunction Organic Light-emitting Diode Devices”, H. Tsuji, C. Mitsui, Y. Sato, and E. Nakamura, *Adv. Mater.*, **21**, 3776-3779 (2009).
- “Imaging Single Molecules in Motion”, M. Koshino, T. Tanaka, N. Solin, K. Suenaga, H. Isobe, and E. Nakamura, *Science*, **316**, 853 (2007).

【Term of Project】 FY2010-2014

【Budget Allocation】 458,700 Thousand Yen

【Homepage Address and Other Contact Information】

<http://www.chem.s.u-tokyo.ac.jp/users/common/NakamuraLab.html>

**【Grant-in-Aid for Specially Promoted Research】
Science and Engineering (Chemistry)**



**Title of Project : Theoretical Study of Complex Electronic Systems
Including d Electron: Fundamental
Understanding and Prediction by New Electronic
Structure Calculation Method for Large Systems**

Shigeyoshi Sakaki
(Kyoto University, Institute for Integrated Cell-Material
Sciences, Professor)

Research Area : Fundamental Chemistry (Physical Chemistry)

Keyword : Electronic Structure, Theoretical Chemistry, Chemical Reaction, Coordination
Chemistry, Metal Complex/Organometallic Catalysts

【Purpose and Background of the Research】

Molecules which have transition metal, non-transition metal, non-metallic heavy elements, and organic groups exhibit varieties of geometry, chemical bond, physicochemical property, and reactivity. As a result, such molecules play important roles in basic and applied chemistry fields. Also, their complex electronic structures are challenging research target in theoretical/computational chemistry and molecular science. However, these molecules are not always investigated well with DFT method which is often applied to large system, because of the presence of large electron-correlation effects.

In this theoretical/computational study, we wish to propose a new hybrid-electronic structure method by combination of our own frontier-orbital-consistent effective potential (FOC-EP) and high-quality computational methods based on wavefunction. Our main purposes here are to present fundamental understanding of geometries, bonding nature, physicochemical properties, and reactivity of complex systems including transition metal, non-transition metal, and/or non-metallic heavy elements and organic group. Our main targets are multi-nuclear transition metal systems containing multiple-bond, complex systems consisting of transition metal, non-transition metal, heavy non-metallic elements and organic groups, nano-scale carbon materials containing transition metal and/or non-transition metal elements, and catalytic reactions by transition metal systems. Some of our targets are shown in Figure 1.

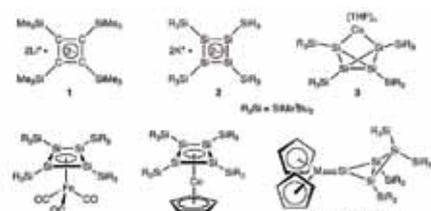


Figure 1 Examples investigated in this work

【Research Methods】

A new hybrid method based on wavefunction is employed here, as well as DFT. The hybrid method is constructed by the combination of FOC-EP and FMO, ONIOM, CASPT2, or SAC/SAC-CI method to perform high-quality calculation with electronic effects of substituent. Also, we will propose an analysis method of complex systems by the linear combination of fragment molecular orbital. Above-mentioned large systems will be investigated with the hybrid electronic structure theory, in which the FOC-EP will be applied to incorporate electronic effects of substituents omitted in model. For instance, multi-nuclear transition metal complexes including multiple metal-metal bond will be investigated by the CASPT2 method combined with the FOC-EP and analyzed.

【Expected Research Achievements and Scientific Significance】

The hybrid electronic structure calculation method presented here can be applied to general large complex systems bearing complicated electronic structure. The theoretical knowledge of metal-metal and metal-non-metal bonds, electronic structures, physicochemical properties, and reactivity of complex systems provides us with non-classical new understanding. We believe that all these findings contribute to new development of molecular science and its application to engineering.

【Publications Relevant to the Project】

- S. Sakaki, Y.-y. Ohnishi, H. Sato, *Chem. Record.*, 10, 29-45 (2010).
- N. Ochi, Y. Matano, Y. Nakao, H. Sato, S. Sakaki, *J. Am. Chem. Soc.*, 131, 10955-10963 (2009).

【Term of Project】 FY2010-2014

【Budget Allocation】 353,500 Thousand Yen

【Homepage Address and Other Contact Information】

<http://www.users.iimc.kyoto-u.ac.jp/~z59354>
sakaki@moleng.kyoto-u.ac.jp

**【Grant-in-Aid for Specially Promoted Research】
Science and Engineering (Engineering)**



**Title of Project : Study on fabrication process of 3-D structured
MOS transistor having atomically flat gate
insulator/Si interface**

Tadahiro Ohmi
(Tohoku University, New Industry Creation Hatchery Center,
Professor)

Research Area : Electronic materials, Electric materials

Keyword : Electrical and electronic materials (semiconductor)

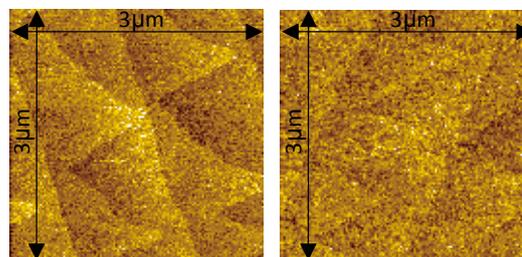
【Purpose and Background of the Research】

The current semiconductor technology can fabricate LSI only on (100) Si surface using 2-D planar structure transistors. Thus, the current silicon technologies are now facing with very severe standstill, and the progress of speed performance of the silicon LSI has completely stopped. In order to overcome these troubles, it is required to create the process technologies for manufacturing the three-dimensional structure MOS transistors, which have the atomically flat interface between the gate insulator film and the silicon substrate, on any crystal orientation silicon surface. The research objective of this project is to create the balanced CMOS silicon LSI having a very excellent speed performance and very low power consumption. Therefore, it is essentially required to develop the flattening technologies for the any crystal orientation silicon surface and silicon sidewall surface of the 3-D MOS transistors.

【Research Methods】

The performance of the silicon LSIs is drastically improved by introducing the following three technologies, (1) Accumulation Mode MOS transistor instead of conventional Inversion Mode MOS transistors, (2) 3-D structure on (551) orientation SOI wafer instead of 2-D planer structure on (100) orientation wafer, (3) atomically flat interface between the gate insulator film and silicon substrate. However, these technologies cannot be realized by using the current silicon technologies. Only by making good use of the new manufacturing system based on the ultra clean technologies and the radical reaction processes, these three technologies can be realized. Figure 1 shows the AFM images of SiO₂/Si interface fabricated by radical oxidation and thermal oxidation on the atomically flat Si(100) surface. The SiO₂/Si interface fabricated by radical oxidation is maintained the mono atomic layer step and the atomically flat terrace, although, that by thermal oxidation is roughened. In this project, we develop the

flattening technologies for the Si surface and Si sidewall surface of the 3-D structure by making good use of the radical reaction based new manufacturing technologies by using the damages free plasma equipments which we have developed.



Radical SiO₂/Si Thermal SiO₂/Si

Fig. 1 AFM images of SiO₂/Si interface

【Expected Research Achievements and Scientific Significance】

By achieving this project, the speed performance of MOS transistors is drastically improved, and the variability of transistor characteristic and 1/f noise are drastically reduced. As the results, the power consumption is lowered with maintaining the reliability. Thus, the realization of the ultra high performance information and communication device with very low power consumption is of great scientific significance.

【Publications Relevant to the Project】

1. R. Kuroda, T. Ohmi, et al., IEEE Trans. Electron Dev., VOL.56, NO.2, pp.291-298, February 2009.
2. T. Ohmi, et al., IEEE Trans. Electron Dev., VOL.54, NO.6, pp.1471-1477, June 2007.

【Term of Project】 FY2010-2014

【Budget Allocation】 474, 400 Thousand Yen

【Homepage Address and Other Contact Information】

<http://www.fff.niche.tohoku.ac.jp/>
Email: ohmi@fff.niche.tohoku.ac.jp

【Grant-in-Aid for Specially Promoted Research】 Science and Engineering (Engineering)



Title of Project : Design of Electronic Properties and Development of High-Mobility Channel Technology for Low Power/High-Speed Nano-CMOS Devices

Shigeaki Zaima
(Nagoya University, Graduate School of Engineering,
Professor)

Research Area : Applied physics, Thin film/Surface and interfacial physical properties

Keyword : Thin film, Interface, Semiconductor, Epitaxial growth

【Purpose and Background of the Research】

In Si ultra-large scale integrated circuit (ULSI) devices, the improvement of current drivability is essential for lowering the power consumption and increasing the speed. The strained-channel technology to obtain higher carrier mobility than bulk Si has already been introduced into ULSI devices in order to overcome the physical properties of Si. This mobility enhancement of Si using strain has also a limit and it is indispensable for future nano-scale ULISs to introduce new materials, which have much higher carrier mobility than strained Si, into the channel region of metal-oxide-semiconductor (MOS) transistors.

In this research project, we focus on the design of electronic properties of Ge using strain and Sn addition and the development of new channel technology using Ge-related materials, aiming to establish the high-mobility channel technology for future nano-scale complementary-MOS (CMOS) devices.

【Research Methods】

It is possible to obtain the high mobility both electrons and holes compared with strained Si by adding the strain of about 1% to Ge. Furthermore, the addition of strain over 1% and 20% Sn into Ge induce the change in the electronic band structures from an indirect- to direct-transition type and hence the electron and hole mobility has been expected to be drastically enhanced.

We will establish the epitaxial growth technology to fabricate the strained-Ge/GeSn/Si heterostructure, examine the electronic and electrical properties of strained Ge and GeSn, and also propose the technology for controlling the MOS interface properties. (Fig. 1)

【Expected Research Achievements and Scientific Significance】

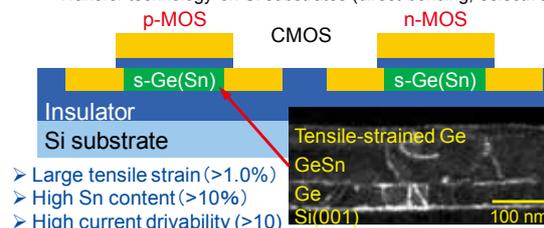
The Sn addition in Ge brings new functionality and flexibility into Group IV semiconductor materials. One of important points is that both n- and p-MOS transistors in future nano-scale CMOS devices are achievable using Ge-related

materials having high compatibility with Si processes. This technology has a potential that the trend of future ULSI technology can be revolutionized and, therefore, the industrial impact is extremely large.

In addition, because these materials with a large strain and a high Sn content are theoretically expected to have a direct band gap, the application for solar cells, optical devices and so forth will be developed.

High-Mobility Channel Technology using Strained-Ge and GeSn

- Heteroepitaxial growth of tensile-strained Ge and GeSn
 - Design of electronic properties by controlling of strain and Sn content
- Integration on Si platform
 - Control technology of insulator/Ge(Sn) interfaces
 - Transfer technology on Si substrates (direct bonding, selective epi)



- Large tensile strain (>1.0%)
- High Sn content (>10%)
- High current drivability (>10)

Fig. 1 Content of this research project

【Publications Relevant to the Project】

- [1] Y. Shimura, N. Tsutsui, O. Nakatsuka, A. Sakai and S. Zaima, "Control of Sn Precipitation and Strain Relaxation in Compositionally Step-Graded Ge_{1-x}Sn_x Buffer Layers for Tensile-Strained Ge Layers", *Jpn. J. Appl. Phys.*, **48**, 04C130-1-4 (2009).
- [2] S. Takeuchi, Y. Shimura, O. Nakatsuka, S. Zaima, M. Ogawa and A. Sakai, "Growth of Highly Strain-Relaxed Ge_{1-x}Sn_x/Virtual-Ge by a Sn Precipitation Controlled Compositionally Step-Graded Method", *Appl. Phys. Lett.*, **92**, 231916 (2008).

【Term of Project】 FY2010-2013

【Budget Allocation】 344, 600 Thousand Yen

【Homepage Address and Other Contact Information】

<http://alice.xtal.nagoya-u.ac.jp/zaimalab/>
zaima@alice.xtal.nagoya-u.ac.jp