Title of Project : Study of Geometric Moduli Theories and Theoretical Applications

Iku Nakamura
(Hokkaido University, School of Science, Professor emeritus)

Research Area : Mathematics, Algebra
Keyword : Algebraic Geometry

【Purpose and Background of the Research】

Some of geometric objects are described by several parameters uniformly. The space determiend by the parameters is called moduli space. The set (the space) consisting of all the natural and stable limits is called compactifi-cation of the moduli space. There are some applications of compactifications of the moduli spaces. Our progress so far is as follows :

1. Nakamura [1][2] constructed two compactifi-cations of the moduli space of abelian varieties with non-commutative levels and proved that The first compactified moduli consists of all the limit objects whose Hilbert points are stable.
2. In his collaboration with statistical economists Kamiya and Takemura, Terao [6] gave a formula of the number of priority models, identifying the moduli space of priority with the moduli space of the complements of hyperplane arrangements.
3. Ono [3] proved that the Betti number version of the Arnold conjecture concerning the upper bound of the number of fixed points is true if any fixed point of a Hamiltonian mapping of a closed symplectic manifold is nondegenerate.
4. Iwasaki [4] formulated Painleve equations moduli-theoretically, and made an extensive study on entropy and chaotic structure of the dynamical system associated with analytic continuation of solutions of the Painleve eqs.

The purpose of this project is to more deeply study the above compactifications to make theoretical applications to distinct fields.

【Research Methods】

(1) Describe in detail the structure of the compactification of moduli space of abelian varieties at good primes. For it, we describe in detail the natural equations defining (degene-rate) abelian varieties, and construct primary Siegel modular forms as coefficients of the equations. Also extend the compactification of moduli space of AVs to bad primes. For it we generalize Katz-Mazur[5] to higher dimension, using Dieudonne theory,.

(2) Make a deeper study of hypergeometric functions, the complements of hyperplane arrangements and pirimitive integrals through algebraic study of hyperplane arrangements. Apply arrangements (algebra) to social scienece through collaboration with social scientists.

(3) Study the connection between the mirror symmetry of Langrange-Floer theory (differen-tial geometry) and the mirror symmetry of deformation theories of Potetail functions, or Givental's theory of mirror symmetry (algebraic geometry and physics).

(4) Using the compactification of the moduli (algebraic geometry) we make similar studies on entropy, chaotic structure of the dynamical system for the other types of Painleve equations.

【Expected Research Achievements and Scientific Significance】

In **(1)**,the moduli functor is representable so that any primary Siegel modular forms will appear in principle. Generalization of Katz-Mazur [5] is a long-standing problem. We may be able to exactly describe the structure of the extended compactifications in detail. It is noteworthy of **(2)** that algebra can be applied to social science. The study of mirror symmetry in **(3)** and the algebro-geometric study of Painleve eqs in **(4)** are new and notable internationally.

【Publications Relevant to the Project】

[1] I.Nakamura, Stability of degenerate abelian varieties, Inv. math., vol. 136, 659-715 (1999).
[2] I. Nakamura, Another canonical compactifi-cation of the moduli space of abelian varieties, ASPM of MSJ., vol. 58, pp. 69-135, (2010).
[3] K.Fukaya, K.Ono, Arnold conjecture and Gromov-Witten inv., Topology, vol. 38 (1999).
[4] M.Inaba, K.Iwasaki, M.-H.Saito, Moduli of stable parabolic connections,…,geometry of Painleve equation of type VI, part I, Publ. Res. Inst. Math. Sci., vol. 42, 987-1089 (2006).
[5] N.M.Katz and B.Mazur, Arithmetic moduli of elliptic curves, Princeton (1985).
[6] H. Kamiya, A. Takemura, H. Terao, Periodicity of hyperplane arrangements …, J. Alg. Comb.,vol. 27, 317-330 (2008).

【Term of Project】 FY2011-2015

【Budget Allocation】 139,300 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.math.sci.hokudai.ac.jp/~nakamura/

Title of Project : Proof of Homological Mirror symmetry

Kenji Fukaya
(Kyoto University, Graduate School of Science, Professor)

Research Area : mathematics
Keyword : Differential Geometry, Topology, Complex manifold, Algebraic geometry

【Purpose and Background of the Research】

Mirror symmetry is a conjecture proposed in 1990's by physisists.

It becomes famous among mathematicians by the conjecture (due to Candelas etc.) that the generating function obtained by cuonting the number of rational curves of Calabi-Yau manifolds satisfies certain differential equation obtained from the deformation theory of another Calabi-Yau manifold, that is called its mirror.

This conjecture itself is solved in many cases by Givental etc. and is called the classical mirror symetry.

Homological Mirror symmetry is proposed by M. Kontsevitch in 1994 and deepen the mirror symmetry conjecture.

It conjectures an equivalence of a category obtained from Lagrangian Floer theory of a symplectic manifold (Fukaya category) and the derived category of coherent sheaves of its mirror.

The conjecture now can be stated rigorously when Lagrangian Floer theory is rigorously established in the general setting by Fukaya-Oh-Ohta-Ono.

The purpose of this research is to prove it.

【Research Methods】

Two methods are proposed toward the proof of homological mirror symmetry conjecture.

One is to use the family Floer homology and the other is to prove it first for toric manifolds and generalize it to its submanifolds.

The first one is closely related to Strominger -Yau-Zaslow's proposal to realize a mirror manifold as a dual manifold. The idea to use family of Floer homology to prove homological mirror symmetry is obtained around 1997 by Fukaya-Kontsevich. We are now close to realize it. The second idea is realted to the proof by Givetal etc. of classical mirror symmetry and also to Hori-Vafa plan of the proof of mirror symmetry.

Fukaya-Oh-Ohta-Ono's recent study of Floer hommology of toric manifolds is a way to perform the proof along this line.

【Expected Research Achievements and Scientific Significance】

The proof of homological Mirror symmetry has the following application to symplectic topology.

Theory of pseudoholomorphic curves are very important method in global symplectic geometry. Gromov-Witen invariant Floer homology etc. are important invariant obtained by using it.

One of the main difficulty to study and use symplectic invariant obtained by using pseudoholomorphic curves is its calculation.

At the heart of the construction there is a modli space of pseudoholomorphic curves. So to calculate those invariant directly from definition requires to determine the set of solution of certain nonlinear PDE that is of course very difficult in general.

(Homological) mirror symmetry provides a way to calculate those invariant by moving the problem to one in complex geometry.

The proof of Homological mirror symmetry is of course useful to the understanding of Mirror symmetry and string theory.

【Publications Relevant to the Project】

K. Fukaya, Y.-G. Oh, H. Ohta and K. Ono, Lagrangian intersection Floer theory-anomaly and obstruction,} International Press/Amer. Math. Soc. (2009).

K. Fukaya, Y.-G. Oh, H. Ohta and K. Ono, Lagrangian Floer theory on compact toric manifolds I, Duke Math. J. 151 (2010), 23-174. ibid II Selecta Math. New Ser. (2011) 17:609–711

Cyclic symmetry and adic convergence in Lagrangian Floer theory, Kyoto J. Math. 50 (2010) 521--590

【Term of Project】 FY2011-2015

【Budget Allocation】 81,600 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.math.kyoto-u.ac.jp/~fukaya/

Title of Project : Concentration Phenomena and Structure of Solution for Nonlinear Evolution Equations

Yoshio Tsutsumi
(Kyoto University, Graduate School of Science,Professor)

Research Area : Mathematical and Physical Sciences, Mathematics, Analysis
Keyword : Functional Equations

【Purpose and Background of the Research】

One of the most important problems in nonlinear partial differential equations is to characterize "concentration phenomena", which are a kind of singularity in a wide sense. This wide-sense singularity does not mean the irregular part of solution unlike the usual usage of the word "singularity". This implies some properties of solutions, which may prevent a possible property we naturally expect of a solution. For example, when we consider the nonlinear scattering problem for nonlinear Klein-Gordon or Schödinger equations with power nonlinearity in the energy space, there is a possibility that a solution may be localized in some region for a long time like a solitary wave, because those equations are invariant under space-time translation and reflection. If one can exclude this possibility of localization, one can construct the nonlinear scattering theory. This kind of wide-sense singularity could happen if some quantity of solution, for instance, the p-integral norm of solution would concentrate on some region in the position space or momentum space. The aim of our research is to analyze the mechanism of formation of wide-sense singularity such as concentration phenomena by using harmonic analysis techniques and numerical simulations for nonlinear dispersive or wave equations, reaction diffusion equations and incompressible Navier-Stokes equations.

【Research Methods】

From a theoretical point of view, we analyze concentration phenomena by using the Fourier restriction norm method, the I-method and the minmum blowup solution argument and we try to improve these methods. From a numerical point of view, we pursue our study about how rigorously we can reproduce the singularity by using the verified numerical computation. For that purpose, we need to establish the theory of verified numerical computation which can cover functions taking infinity as values. Since mathematical theory handles abstract objects, it is important that we discuss problems with each other face to face. So, we make every effort to invite and send researchers to Kyoto University and other institutes as well as to organize scientific meetings. Furthermore, we invite young researchers to join us in this project to hire postdocs.

【Expected Research Achievements and Scientific Significance】

The Fourier restriction norm method is helpful for the close investigation of time local estimates and the I-method has been developed to the time global estimates of weak solutions. The minimal blowup solution argument recently exploited is useful for the classification of global behavior of general solutions. We try to combine these three methods to analyze the concentration phenomenon. As a result, we expect to have an improvement of these methods, which would be very helpful for the global existence theory and the nonlinear scattering theory of weak solution. Moreover, it is also important how one can handle the concentration phenomenon numerically. In this direction, we may expect to develop the scheme which can cover the infinity. In this respect, one may expect that our prospective results could be applied to problems in other fields.

【Publications Relevant to the Project】

・K. Nakanishi, H. Takaoka and Y. Tsutsumi, Locla well-posedness in low regularity of the mKdV equation with periodic boundary condition, Discrete Contin. Dyn. Syst., 28(2010), 1635-1654.
・J. Ginibre, Y. Tsutsumi and G. Velo, On the Cauchy problem for the Zakharov system, J. Funct. Anal., 151(1997), 384-436.

【Term of Project】 FY2011-2015

【Budget Allocation】 57,700 Thousand Yen

Title of Project : Stellar evolution and chemical enrichment from the first stars to the Milky Way formation

Wako Aoki
(National Astronomical Observatory of Japan, Optical and Infrared Astronomy Division, Assistant Professor)

Research Area : Astronomy
Keyword : Optical-infrared astronomy, Theoretical astronomy

【Purpose and Background of the Research】

Since the Big Bang of the universe 13.7 billion years ago, a variety of elements have been synthesized by stars and supernova explosions. The first generations of stars are believed to have key to understanding of such history of the universe. Among such stars formed from the gas clouds including only hydrogen and helium, massive stars that are much heavier than the Sun are dominant, and have provided amount of heavy elements through supernova explosions.

The dust grains formed from the heavy elements should have promoted the next generations of stars including less massive stars. The long lifetime of low-mass stars enables some of them survive until now.

Such objects still contain smaller amount of heavy elements than the Sun, and can be distinguished by measurements of chemical compositions based on stellar spectroscopy. The purpose of our project is to investigate such old stars in the Milky Way and surrounding small galaxies to understand the star formation and supernova explosions in the early universe, as well as subsequent chemical enrichment, dust formation, and formation of small galaxies.

【Research Methods】

We have been working on the survey and chemical abundance measurements for old stars in the Milky Way using the spectrograph mounted on the Subaru Telescope (NAOJ). We will extend such studies to objects in dwarf galaxies around the Milky Way. The efficiency of the observations for such objects will be enhanced by upgrading the instrument through this project.

Observational results will be combined with previous studies by constructing a database of metal-poor stars. Theoretical studies for supernova nucleosynthesis, dust formation after supernovae, low-mass star formation at low metallicity, and formation of dwarf galaxies will be conducted.

The dwarf galaxy Sextans A (observed with the Subaru Telescope. Such small galaxies would have been formed in the early Galaxy.

The Subaru Telescope (NAOJ)

【Expected Research Achievements and Scientific Significance】

Recent studies for limited number of stars in dwarf galaxies around the Milky Way suggest that the chemical composition of such small galaxies show unexpectedly large variations. Our project will conduct such observations for significantly large number of objects and will reveal the variations of dwarf galaxies and their similarity to, or differences from, the Milky Way stars. Our observations and theoretical studies will contribute to understanding the first generations of massive stars and their supernova explosions, as well as the low mass star formation and evolution through the history of the Galaxy formation.

【Publications Relevant to the Project】

"Nucleosynthesis signatures of the first stars" Frebel, A., Aoki, W., et al., 2005, Nature 434, 434, 871-873
"The first chemical enrichment in the universe and the formation of hyper metal-poor stars" Iwamono, N., Umoede, N., Tominaga, N., Nomoto, K. Maeda, K., 2005, Science 309, 451
"Formation and evolution of dust in type IIb supernovae with application to the Cassiopea A supernove remnant" Nozawa, T., Kozasa, T. Tominaga, N. et al., 2010, Astrophy. J., 713, 356

【Term of Project】 FY2011-2015

【Budget Allocation】 90, 500 Thousand Yen

【Homepage Address and Other Contact Information】

http://optik2.mtk.nao.ac.jp/~waoki/

Title of Project : The Origin of Morphologies of Galaxies : Explorations with Multi-Object andIntegral-Field Spectroscopic Observations

Nobuo Arimoto
(National Astronomical Observatory of Japan, Optical and Infrared Astronomy Division, Professor)

Research Area : Astronomy
Keyword : Optical and Infrared Astronomy, Extragalactic Astronomy

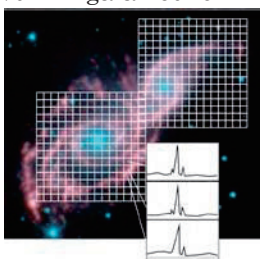
【Purpose and Background of the Research】

Red-shifted optical spectra of distant galaxies can be measured by infrared spectrographs. One of Subaru Telescope's major instruments, multi-object infrared camera and spectrograph (MOIRCS) has revealed some aspect of evolutionary behaviour of galaxies at z=2-3. It is still poorly understood, however, how these galaxies have evolved and have become the present day galaxies with well designed morphologies. To reveal the origin of galaxy morphologies, it is crucial to study the internal gas motion, such as the rotation and random motion, and to know the detailed star formation histories of galaxies.

We will upgrade MOIRCS with newly designed integral-field spectrograph (IFS) and new CCDs. With this upgraded MOIRCS, we will investigate the internal structure and gas motion and will carry out an intensive spectroscopic survey of star forming activity and metallicities of high-z galaxies to uncover how galaxies evolve from active star forming galaxies of irregular shapes to passive elliptical galaxies in the present Universe.

【Research Methods】

① The origin of galaxy morphologies explored with multi-object and integral field spectroscopic observations – We study the internal structure and gas motion of star forming galaxies at z=0.5-1.5, which is just after the period when the star forming activity of the Universe has attained the maximum peak and then declined gradually; at the same time, the regular morphologies of galaxies has appeared. With integral-field spectroscopy of galaxies at different redshift from z=1.5 to 0.5, we will learn how dynamical mass controls star forming, and how gas flows in galaxies of various irregular morphologies. Systematic survey of galaxies will hopefully provide us a crucial key to open the door of mysterious box with a label written as " galaxy evolution".

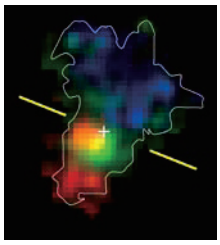


(Fig.1 IF Spectroscopy)

② Star formation and galaxy morphologies explored with multi-object spectroscopic observations – We will measure the metallicities of large number of galaxies at z=0.5-1.5. The metallicities of galaxies, a fossil of star formation in the past, would uncover how galaxy morphologies correlate tightly with star formation histories.

【Expected Research Achievements and Scientific Significance】

Why the star forming activity of galaxies has peaked at around z=2-3 and then declined gradually? Why star forming massive galaxies with irregular morphologies have become grand designed spirals or ellipticals of the local Universe? These are the questions we wish to answer by spectroscopic survey with new MOIRCS.



(Fig.2 Rotating Disk Galaxy @ z=2.4)

Next generation telescopes such as TMT (30m) will fully use the power of IFS to reveal the details of galaxy formation. The IFS is the crucial technique for the next generation ground telescopes and this research will contribute a lot to develop such technique for Japanese astronomical community of post Subaru.

【Publications Relevant to the Project】

Onodera,M., Daddi,E., Gobat,R., Cappellari,M., Arimoto,N. et al. "A z=1.82 Analog of Local Ultra-Massive Elliptical Galaxies", ApJ 715, L6-L11, 2010

Onodera,M., Arimoto,N., Daddi,E., Renzini,A., Kong,X. et al. "A Wide Are Survey for High-Redshift Massive Galaxies. II. Near-Infrared Spectroscopy of BzK-Selected Massive Star-Forming Galaxies", ApJ 715, 385-405, 2010

【Term of Project】 FY2011-2014

【Budget Allocation】 165,600 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.naoj.org/Projects/newdev/nm/

Title of Project : Systematic Study of Double-Hypernuclei with Nuclear Emulsion

Kazuma Nakazawa
(Gifu University, Faculty of Education, Professor)

Research Area : Elementary particle physics, Nuclear physics, Cosmic ray, Cosmic physics
Keyword : Nuclear physics (experiment)

【Purpose and Background of the Research】

One of the most important issues on nuclear physics is an understanding of interaction between baryons with strangeness.

Nuclear force under the system with proton and neutron was precisely studied for more than 50 years, thus we have obtained fruitful informations about that. The knowledge of the interaction between hyperon(Y) and nucleon is rapidly proceeding with the technique of gamma ray spectroscopy. Therefore the next challenge is research on Y-Y interaction.

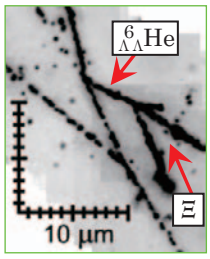
The unique expedient is study of structures of many double-hypernuclei. The most effective method to produce double-hypernuclei is nuclear emulsion experiment which we have developed for long time. With use of the emulsion, we have detected 8 events of double-hypernuclei in these 20 years. Among them, Nagara event was fixed as a new species of nucleus formed by a ^{4}He and two Λ hyperons ($_{\Lambda}^{6}{}_{\Lambda}$He) and provided an interaction energy between two hyperons, successfully. However, for a firm understanding of Y-Y interaction with less uncertainty by nuclear structure, the masses have to be measured in some more double-hypernuclei other than $_{\Lambda}^{6}{}_{\Lambda}$He nucleus.

Since the K$^-$ beam with good separation from others and high intensity becomes available at J-PARC, we will carry out an experiment (E07) which provides 100 times' double-hypernuclei than before.

【Research Methods】

We will expose K$^-$ beam to the emulsion with its volume of 3 times larger than that of the previous experiment (KEK-E373), where the K/beam ratio of J-PARC becomes nearly 4 times better than that of KEK-PS. At the exposure, we use electric detectors, e.g. counters, chambers and so on, which inform us of the production of Ξ$^-$ hyperon with two units of strangeness. Especially, Ge detector located in upstream of the emulsion will work for the energy shifts measurement of X-ray from Ξ-atom, where the shifts provide us the information of Ξ-nucleon interaction for the first time. By this hybrid emulsion method, we can expect 10 times more events of double-hypernuclei than before.

In the above hybrid method, we fail to tag 90% Ξ$^-$ hyperon production due to the efficiency and acceptance of the electric detectors. We can find three vertices in the decay of double-hypernucleus, as shown in the figure. If the events with such topology can be scanned in overall area of the emulsion, it is expected an additional 10 times more double-hypernuclei than those obtained by the hybrid method.



We are developing systems for whole-area scanning to complete detection for a few years.

The measurement of scattering and energy-loss can be done for decay daughters of double-hypernuclei and the binding energies of two hyperons are provided to study Y-Y interaction.

【Expected Research Achievements and Scientific Significance】

Unified understanding of the baryon-baryon interaction can be obtained in SU(3) symmetry with strangeness. It is expected that new species of double- hypernucleus shall be found and further we will get the know-how for the step of the study on triple-hypernuclei and/or charm-hypernuclei.

【Publications Relevant to the Project】

1. "Observation of a $^{6}_{\Lambda\Lambda}$He Double Hypernucleus". H.Takahashi *et al.*, Phys. Rev. Lett. Vol.87, 212502 (2001)
2. "Experimental Study of Double-Λ Hypernuclei with Nuclear Emulsion". K.Nakazawa and H.Takahashi, Prog. Theor. Phys. Suppl. 185, 335-343 (2010)

【Term of Project】 FY2011-2015

【Budget Allocation】 151, 600 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.phys.ed.gifu-u.ac.jp/index.htm

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

Title of Project : Search for New Physics Beyond the Standard Model with Rare Neutral Kaon Decays

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

Research Area : Physics
Keyword : Experimental Particle Physics, Neutral Kaons, CP violation

【Purpose and Background of the Research】

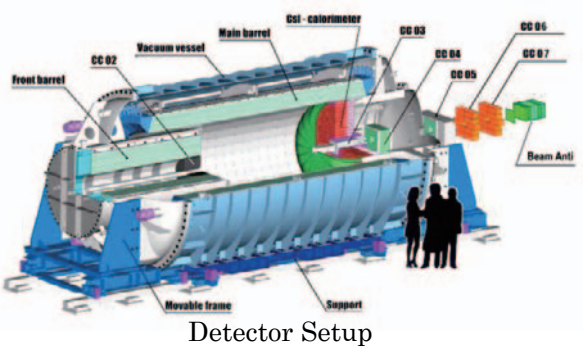
At the beginning of the universe, there were the same number of particles and antiparticles; but today, there are almost no antiparticles left. This is because particles and antiparticles behave slightly differently. This is called CP violation. In laboratories, CP violation was discovered in Kaons and B-mesons, and its mechanism was theoretically explained by Kobayashi and Maskawa. However, the CP violation mechanism in the standard model is still too small to explain why the antiparticles disappeared from the universe. This imbalance in the universe must have been produced by a CP-violating mechanism in a new physics beyond the standard model.

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

【Research Methods】

We will search for CP violation caused by new physics in a neutral kaon decay mode, K_L decaying into a neutral pion and neutrino pairs. The standard model predicts it branching ratio to be small, 3×10^{-11}, and its theoretical uncertainty is only a couple of %. If a particle of new physics, such as super symmetric (SUSY) particle or a 4th generation quark contribute to this decay mode, the branching ratio can be largely enhanced. Thus we will search for the decay down to the level predicted by the standard model, and measure its branching ratio.

To observe this rare decay, we will produce a large number of neutral kaons by hitting a target by protons accelerated by the J-PARC high intensity proton accelerator located in Ibaraki, Japan. The signature of the decay is that there are only two photons coming out from the decay. Other decay modes have charged particles or more than three photons in the final states. As shown in the next figure, an electromagnetic calorimeter is located downstream of the decay region to measure the energy and hit positions of the two photons. The decay region is surrounded by charged and photon veto detectors to reject all other decay modes which have extra particles.



Detector Setup

【Expected Research Achievements and Scientific Significance】

If we measure a branching ratio larger than the standard model prediction, it signifies the existence of a new physics, and gives the size of its effect. Even if we do not find the decay, we can still place constraints on new physics models and their parameters. In addition, by combining with results expected from a charged kaon decay experiment at CERN and B-meson results from new B-factory at KEK, both under construction, we can apply further constraints. If the proton-proton collider experiments at CERN LHC finds SUSY particles, we can give information on flavor structure of SUSY particles.

【Publications Relevant to the Project】

1. "Experimental Study of the Decay $K_L \to \pi^0 \nu \nu$", J.K. Ahn *et al.*, Phys. Rev. D **81**, 072004 (2010).
2. "Testing the CKM Model with Kaon Experiments", E. Blucher, B. Winstein and T. Yamanaka, Prog. Theo. Phys. **122**, 81 (2009).

【Term of Project】 FY2011-2015

【Budget Allocation】 171,500 Thousand Yen

【Homepage Address and Other Contact Information】

http://koto.kek.jp/

Title of Project : Effects of tensor forces in nuclear structure and search for hidden interactions in nuclei

Isao Tanihata
(Osaka University, Research Center for Nuclear Physics, Professor)

Research Area : Nuclear Physics

Keyword : theoretical nuclear physics, experimental nuclear physics, tensor forces

【Purpose and Background of the Research】

Present proposal aim for studying effects of the strong tensor forces caused by pion exchange interactions in stable and unstable nuclei through observations of characteristic changes of nuclear orbitals and high-momentum components in nucleon motion in nuclei. Since the invention of radioactive nuclear beams (RIB), new structures and phenomena have been discovered and that become a driving force of science with RIB in the world. Such discoveries and new suggestions include, neutron halo, neutron skin, soft mode of excitation, new magic numbers.

An appearance of the new magic number (N=16) among other data in neutron rich nuclei triggered a new view to the nuclear interactions that affect orbitals in nuclei. In particular the importance of the tensor forces, that have not played an important roles in shell models, has been pointed out recently. The tensor forces, that are originated from the pion exchange nucleon-nucleon interactions, has been known to play important roles for binding a deuteron and an alpha.

Theoretically, an effect of the tensor force on the internal momentum distribution of nucleon have been published by several authors. All papers show an enhancement of high-momentum component at around 2 fm-1 due to the tensor correlations between two nucleons. It is also clear that this high-momentum component appears only in p-n pair coupled to S=1. No such correlation exist in between n-n, for example, pair with S=0. Therefore the comparison of the high-momentum component between S=1 and S=0 pairs is a sensitive method to see the tensor correlations.

【Research Methods】

To study the effects of tensor interactions on nuclear structure, we plan to studies,

1. to establish the high-momentum components in the nucleon wave function in nuclei though high energy transfer reactions, (experimental)
2. to reveal tensor and other unknown interaction in nuclei though the systematic studies of nuclear structure by precise spectroscopies, (experimental)
3. to establish nuclear structure theory that include tensor forces explicitly and compare the prediction with experimental observations. Then also form a view of nuclei including pions. (theoretical)

【Expected Research Achievements and Scientific Significance】

We would like to confirm the importance of the high-momentum nucleon on the structure of nuclei. Then we build a new theory of nuclei that explicitly include the effect of tensor forces, thus pion interactions.

The theory will be a powerful tool to predict the structure and properties of nuclei far from the stability line that would not be obtained experimentally by the present days technology and thus useful for understanding the nucleo-synthesis path such as R-process.

【Publications Relevant to the Project】

1. "Searching for effects of tensor forces in nuclei", Modern Physics Letters A 25 (2010) 1886.
2. "Extended relativistic chiral mean field model for finite nuclei", Y. Ogawa, H. Toki, S. Tamenaga, and A. Haga, Progr. Theor. Phys. 122 (2009) 477.

【Term of Project】 FY2011-2015

【Budget Allocation】 161,400 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.rcnp.osaka-u.ac.jp/Divisions/cnp/

Title of Project : Study of Quantum Magnetic Phases by High Magnetic Field Neutron Scattering and XMCD

Hiroyuki Nojiri
(Tohoku University, Institute for Materials Research, Professor)

Research Area : Physics, Magnetism
Keyword : X-ray・Neutron, High Magnetic Field, Quantum Phase Transition

【Purpose and Background of the Research】

A variety of states are induced in matter by the application of high magnetic field and/or low temperature. We call each state of a matter as phase. The translation between these phases is called as phase transition. It is an important subject of condensed matter physics to find out novel phases in extreme conditions and to examine the origin of such phases. In phase transition, fluctuation plays an essential role. There are two types of fluctuations, thermal fluctuation and quantum fluctuation. The phase transition driven by the quantum fluctuation is called quantum phase transition and unexpected strange phases appear.

It is important to suppress the thermal fluctuation to examine the quantum phase transitions. The application of high magnetic field at low temperature is the best way to exclude the thermal effect and to pick up the intrinsic quantum effect. Another important point in our research is to use the microscopic probes such as neutron and X-ray to examine the quantum phase transitions. The combination of X-ray and neutron with the high magnetic field is very difficult task and so the example has been quite limited. Recently, we have established the world record of high magnetic field X-ray and neutron experiments and these successes are the basis of the present project.

【Research Methods】

We are aiming at generating 50 T, which is 1 million times as intense than geomagnetic field. To realize this, we use the pulsed magnetic field method. In pulsed magnet, more than 10 kA current flows by the capacitor bank discharge. The unique point of our system is to use the mini coil as shown in the photograph. The coil is very small and so the installation is easy. It increases dramatically the opportunities of high magnetic field experiment in X-ray and neutron facilities. In fact, our method is employed in abroad such as France and United States.

The key points of measurement are uses of X-ray and neutron. In X-ray, we can evaluate the magnetization in element selective manner for the difference of absorption edges in different elements. If we use this method, we can pick up the magnetic contribution of specific element in microscopic manner.

Another probe is the neutron, which is the atomic size small magnet. For this property, we can determine directly the arrangement of magnetic moments in matter with the atomic resolution. The powerfulness of the combination of high magnetic field with the X-ray and neutron will uncover the exotic properties of various quantum phases.

【Expected Research Achievements and Scientific Significance】

Our project would contribute to the understanding of quantum phase transition and quantum phases. Such understanding will be the basis of developing new functional materials such as multiferroics, quantum magnets, magnets with ubiquitous elements and so on.

【Publications Relevant to the Project】

(1)H. Nojiri *et al.* Neutron Laue Diffraction Study on the Magnetic Phase Diagram of Multiferroic $MnWO_4$ under Pulsed High Magnetic Fields, Phys. Rev. Lett. **106** (2011) 237202.

(2)T. Nakamura, Y. Narumi *et al.*, Soft X-ray Magnetic Circular Dichroism of a CoFe/MnIr Exchange Bias Film under Pulsed High Magnetic Field, Applied Physics Express **4** (2011) 066602.

Fig. 1 Minicoil with 3 cm diameter

【Term of Project】 FY2011-2015

【Budget Allocation】 163, 000 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.hfpm.imr.tohoku.ac.jp/

Title of Project : Electronic states of novel functional materials studied by ultrahigh-resolution three-dimensional spin- and angle-resolved photoemission spectroscopy

Takashi Takahashi
(Tohoku University, WPI-AIMR, Professor)

Research Area : Mathematical and Physical Sciences
Keyword : spintronics, photoemission spectroscopy, topological insulator, surface

【Purpose and Background of the Research】

Recent discovery of novel functional materials such as topological insulators and GMR compounds has accelerated intensive researches on the basic sciences and device applications. While the complete understanding of the novel physical properties requires the experimental elucidation of the spin-dependent electronic states, there have been very few studies so far, mainly due to the difficulty in directly detecting the spin itself. In this project, we investigate the basic electronic states in the vicinity of the Fermi level for spintronics-related functional materials where the spin-dependent quantum transport plays an essential role in characterizing the physical properties.

【Research Methods】

To elucidate the fine electronic states of new functional materials, we develop an ultrahigh-resolution three-dimensional spin-resolved photoemission spectrometer which achieves the world best energy, momentum, and spin-resolutions. By utilizing the ultrahigh-resolution capability of the constructed spectrometer, we perform spin- and angle-resolved photoemission spectroscopy on topological insulators, Rashba metals, GMR compounds, and half-metals. We investigate the Fermi surface, energy band dispersion, spin polarization, spin vector, and quasiparticle dynamics by separately observing the electronic states from the bulk, surface, and interface.

【Expected Research Achievements and Scientific Significance】

(1) A systematic high-resolution ARPES study by changing the crystal structure, the composition, and the doping level on several candidate materials would reveal the essential key electronic structure for the topological insulator, leading to discovery/design of new non-trivial topological insulators.

(2) By spin-resolved ARPES, we map out the spin polarization and the spin vector in the whole momentum space. We investigate the relationship between the Fermi-surface warping and the out-of-plane spin component to reveal the key factor dominating the spin polarization vector.

(3) We examine the theoretical prediction for the topological phase in an ultrathin Bi film by comparing the experimental result with the theory. In addition, we prepare ultrathin films of heavy-elements such as Pb, Tl, and Au, and seek for new materials having a large Rashba splitting.

(4) We investigate the electronic structure of GMR materials and half-metals prepared by the PLD method. We also perform spin-resolved ARPES on hetero-structured oxide thin films and elucidate the origin for the anomalous magnetism and conductivity of the interface.

【Publications Relevant to the Project】

[1] T. Sato et al., Direct Evidence for the Dirac-cone Topological Surface States in the Ternary Chalcogenide $TlBiSe_2$, Phys. Rev. Lett. **105**, 136802-1-4 (2010).

[2] S. Souma et al., Direct Measurement of the Out-of-Plane Spin Texture in the Dirac Cone Surface State of a Topological Insulator、Phys. Rev. Lett. **106**, 021680-1-4 (2011).

[3] A. Takayama et al., Giant Out-of-Plane Spin Component and the Asymmetry of Spin-Polarization in Surface Rashba States of Bismuth Thin Film, Phys. Rev. Lett. **106**, 166401-1-4 (2011).

【Term of Project】 FY2011-2014

【Budget Allocation】 162,300 Thousand Yen

【Homepage Address and Other Contact Information】

http://arpes.phys.tohoku.ac.jp

Title of Project : Study on relativistic electron accelerations with a development of wave-particle interaction analyzer

Takayuki Ono
(Tohoku University, Graduate School of Science, Professor)

Research Area : Earth and planetary science
Keyword : solar-terrestrial physics, radiation belts, electron acceleration, space weather

【Purpose and Background of the Research】

In geospace (inner magnetosphere), there exist the radiation belts that consist of trapped relativistic electrons and ions. Recent advances of theoretical and computer simulation studies suggest that whistler mode chorus emissions play an important role to generate relativistic electrons. The direct measurement of the relative phase between the cyclotron motion of an electron and wave field vector is essential for the identification of the energy transfer process between particle and waves. In conventional observations, the particle distribution function is derived from the integrations of the particle counts in the velocity space, which conceals the energy transfers between particle and waves.

We have proposed the new measurement concept of wave-particle interaction analyzers (WPIA) that can correlate the phase between an electron and wave, which can provide definitive evidence on the energy transfer via wave-particle interactions. In this project, we will realize this idea as a software program in CPU onboard the satellite. This Software-type WPIA (S-WPIA) system will be installed in the satellite and sounding rocket for in-situ observations, which will establish the new measurement methods of space plasma

【Research Methods】

In this research project, the following three subjects are conducted.

1) Development of S-WPIA simulator
2) Development of S-WPIA system
3) Operational tests of S-WPIA system with sounding rocket and satellite programs.

1) We study the chorus generation as well as the electron acceleration processes by a comprehensive simulation combined with the global simulation for the inner magnetosphere and the micro simulation for the wave-particle simulation. The developed pseudo-S-WPIA observations will be conducted using the S-WPIA simulator, which can be used for a design of measurement algorithm and observation plan.
2) We develop the pulse conversion unit of the particle measurement, onboard plasma density measurement unit, and timing synchronization unit that are essential components of the S-WPIA system. Taking into consideration of the study of subject 1), we develop software for the S-WPIA systems.
3) The S-WPIA observation system is established by in-situ observation for wave-particle interactions with sounding rocket and the satellite.

【Expected Research Achievements and Scientific Significance】

The S-WPIA system developed by this project realizes the direct measurement method for wave-particle interactions in space plasma. The concept of S-WPIA is an innovative method of space plasma measurements, which contributes a great advance for understanding of wave-particle interactions and particle acceleration mechanism.

【Publications Relevant to the Project】

- Fukuhara, H., H. Kojima, Y. Ueda, Y. Omura, Y. Katoh, and H. Yamakawa, A new instrument for the study of wave-particle interactions in space: One-chip wave-particle interaction analyzer, Earth Planets Space., 61, 756-778, 2009.
- Miyoshi, Y., et al., Geospace exploration mission: ERG project, Trans. Japan Soc. Aer. Space Science, 8, ists27, 2010.

【Term of Project】 FY2011-2015

【Budget Allocation】 162, 200 Thousand Yen

【Homepage Address and Other Contact Information】

http://stpp.gp.tohoku.ac.jp/s-wpia/
ono@stpp.gp.tohoku.ac.jp

Title of Project : Growth of the Second Continent and Mantle Dynamics: Insights from a History of Continental Growth and Tectonic Erosion

Shigenori Maruyama
(Tokyo Institute of Technology, Graduate School of Engineering, Professor)

Research Area : Mathematical and physical sciences
Keyword : Earth History, Tectonics, Terrestrial and planetary evolution

【Purpose and Background of the Research】

Tectonic erosion could drive a surface to mantle transportation of continental materials (Fig. 1), however any quantitative approach has done about the volume and effect of the subducted materials. We aim to develop a new scenario for the Earth evolution including the recycling effect of the continental materials.

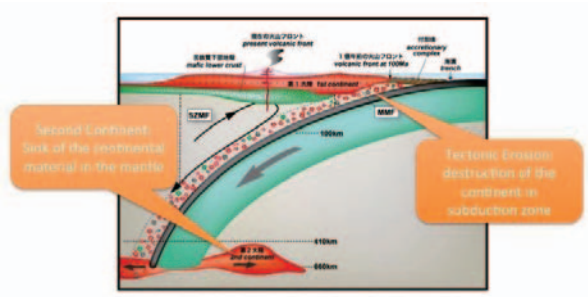


Fig.1 Tectonic erosion and the 2nd continent

【Research Methods】

We organize five interdisciplinary groups for the subject. Geology, geochemistry, high-P experiment, seismology, and numerical simulation will be integrated to a new comprehensive model for the Earth evolution.

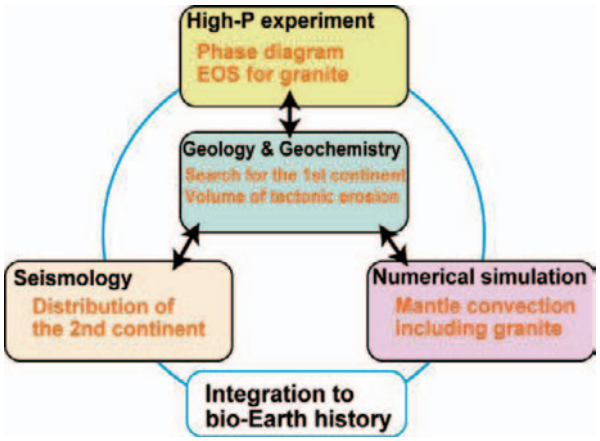


Fig. 2 Organization

【Expected Research Achievements and Scientific Significance】

Continental material could be the significant radiogenic heat source in the mantle, however its effect to the mantle dynamics has been underestimated. Our multidisciplinary approach is a unique and never has done. Expected results will renovate a scenario how the Earth has been cooled, consequently it will contribute to understand how the Earth became a habitable planet.

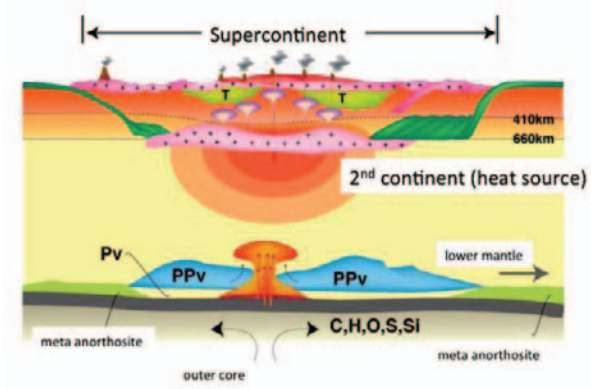


Fig.3 Expected model for the mantle dynamics including recycled continental materials.

【Publications Relevant to the Project】

Kawai, K., Tsuchiya, T., Tsuchiya, J., and Maruyama, S. (2009). Lost primordial continents. Gondwana Res 16, 581-586.

Maruyama, S., Omori, S. , Senshu, H., Kawai K., and Windley, B.F., (2011) Pacific-type Orogens: New Concepts and Variations in Space and Time from Present to Past, J. Geography, 120. 115-223

【Term of Project】 FY2011-2015

【Budget Allocation】 162, 900 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.geo.titech.ac.jp/lab/maruyama/maruyamalab/maruyamalab.html

Title of Project：Isotopomer Material Cycle Analysis

Naohiro Yoshida
（Tokyo Institute of Technology, Interdisciplinary Graduate School of Science and Engineering, Professor）

Research Area：Environmental chemistry, Geochemistry, Environmental behavior analysis
Keyword：material cycle analysis, isotopomer

【Purpose and Background of the Research】

Global environmental issues are caused mostly by anthropogenic disturbances to the natural cycles of environmental materials. The cycle of such materials need be analyzed quantitatively and precisely to help understanding the natural and anthropogenic processes regarding their cycles. We proposed the use of 'isotopomers' which are known to be powerful tracers to reduce the uncertainties regarding the biological, chemical, and physical source and sink processes of environmental materials.

'Isotopomers' are defined as isotopically substituted molecules of a molecular species. Bio-elements such as hydrogen and sulfur have one to four isotopes. And there are numerous isotopomers for each molecule with different sites and different combinations of isotopes. We have dedicated ourselves to the analysis of the cycle of greenhouse gases in terms of their own isotopomers, their source materials and their sink products to reduce uncertainties concerning their sources and sinks.

During the past years the following technologies have been developed in the field of isotopomer analysis:

1) Measurements for mass-independent fractionation (MIF) in some compounds containing oxygen and sulfur.

2) Precise measurements of molecules containing more than one rare isotope (clumped-isotope), which potentially may be used as a new thermometer and atmospheric tracer.

3) Position-specific isotopic analysis (PSIA) for some structurally-complex biomolecules.

Our final goal is the generation of a novel isotopomer material cycle analysis which is applicable to all environments from cells to the Earth system.

【Research Methods】

We advance the formulation of new material cycle analysis by integrating cutting-edge measurement technologies, theoretical calculations, and numerical models.

Our main focus includes:

1) Analytical development for isotopomers of biomolecules such as acetic acid using mass spectroscopy and NMR, and its application to environmental and microbial samples.
2) Analytical development for MIF and clumped-isotope of gaseous and aerosol species relevant to climate change.
3) Theoretical calculation of rate constants for the atmospheric reactions of isotopomers
4) Clarification of N_2O cycle and sulfur cycle using isotopomer models and available data.

【Expected Research Achievements and Scientific Significance】

The generation of a new material cycle analysis is expected to refine the estimation of global cycles of greenhouse gases and related materials. The new isotopomer material cycle analysis will be effective not only for refinement of greenhouse gas cycles but also for better understanding of biogeochemical processes.

【Publications Relevant to the Project】

Yoshida, N., and S. Toyoda, Constraining the atmospheric N_2O budget from intramolecular site preference in N_2O isotopomers, *Nature*, **405**, 330-334, 2000.

Ueno, Y., M. S. Johnson, S. O. Danielache, C. Eskebjerg, A. Pandey, and N. Yoshida, Geological Sulfur Isotopes Indicate Elevated OCS in the Archean Atmosphere, Solving Faint Young Sun Paradox, *Proc. Nat. Acad. Sci., USA.*, **106**, 14784-14789, 2009.

【Term of Project】 FY2011-2015

【Budget Allocation】 160,300 Thousand Yen

【Homepage Address and Other Contact Information】

http://nylab.chemenv.titech.ac.jp/
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Title of Project : Self-Organization of Magnetospheric Plasma Confinement --- nonlinear effect of space-time distortion cause by inhomogeneous magnetic field

Zensho Yoshida
(The University of Tokyo, Graduate School of Frontier Sciences, Professor)

Research Area : Plasma Science
Keyword : Plasma Physics, Self-organization, Vortex, Magnetosphere

【Purpose and Background of the Research】

Magnetospheres are self-organized structures found commonly in the Universe. A dipole magnetic field sets the stage for charged particles to cause a variety of interesting phenomena. We can explain the self-organization process by the nonlinear effect of "space-time distortion" represented as a "vortex" (Fig. 1); a strongly inhomogeneous magnetic field distorts the space-time metric of the magnetized particle, giving rise to various interesting phenomena. The aim of this project is to elucidate the physical mechanisms in a magnetospheric vortex and demonstrate their applications.

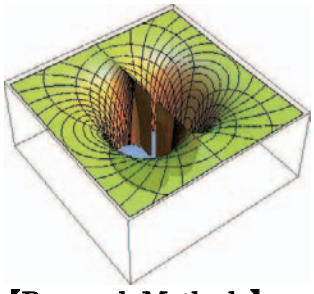


Fig. 1: The distorted metric of space-time dictating the motion of charged particles in the vicinity of a dipole magnetic field.

【Research Methods】

Recently a "laboratory magnetosphere" has been created; the RT-1 device levitates a superconducting ring magnet in a vacuum chamber and produces a magnetospheric plasma (Fig. 2). By the electron-cyclotron heating a high temperature plasma is produced proving high-beta stable confinement (simultaneous electron parameters: temperature $\gtrsim$10keV, density $\lesssim 10^{17}\mathrm{m}^{-3}$, beta $\gtrsim$0.7, energy confinement time $\gtrsim$0.5s).

In this project, we will explore a new regime of parameters on RT-1: (1) Developing an ion-cyclotron heating (ICH) system, we will heat ions to produce high ion beta (~0.1), and demonstrate high-performance confinement. (2) By the strong inhomogeneity of the dipole magnetic field, the nonlinear magnetic beach heating in ICH will become possible. We will study the mechanism of heating developing Pockels sensor measurement. (3) Measuring the internal structure (density and temperature distributions, flow velocity, density and electric field fluctuations), we will explore the nonlinear structure of the magnetospheric vortex. Fast rotation will emerge as the ions are heated (predicted Alfvén Mach number $\sim(\beta_{ion})^{1/2}$).

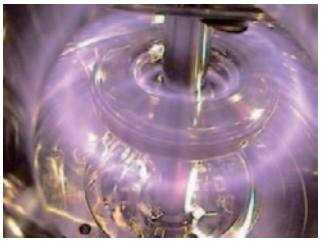


Fig. 2: RT-1plasma device; a levitated superconducting ring magnet produces a magnetospheric configuration, which confines high- temperature plasma.

【Expected Research Achievements and Scientific Significance】

The mechanism of plasma confinement in the magnetospheric system is totally different from those of tokamaks or helicals; it represents the realm of natural plasmas. The RT-1 plasma will have scaling parameters (Reynolds number, Hall parameter, etc.) comparable to space and astronomical systems, making it possible to study the mechanisms of in the Universe. The high-beta plasma in a magnetospheric system will open up the possibility of "advanced fusion" burning, for example, D-^{3}He fuel.

【Publications Relevant to the Project】

1. Z. Yoshida *et al.*; Magnetospheric vortex formation: self-organized confinement of charged particles, Phys. Rev. Lett. **104** (2010), 235004 1-4.
2. S.M. Mahajan and Z. Yoshida; Twisting space –time--Relativistic origin of seed magnetic field and vorticity, Phys. Rev. Lett. **105** (2010), 095005 1-4.

【Term of Project】 FY2011-2015

【Budget Allocation】 81,800 Thousand Yen

【Homepage Address and Other Contact Information】

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

Title of Project : Development of Density Functional Theory

Kimihiko Hirao
(RIKEN, Advanced Institute for Computational Science, Director)

Research Area : Theoretical Chemistry
Keyword : electronic structure theory, density functional theory (DFT), LC functional

【Purpose and Background of the Research】

Density functional theory (DFT) has emerged as a powerful computational tool for the chemical systems. However, there is no means of systematically improving DFT energies. Our long-range corrected density functional theory (LC-DFT) solves many problems of the conventional DFT. The purpose of this project is to establish LC-DFT as the standard of the electronic structure theory.

There are two approaches in the electronic structure theory, the wave function method and the density functional theory. For wave function method, a huge and very successful effort has been done in the last 30 years leading to accepted state-of-the-art methodology. Accurate results can be obtained for small systems but it is rather difficult to handle very large systems due to the steep N-dependence. DFT is not reached such a mature stage as wave function method but DFT is simple, conceptual, and applicable to large systems. However, the accuracy depends on the *xc* functional employed. DFT fails to describe induced/response properties. The failures arise mainly from the wrong long-range behavior due to the local character of the approximate *xc* functionals. We have developed new functionals based on the long-range correction scheme. The exchange functional is partitioned with respect to the interelectronic separation into long-range and short-range parts using a standard error function

$$\frac{1}{r_{12}} = \frac{1-erf(\mu r_{12})}{r_{12}} + \frac{erf(\mu r_{12})}{r_{12}}$$

LC solves many of the conventional DFT problems. Very recently we have demonstrated that LC satisfies DFT-Koopmans' theorem. This implies that the orbitals and the orbital energies of the LC-Kohn-Sham theory do have a strict physical meaning.

In this project, we will further develop LC-DFT theoretically. We will extend LC-DFT to more practical one by collaborating with experimental and other field theoretical investigators. Using this new theory, we will clarify the mechanisms of significant photo- and electro-chemical reactions and suggest new functional materials. LC-DFT will be established as the standard of the electronic structure theory.

【Research Methods】

In this project, we feature new developments of photo- and electro-chemical reaction theories and its high-speed computational algorithms for using on next-generation supercomputer "K", and the eludations of significant reaction mechanisms and the designs of new functional materials in photo- and electrochemistry:

1. New developments of photo- and electro-chemical reaction theories:
   - A nonadiabatic interaction calculation theory on time-dependent DFT (TDDFT)
   - A multiconfigurational DFT
   - An open-shell TDDFT with spin-orbit effects
   - A new reaction analysis method on orbital
2. Developments of high-speed computational algorithm of DFT used on K supercomputer:
   - An order-N algorithm of LC-DFT
   - An order-N algorithm of LC-TDDFT
3. Reaction mechanism analyses and new functional material designs on:
   - Electron transfers in fuel cell
   - Photosynthetic reactions of purple bacteria

【Expected Research Achievements and Scientific Significance】

Our LC will evolve DFT into the higher stage. As the accomplishments of this project, we will obtain new photo- and electro-chemical reaction theories and an analysis method on orbital, and a new software with high-speed computational algorithms of DFT adapted to the K supercomputer architecture. This software enables us to analyze photochemistries of several thousands atoms and charge transfers in the interfaces, which cannot be treated even by the state-of-the-art method.

【Publications Relevant to the Project】

- Y. Tawada, T. Tsuneda, S. Yanagisawa, T. Yanai and K. Hirao, "A long-range- corrected time-dependent density functional theory", *J. Chem. Phys.* 120, 8425 – 8433 (2004).
- T. Tsuneda, J. Song, S. Suzuki, and K. Hirao, "On Koopmans' theorem in density functional theory", *J. Chem. Phys.*, 133, 174101(1-9) (2010)

【Term of Project】 FY2011-2015

【Budget Allocation】 165,500 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.aics.riken.jp/

Title of Project : Rapid synthesis of complex molecules using super Brønsted acid catalysis

Hisashi Yamamoto
(Chubu University, Professor)

Research Area : organic synthesis
Keyword : selective organic synthesis, molecular acid catalysis

【Purpose and Background of the Research】

Selective organic synthesis was refined significantly during the last century and we now have numerous reliable tools for chemical transformations using transition metal catalysis. The recent high demand for green chemistry, however, has required environmentally benign chemical processes, particularly the non-metal catalysis protocols. The present project will attempt to introduce new strong organic non-metal acid catalysis, which is expected to be one of the major tools of organic synthesis of the next generation, and to apply these new catalysts for various organic transformations. Further, the project will attempt to design new super Brønsted acid catalysts, which will give us opportunities to make complex molecules by combining their use with super-silyl reagents. These new processes will establish an unusually short synthetic route to construct complex three-dimensional molecules for which very few synthetic methods are currently available.

【Research Methods】

Combined use of super Brønsted acid catalyst and super-silyl reagent would provide simple and reliable methods to control the otherwise nonstop polymerization process so that it terminates at three or four steps. The super Brønsted acid catalyst serves as an important tool to accelerate and/or decelerate these chemical processes. Further, chiral Brønsted acid catalyst will open a new approach for an asymmetric version of these successive reactions.

Specifically, the super-silyl groups generate a specially designed molecular reaction template within which the polymerization reaction can be stopped by strong stereochemical demands. Thus, we will be able to stop the second, third, and fourth successive reactions for various transformations by choosing the proper reaction conditions and catalysis. For example, the double or triple aldol products could be prepared with high chemoselectivity as well as diastereo stereoselectivity. Using alpha alkoxy or amino silyl enol ethers, we would be able to obtain all the functional polyhydroxy linear carbon chain or amino-hydroxy chains stereo- and regioselectively.

The concept can also be applied to 1,3-butadiene polymerization as well as terminal olefins polymerization processes. Employing these new protocols, we would be able to prepare isoprenoid structures in significantly short steps or 1,3-siloxy derivatives stereoselectively.

【Expected Research Achievements and Scientific Significance】

Flexible and reliable molecular engineering is one of the most sought-after scientific targets of our century. The present proposed strategy would contribute the molecular engineering by providing rapid access of three-dimensional molecules with high stereo- and regioselectivities. The method would be very useful not only for medicinal chemistry but also for material sciences. The Brønsted acid catalyst, which was developed mainly in the principal investigator's laboratories, is the key catalyst for the present proposal. The same catalyst, however, would contribute to numerous other fields of synthesis as an environmentally acceptable green catalyst.

【Publications Relevant to the Project】

(1) Cheon, C.H., Yamamoto, H., A Brønsted Acid Catalyst for the Enantioselective Protonation Reaction, *J. Am. Chem. Soc.*, **2008**,130, 9246-9247.
(2) Boxer, M. B., Yamamoto, H., Ketone Super Silyl Enol Ethers in Sequential Reactions: Diastereoselective Generation of Tertiary Carbinols in One Pot, *J. Am. Chem. Soc.*, **2008**,130, 1580-1583.
(3) Boxer, M. B., Yamamoto, H. "Super Silyl" Group for Diastereoselective Sequential Reactions: Access to Complex Chiral Architecture in One Pot, *J. Am. Chem. Soc.*, **2007**, 129, 2762.

【Term of Project】 FY2011-2015

【Budget Allocation】 165, 600 Thousand Yen

【Homepage Address and Other Contact Information】

hyamamoto@isc.chubu.ac.jp

Title of Project : Mesoscopically Sized and Restricted Polymer Thin Films for Creation of New Photoresponsive Functions

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

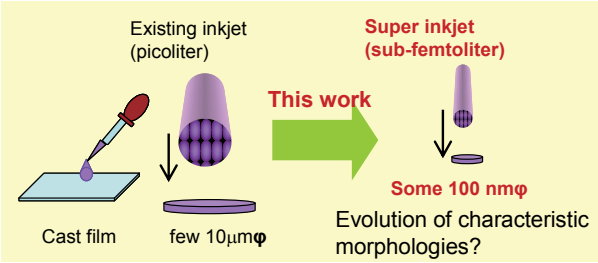
Research Area : Polymer Chemistry
Keyword : polymer thin films, mesoscopic restriction, wrinkle formation, photoresponse

【Purpose and Background of the Research】

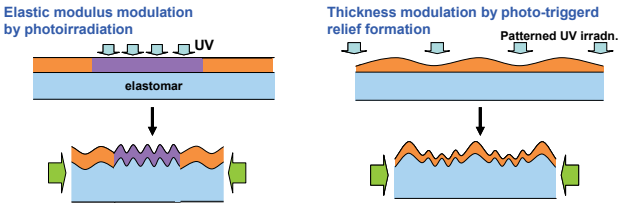
We have been accumulated a number of knowledge on smart photoresponsive films that exhibit molecular alignment and morphology evolutions in response to light. However, the investigations so far are limited to large area film systems. This project is planned to deal with mesoscopically (10 – 100 nm regime) restricted films prepared by a super-inkjet system (whole area divided) and surface wrinkling (patterned area divided). The materials will involve polymer blends, block copolymers, organic-inorganic hybrid materials. This project is intended to elucidate the characteristic morphology formation of phase separation structure whose feature size is less or comparable to the total film size. Based on the precise understandings of the film properties, the project also intends to create new photoresoponsive materials via introducing photoreactive unit such as azobenzene.

【Research Methods】

Mesoscale sized film will be prepared with a recently developed super-inkjet apparatus which is able to eject a droplet of sub-femtoliter levels. This allows formation of a film of less than one mirometer (mesoscopic film). Using this method, phase separation behaviors of the resulting films of polymer blends, block copolymers and organic-inorganic hybrids will be evaluated.



The surface wrinkling formed on an elastomer film is a subject of intensive study in recent years. In this project, we will use a various type of photoresponseive polymer thin films as the top coat layer. We expect that the patterned photomodulatins of the top layer can provide on-demand extended variations in the wrinkle formation phenomena.



【Expected Research Achievements and Scientific Significance】

New and versatile possibilities in pattern formation are proposed in this project, which is expected to contribute a great deal to polymer chemistry, physics and processing technologies. Based on the knowledge obtained, the fabrication of more precisely designed photoresponsive materials for photomechanical functions is anticipated.

【Publications Relevant to the Project】

1. J. Isayama, S. Nagano, T. Seki, Photo-triggered mass migrating motions in liquid crystalline azobenzene polymer films with systematically varied thermal properties, *Macromolecules*, **43(9)**, 4105–4112 (2010).
2. T. Seki, Light-directed smart responses in azobenzene-containing liquid crystalline polymer thin films, in *Functional Polymer Films* (R. Advincula & W. Knoll eds,), Vol. 2, Wiley-VCH , chapter 31, pp. 961-982 (2011).

【Term of Project】 FY2011-2015

【Budget Allocation】 144,000 Thousand Yen

【Homepage Address and Other Contact Information】

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

Title of Project : Creation of Functional Materials Using Polymer Self Assembly and Biomedical Application

Mitsuru Akashi
(Osaka University, Graduate School of Engineering, Professor)

Research Area : Polymer Chemistry
Keyword : Nano Structure Controlled Biomaterial, Polymer Thin Film, Interface, LbL

【Purpose and Background of the Research】

Polymer-polymer interaction arises strongly, even if it is weak interaction at low molecular level individually. We have reported the creation of medical materials and regular nanospace using layer by layer (LbL) assembly, taking advantages of polymer-polymer interaction. LbL method is the unique technique for thin film preparation, dipping the substrate into two kinds of polymer solutions alternatively, which associates with each other. For example, we have prepared hollow nanoparticle with biodegradable polylactides by stereocomplex formation. In 2000, we have revealed the "weak interaction", such as Van der Waals interaction, could apply to LbL method.

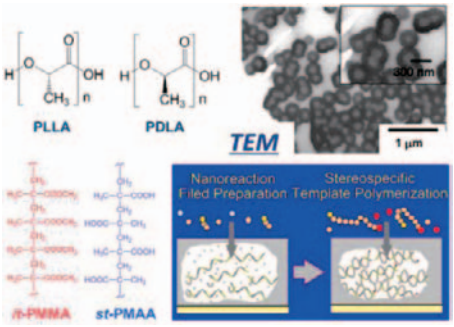


Figure 1. Nanomaterials by LbL method.

In this study, we collect the basic information on the LbL method with "weak polymer-polymer interaction", which we have firstly developed in the world. The technique is applied to create the novel safe functional materials, using biocompatible polymers with various components and substrate shapes. After the evaluation of the material functionalities, the cell experiments, the experiments *in vitro* and *in vivo*, and translational research are carried out in order to show that the polymer chemistry contributes the human society.

【Research Methods】

The LbL methods have been mainly achieved with 2 dimensional substrates. We expand the LbL materials for 0 dimensional, 1 dimensional, and 3 dimensional substrates, such as cell, tube, and various structures. The approach advantages the proper biomedical materials, shown in Figure 2.

The chemical and physical characters are analyzed for the LbL materials with biocompatible polymers, and the safety test is performed to establish technologies for translational research.

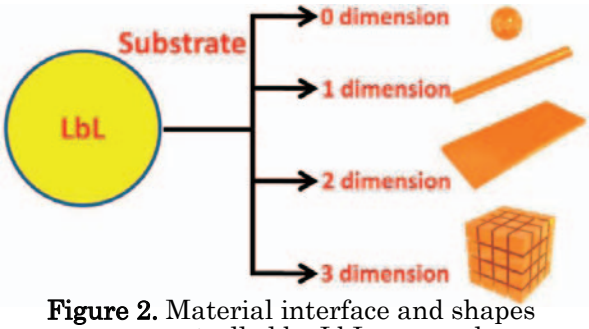


Figure 2. Material interface and shapes controlled by LbL approaches.

【Expected Research Achievements and Scientific Significance】

Important insights regarding polymer assembly are obtained. Polymer biomedical materials are fabricated, which are controlled with interface and form. The results will be utilized for novel medical treatment and future development of healthcare.

【Publications Relevant to the Project】

1. Takeshi Serizawa, Ken-ichi Hamada, Mitsuru Akashi, "Polymerization within a molecular scale stereoregular template" *Nature* **2004**, *429*, 52-55.
2. Michiya Matsusaki, Kohji Kadowaki, Yoshio Nakahara, Mitsuru Akashi, "Fabrication of cellular multilayers with nanometer-sized extracellular matrix films" *Angew. Chem. Int. Ed.* **2007**, *46*, 4689-4692.

【Term of Project】 FY2011-2015
【Budget Allocation】 163,900 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.chem.eng.osaka-u.ac.jp/~akashi-lab/

Title of Project : Development of Electronic Multifunction Based on Organic Triangular Spin Lattice

Gunzi Saito
(Meijo University, Research Institute, Professor)

Research Area : Chemistry
Keyword : Electric/Magnetic function, Crystal structure, Organic electronic materials/devices

【Purpose and Background of the Research】

Quantum spin liquid, that was first proved experimentally by our group for organic triangular spin lattice κ-$(ET)_2Cu_2(CN)_3$, remains wave nature of electron spins down to extremely low temperatures and competes with several electronic phases (Mott insulating, metal, and superconducting phases). For the triangular spin lattice system, the magnitude (t) and its anisotropy (t'/t; Fig. 1) of transfer integrals can be controlled by selecting component molecules and designing the assemblies, and therefore, systematic material exploration including the adjacent electronic phases is an urgent issue. In this project, we will systematically develop the triangular spin lattice system, control the t and t'/t values with applying pressure utilizing the characteristics of organic matters (soft lattice and electronic state), and inject the carriers by electric field and light irradiation, with the aim of exploration of new quantum spin lattice system and electronic multifunctions.

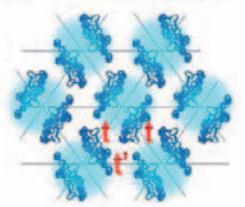


Figure 1 ET packing in κ-$(ET)_2X$ (Light blue circle: $(ET)_2^{\bullet+}$ dimer).

【Research Methods】

On the basis of accumulated knowledge, we will develop new triangular spin lattice system composed of molecular units with S = 1/2 spin (e.g., cationic radical dimer for TTF system, and anionic radical monomer for C_{60} system) by designing and selecting component molecules (ref. 1). In addition, we will establish (1) the chemical control method of localization and symmetry of electronic system, (2) the control method of geometrical spin anisotropy and bandwidth by applying uni-axial stress and hydrostatic pressure, (3) the T-P phase diagram around the quantum spin liquid phase, (4) the novel pressure-induced superconducting phase and external field induced metal-insulator transition associated with the spin frustration, (5) the ionic liquids for improving FET device performance, and (6) the non-equilibrium dynamics of excitation state for electron and lattice systems on a wide energy and time (fs ~ ms) scales.

【Expected Research Achievements and Scientific Significance】

Exploration of new quantum spin liquid system and their comprehensive understanding would allow the elucidation of quantum spin liquid behavior. Although seven quantum spin liquid materials (one being organic matter and the other being inorganic matters) have been found after our discovery, the phase neighboring the superconducting one is still limited for κ-$(ET)_2Cu_2(CN)_3$. Therefore, our project is a leading and ingenious one that faces the nature of quantum spin liquid, with the aim of the derivation of the relationship between quantum spin liquid and superconductivity. We also promote construction of new principle devices, and lay an innovative and advanced foundation of material science, by chemical and physical control (i.e., temperature, pressure, electric field, light, magnetic field, etc).

【Publications Relevant to the Project】

1. G. Saito and Y. Yoshida "Development of Conductive Organic Molecular Assemblies: Organic Metals, Superconductors and Exotic Functional Materials" *Bull. Chem. Soc. Jpn.*, **80**, 1-137 (2007).
2. D. V. Konarev, S. S. Khasanov, A. Otsuka, M. Maesato, G. Saito, and R. N. Lyubovskaya, "A Two-Dimensional Organic Metal Based on Fullerene" *Angew. Chem. Int. Ed.*, **49**, 4829-4832 (2010).
3. Y. Shimizu, H. Kasahara, T. Furuta, K. Miyagawa, K. Kanoda, M. Maesato, and G. Saito "Pressure-Induced Superconductivity and Mott Transition in Spin-Liquid κ-$(ET)_2Cu_2(CN)_3$ Probed by ^{13}C NMR" *Phys. Rev.*, **B81**, 224508/1-5 (2010).

【Term of Project】 FY2011-2015

【Budget Allocation】 188,400 Thousand Yen

【Homepage Address and Other Contact Information】

In preparation

Title of Project : The development of plasmonic antennae realizing light harvesting/localization and its application to solar cells

Hiroaki Misawa
(Hokkaido University, Research Institute for Electronic Science, Professor)

Research Area : Photochemistry
Keyword : localized plasmon, nanomaterials, optical physics

【Purpose and Background of the Research】

The development of a high-efficiency solar cell is critical to the development of a future low-carbon society. To produce a solar cell with high photoelectric conversion efficiency, we need to develop a system that responds to a wide spectrum of solar light, from visible to near-infrared wavelengths. However, the photoelectric conversion characteristics of an amorphous silicon solar cell commonly used today are known to drastically decrease in wavelength ranges longer than 700 nm. However, the spectral distribution in an infrared wavelength region longer than 800 nm accounts for ~40% of the entire solar energy observed on earth, and only a few solar cells can efficiently convert solar energy with such a long wavelength to electrical energy. We have recently demonstrated the first successful plasmonic photoelectric conversion from visible to near-infrared wavelengths using electrodes in which gold nanostructures are elaborately arrayed on the surface of TiO_2 single-crystal electrodes via a top-down nanostructuring process. In this study, we aim to develop plasmon enhanced photocurrent generation system with a function of optical antennae realizing light harvesting and localization, and we will optimize a structural design which can realize the efficient electronic transition from a gold nanostructure to TiO_2.

【Research Methods】

To construct an efficient solar cell that responds to near-infrared light, it is necessary to elucidate a relationship between photocurrent generation and plasmonic enhancement effects. Therefore, we will fabricate gold nanoblocks with nanometric accuracy with the following characteristics: strong field enhancement and radiation suppression owing to Fano effect or Rabi oscillation, and sharper features at the edges using an ultra-high-resolution electron beam lithography system with an acceleration voltage of 125 kV. We will improve the function of "an optical antenna" to a limit, and try improvement in the photoelectric conversion efficiency

【Expected Research Achievements and Scientific Significance】

The plasmon-assisted photocurrent generation system has the outstanding function "the optical antenna" which enables to light harvesting and localization to the nanospace of gold nanostructure/TiO_2 electrode interface. In this study, it has originality which aims at realization of the infrared light solar cell with high photoelectric conversion efficiency by improving the characteristic "optical antenna" function to a limit. Furthermore, this research also gives various knowledge to the research on the interaction between localized surface plasmon and materials in which many points remaining which are not solved scientifically, so that the acquired knowledge will give a big impact to the researchers in this field.

【Publications Relevant to the Project】

1. Y. Nishijima, K. Ueno, Y. Yokota, K. Murakoshi, H. Misawa, *J. Phys. Chem. Lett.*, **1**, 2031-2036 (2010).
2. S. Gao, K. Ueno, H. Misawa, *Accounts. Chem. Res.*, **44**, 251-260 (2011).
3. K. Ueno, S. Juodkazis, T. Shibuya, Y. Yokota, V. Mizeikis, K. Sasaki, H. Misawa, *J. Am. Chem. Soc.*, **130**, 6928-6929 (2008).
4. K. Ueno, S. Juodkazis, V. Mizeikis, K. Sasaki, H. Misawa, *Adv. Mater.*, **20**, 26-30 (2008).

【Term of Project】 FY2011-2015

【Budget Allocation】 166,400 Thousand Yen

【Homepage Address and Other Contact Information】

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Title of Project : Research on the high frequency spintronics

Yoshishige SUZUKI
(Osaka University, Graduate School of Engineering Science, Professor)

Research Area : Applied solid state physics
Keyword : (S) Spintronics

【Purpose and Background of the Research】

Recently, not only a charge-flow but also a spin-flow in solids started to be controlled. In this study, we establish a systematic understanding of high frequency spintronics, which has basis on the excitation of precession of a magnetization in a frequency range from GHz to THz.

【Research Methods】

1. High performance spin-torque oscillator

(a) Clarification of a mechanism giving a oscillation linewidth

From real time measurements of the oscillation signals, an origin of the oscillation linewidth will be clarified.

(b) Clarification of a coupled oscillation

By investigating effects of an external high frequency signal or a mutual coupling, we reveal a mechanism of the coupled oscillation operation.

(c) Development of over 50GHz oscillator and its characterization technique

Coupling between optical mode in multilayer to the injected current will be investigated. We develop a characterization method in over 50GHz range in collaboration with Prof. Rasing of Radboud University.

2. Investigation of an ultra-high sensitive field sensor

From observations about oscillation amplitude, phase fluctuation, and response to an external field, we clarify a performance of the spin-torque oscillator as an ultra-high sensitive field sensor.

3. Ultra-high sensitive spin-torque diode

Non-linear response of the magnetization to the spin-current and effects to the diode effect will be investigated. Detection limt of the spin-torque diode signal from very small magnetic objects will be investigated.

【Expected Research Achievements and Scientific Significance】

Establishment of a systematic understanding of high frequency spintronics, which has basis on excitations of precession of a magnetization in a frequency range from GHz to THz is expected.

From the knowledge a spin-torque oscillator with a high output power, high-Q, and over 50GHz operation, a spin-torque diode with high sensitivity, which surpasses that of semiconductor diodes, will be realized. Also highly sensitive nano-scale magnetic sensor, which may detect a stray field from paramagnetic particles will be realized. Further, a principle to detect a single spin will be clarified.

The results are expected to provides a new principle of the information storage and considerable influences to chemistry, biophysics, medical science, etc.

【Publications Relevant to the Project】

[1] H. Kubota, A. Fukushima, K. Yakushiji, T. Nagahama, S. Yuasa, K. Ando, H. Maehara, Y. Nagamine, K. Tsunekawa, D. D. Djayaprawira, N. Watanabe, and Y. Suzuki, “Quantitative measurement of voltage dependence of spin-transfer torque in MgO-based magnetic tunnel junctions”, Nature Physics 4, 37-41 (2008).

[2] A. M. Deac, A. Fukushima, H. Kubota, H. Maehara, Y. Suzuki, S. Yuasa, Y. Nagamine, K. Tsunekawa, D. D. Djayaprawira and N. Watanabe, “Bias-driven high-power microwave emission from MgO-based tunnel magnetoresistance devices”, Nature Physics Vol 4. No 8. 803-809 (2008).

[3] A. A. Tulapurkar, Y. Suzuki, A. Fukushima, H. Kubota, H. Maehara, K. Tsunekawa, D. D. Djayaprawira, N. Watanabe & S. Yuasa, “Spin-torque diode effect in magnetic tunnel junctions”, Nature, Vol 438, 339 (2005).

【Term of Project】 FY2011-2015

【Budget Allocation】 165,700 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.suzukiylab.mp.es.osaka-u.ac.jp/

Title of Project : Demonstration of ultrafast electron diffraction with fast electron pulse generated in plasma by intense femtosecond laser pulses

Shuji Sakabe
(Kyoto University, Institute of Chemical Research, Professor)

Research Area : Eng., Applied Phys., Thin film/surface and interfacial physical properties
Keyword : Electron microscopy

【Purpose and Background of the Research】

As a technology to observe structural dynamics such as superfine state transition in matter directly in the temporal scale as short as vibration of a single atom (< several 100fs), time resolved electron diffraction (TRED) is promising. With the TRED phase transition in solid, transitional molecular structure in gas, and surface dynamics have been studied. However, the temporal resolution in the TRED experiments is not shorter than several ps up to now. To observe structural dynamics directly in femtosecond temporal resolution by electron diffraction, intense femtosecond electron pulses are absolutely necessary. In recent research the electron pulses are generated from a photo -cathode irradiated by a low power femtosecond laser. In this method electron pulses must be accelerated to several 100keV, which is suitable to electron diffraction in matter, in an external electric field, and during the acceleration the pulse expands much by space charge effect. By only one pulse in which the number of electrons is reduced to avoid pulse expansion due to the space charge effect, electron diffraction cannot be imaged and multiple pulses are required, consequently it is not available to the observation of irreversible phenomena.

Radiation emitted from plasma produced by an intense femetosecond laser pulse is in general featured by point, pulse, high bright -ness, and compactness. In this research, to avoid the space charge effect mentioned above, we use and control the electrons, which are accelerated instantaneously to several 100keV in plasmas by an intense femtosecond laser pulse light. The specification of electron source required for ultrafast electron diffraction (UED) is estimated to be several 100keV, shorter than several 100fs, and more than one million in number. The present laser accelerated electron pulse can image diffraction by a single pulse, which cannot be done by the conventional photocathode electron source.

Though it is known that high-energy electrons are generated from solid or gas irradiated by an intense femtosecond laser pulse, generation and control of high quality electron source of several 100keV suitable to UED is not studied in both foreign and domestic institutes. The purpose of the present research is generation and acceleration of high-energy (several 100keV), short pulse (<several 100fs), and intense (>1 million electrons) electron source by intense femtosecond laser pulse light, and demonstration of single pulse UED with temporal resolution as short as several 100fs.

【Research Methods】

With an intense femtosecond laser, high quality electron pulses are generated, controlled, and compressed. Short pulse light is irradiated in advance on an object sample, and with some delay the electron pulse is irradiated it on to see the dynamical change through the electron diffraction. We are aiming single shot UED. Major theme and methods are (1) high density electron source <- use of metal foil <- reduction of laser pre-pulse <- development of plasma mirror, (2) low emittance electron source <- use of isolated micro foil <- development of laser driven foil flying, (3) short pulse electron source <- self pulse compression by phase reversal, (4) construction of laser pump & electron probe system, (5) construction of UED system and demonstration of single shot UED. The team organized by professionals of laser, laser plasma physics, radiation science, electron microscopy, and crystal science perform the present research.

【Expected Research Achievements and Scientific Significance】

The present research is advanced in the world. The completeness of the UED will bring much innovation in the fields of material science and nano science. By the combination with advanced electron microscopy technologies, we can observe ultrafast phenomena under various environments. Additionally the research on interactions of intense femtosecond laser with isolated micro thin foil is available to other radiations, and will contribute on the development of the next generation radiation sources.

【Publications Relevant to the Project】

○S. Tokita, M. Hashida, S. Sakabe, *et al.*, "Single-Shot Femtosecond Electron Diffraction with Laser-Accelerated Electrons:Experimental Demonstration of Electron Pulse Compression," Physical Review Letters **105**, 215004(4) (2010).
○S. Tokita, M. Hashida, S. Sakabe, *et al.*, "Single -shot ultrafast electron diffraction with a laser-accelerated sub-MeV electron pulse," Applied Physics Letters, **95**, 111911(3) (2009).

【Term of Project】 FY2011-2015

【Budget Allocation】 129, 200 Thousand Yen

【Homepage Address and Other Contact Information】

http://laser.kuicr.kyoto-u.ac.jp

Title of Project : High Harmonic Generation in the 1-keV region and their Application to Attosecond Soft-X-ray Spectroscopy

Jiro Itatani
(The University of Tokyo, The Institute for Solid State Physics, Associate Professor)

Research Area : Applied Physics
Keyword : Quantum electronics

【Purpose and Background of the Research】

Recent progress in intense laser technologies has realized the generation of coherent attosecond optical pulses by the process called high harmonic generation (HHG). The practical wavelength of HHG is, however, limited to about 10 nm (~ 100 eV in photon energy). This limit is set by the fact that the minimum wavelength of high harmonics is inversely proportional to the square of the driving laser's wavelength, where we usually use Ti:sapphire lasers operated at 800 nm. The purpose of this research is to break this limit by newly developed intense ultrafast light sources in infrared. If such novel light sources are realized, high harmonics can cover the spectral range down to 1 nm (or 1 keV in photon energies). Such soft X rays can interact with matters strongly and matches well with the absorption edges of light elements and transition metals. Using these absorption edges, we will aim to realize new methods to probe transiently excited states of matters on extremely short time scales. These efforts will open the field of ultrafast soft-X-ray spectroscopy.

【Research Methods】

We will develop a novel intense light source in infrared based on optical chirped pulse amplification. This concept was originally proposed by our group, and its proof-of-principle was recently demonstrated. This light source consists of a Ti:sapphire oscillator and amplifiers, whose outputs are used in parametric optical amplifiers for producing nearly-single-cycle phase-stabilized intense optical pulses at a 1-kHz repetition rate. Such high repetition rate and phase stabilization are crucial for spectroscopic applications. Using this new light source, we will produce high harmonics extended to 1-keV photon energies. Using the attosecond pulses in soft X rays, we will firstly work on the attosecond photoelectron spectroscopy in gas-phase molecules to establish time-resolved measurement techniques. We will then extend the methods to condensed matters to explore the possibilities of photo-emission spectroscopy and absorption spectroscopy on femtosecond to attosecond time scales.

【Expected Research Achievements and Scientific Significance】

Our new intense light source will realize the generation of soft X-ray pulses on femtosecond to attosecond time scales, opening the route to ultrafast soft-X-ray spectroscopy with the laboratory-scale setup. Such new instruments will allow us to probe photo-induced dynamics of atoms, molecules and condensed matters that occur on extremely-short time scales. Extension of the wavelength of intense light sources towards infrareds will also allow us to control various freedoms in matters, which will be useful to understand and control the non-equilibrium dynamics in photo-induced processes in molecular physics and condensed matter physics.

【Publications Relevant to the Project】

[1] N. Ishii, K. Kitano, T. Kanai, S. Watanabe, J. Itatani, "Carrier-envelope-phase-preserving, octave-spanning optical parametric amplification in the infrared based on BiB_3O_6 pumped by 800 nm femtosecond laser pulses," Appl. Phys. Express vol.4, p.022701-1-3 (2011),

[2] J. Itatani, J. Levesque, D. Zeidler, H. Niikura, H. Pepin, J. C. Kieffer, P. B. Corkum, "Tomographic imaging of molecular orbitals with high-harmonic generation," Nature vol. 432, p.867-871 (2011).

【Term of Project】 FY2011-2015

【Budget Allocation】 119,800 Thousand Yen

【Homepage Address and Other Contact Information】

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Title of Project : Adaptively controlled multistage nanofocusing systemfor x-ray free electron laser

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

Research Area : ultraprecision machining, optical fabrication and metrology, x-ray optics
Keyword : ultraprecision machining, optical sensing, x-ray optics

【Purpose and Background of the Research】

Third generation synchrotron radiation facilities are now producing high-quality light with wavelengths ranging from the infrared to hard-x-ray regions. The use of hard x-rays in conjunction with analysis methods such as x-ray diffraction, x-ray fluorescence, x-ray absorption, and x-ray photoelectron spectroscopy has unique advantages for investigating the structure, elemental distribution, and chemical bonding state of advanced materials and biological samples. In these analytical methods, the resolution, signal strength, and contrast must be as high as possible. In this regard, the development of a hard-x-ray focusing device is important to meet these requirements.

In the past decade, we have attempted to condense synchrotron radiation x-rays by using a mirror optical system, which has many advantages such as achromaticity, high focusing efficiency, and long working distance. In scanning microscopy, we broke the 10nm barrier in beam size by achieving 7nm×8nm spot size (Nat. Phys. (2010)). Moreover, in the diffraction microscopy, we achieved a 3nm resolution (Nano Lett. (2010)). In this study, we will attempt to realize high-precision multistage mirror optics for the single-nanometer focusing of next generation x-ray free electron lasers (XFELs).

【Research Methods】

The XFEL has very small source divergence, which is theoretically limited by a diffraction; thus, the beam size of the XFEL at the experimental hutch becomes very small, such as smaller than 200μm. To condense an x-ray with a wavelength shorter than 1Å into a single-nanometer spot size, the numerical aperture (NA) must be larger than 10^{-2}. In this study, we plan a multistage nanofocusing system to optimally control the NA at the final stage. Additionally, we will develop in situ wavefront measurement and correction methods to enable the construction of a novel adaptive optical system. Adaptive compensation may be a key technology that can be used to satisfy the Rayleigh quarter-wavelength rule and to overcome the unprecedented accuracy required in an ultimately high precision optical system. In this multistage focusing, we propose two-stage focusing as an intial trial. The mirror on the first stage will play the roles of changing the NA and prefocusing the XFEL down to micrometer size. The mirror on the second stage will be multlayer-coated and will have a large NA to focus the beam down to a single-nanometer size. The First mirror is planned to be controlled adaptively to enable the wavefront compensation.

【Expected Research Achievements and Scientific Significance】

The XFEL has a spatially fully coherent and ultrashort-pulse beam. The peak intensity is 10^9 times higher than that of the x-rays provided at SPring-8. Such x-rays will enable us to explore the forefront of x-ray science and technology such as x-ray nonlinear optics, high density-plasma physics, and single-molecule diffraction microscopy. In particular, the structural analysis of a single protein molecule will be possible by diffraction microscopy. In addition, the development of the high-precision optics will contribute to next-generation optical fabrication technology.

【Publications Relevant to the Project】

[1] H. Mimura, S. Handa, T. Kimura, H. Yumoto, D. Yamakawa, H. Yokoyama, S. Matsuyama, K. Inagaki, K. Yamamura, Y. Sano, K. Tamasaku, Y. Nishino, M. Yabashi, T. Ishikawa, and K. Yamauchi, "Breaking the 10 nm barrier in hard-X-ray focusing," Nature Physics, vol. 6, 2010, pp. 122-125.

[2] Y. Takahashi, N. Zettsu, Y. Nishino, R. Tsutsumi, E. Matsubara, T. Ishikawa, and K. Yamauchi, "Three-dimensional electron density mapping of shape-controlled nanoparticle by focused hard X-ray diffraction microscopy.," Nano letters, vol. 10, 2010, pp. 1922-6.

【Term of Project】 FY2011-2015

【Budget Allocation】 166,100 Thousand Yen

【Homepage Address and Other Contact Information】

http://www-up.prec.eng.osaka-u.ac.jp

Title of Project : Investigations on Multi-Hierarchical Structures of Turbulent Premixed Flame by Multi-Dimensional Combined Laser Diagnostics and GPU Cloud DNS

Toshio Miyauchi
(Tokyo Institute of Technology, Graduate School of Engineering, Professor)

Research Area : Engineering
Keyword : Combustion, Turbulence, Experimental fluid mechanics, Computational fluid dynamics, Energy utilization

【Purpose and Background of the Research】

Combustion technology of fossil fuels still covers about 85% of total primary energy supply in Japan. Combustors such as IC engine and gas turbine are required to be more efficient and lower emissions. These improvements directly resolve the global/urban environmental problems. The flow fields in many combustors used in engineering applications are in complex turbulent combustion state in which strong interactions between complex chemistry and turbulence occur. Characteristics of turbulent combustion are dominated by hierarchical structures of turbulence and flame. It can be expected that a hierarchical structure inside flame is newly caused by chemical reactions at high Reynolds number conditions, since interactions between flame surface and coherent fine scale eddies in turbulence are enhanced. At high pressure, the instability mode of flame and the hierarchical structures of flame surface and inside flame are considered to have complex interactions.

In this research project, the hierarchical structures of flame surface and inside flame in turbulent premixed flames are investigated by the world's most sophisticated laser diagnostics and direct numerical simulation. Turbulent flame structures at high Reynolds number and high pressure which can be observed in practical combustors will be clarified and modeled.

【Research Methods】

The most advanced laser diagnostics and direct numerical simulation of turbulent combustion in the world are conducted to investigate the hierarchical structures of flame surface and inside flame in turbulent premixed combustion, and the turbulent flame structures at high Reynolds number and high pressure. Simultaneous measurements of several chemical species and fluid velocity in multi-dimensions are developed by combining planar laser induced fluorescence (PLIF) and stereoscopic particle image velocimetry (PIV) in the experimental approach, and cloud computing technology of massive parallel graphic processing unit (GPU) is combined with direct numerical simulation technology of turbulent combustion in the numerical approach.

【Expected Research Achievements and Scientific Significance】

Turbulent combustion mechanism in the practical combustors is going to be revealed in this research project. The clarified turbulent combustion mechanism will be applied to the development of more efficient and lower emission combustors, which will contribute to the resolution of global/urban environmental problems in the medium- and long-term.

【Publications Relevant to the Project】

・Y.-S. Shim, S. Tanaka, M. Tanahashi and T. Miyauchi, Local Structure and Fractal Characteristics of H_2-Air Turbulent Premixed Flame, Proc. Combust. Inst., Vol. 33 (2011), pp. 1455-1462.
・M. Shimura, T. Ueda, G.-M. Choi, M. Tanahashi and T. Miyauchi, Simultaneous Dual-plane CH PLIF, Single-Plane OH PLIF and Dual-plane Stereoscopic PIV Measurements in Methane-Air Turbulent Premixed Flames, Proc. Combust. Inst., Vol. 33 (2011), pp. 775-782.
・M. Tanahashi, S. Taka, M. Shimura and T. Miyauchi, CH Double-Pulsed PLIF Measurement in Turbulent Premixed Flame, Exp. Fluids, Vol. 45, No. 2 (2008), pp. 323-332.

【Term of Project】 FY2011-2015

【Budget Allocation】 161, 500 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.navier.mes.titech.ac.jp/kiban-s-2011/index.html

Title of Project：Super-microsurgical robotic platforms and investigation of precise manufacturing technologies

Mamoru Mitsuishi
（The University of Tokyo, Graduate School of Engineering, Professor）

Research Area：Mechanical Engineering, Intelligent mechanics/Mechanical systems
Keywords：Robotics, Medical Robots, Surgical Robots, Microsurgery

【Purpose and Background of the Research】

This project aims to develop robotic platforms for microsurgical applications providing highly advanced treatments. Super-microsurgery is difficult to perform, even for skilled surgeons. Thus, surgical robotic and precision manufacturing technologies can contribute to the realization of less invasive and more accurate microsurgery. We will integrate our previous achievements and develop new platforms for use in several surgical fields.

【Research Methods】

We propose three robotic platforms: (1) a surgical robotic platform for handling soft tissue, (2) a bone-cutting robot, and (3) intravascular microrobots. The first year will be dedicated to the development of the robotic platforms. Miniaturized components, manufactured using the latest technologies, will be implemented before the development of advanced robotic controls. This project is a multi-disciplinary research project, involving partners from universities, hospitals, and companies. Our collaboration will lead to early clinical applications as well as the prompt commercialization of results.

【Expected Research Achievements and Scientific Significance】

(1) Surgical robotic platform for handling soft tissue (Fig. 1)

We will develop multi-DOF forceps using miniaturized components. The forceps will be mounted on a master–slave surgical robotic platform. Robotic control and force–feedback control methods will be investigated to advance a new discipline in microsurgical robotics.

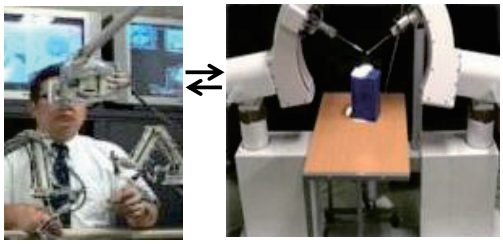

Fig.1 Master–slave surgical robotic platform

(2) Robot for bone-cutting and machining bio-materials (Fig. 2)

We have investigated some micro-scale phenomena of bone cutting. In this project, we will develop optimized bone-cutting techniques, facilitating the regeneration of bone tissue after cutting. We will also integrate tool path generation methods to minimize operation time and skin incision.

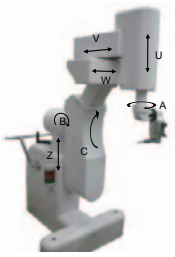

Fig. 2 Bone-cutting robot

(3) Intravascular microrobots (Fig. 3)

We will develop the electromagnetic control of tetherless microrobots and investigate their further miniaturization using the latest manufacturing technologies.

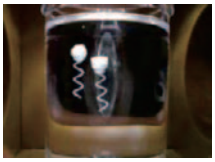

Fig. 3 Microrobots

【Publications Relevant to the Project】

・Ida, Y., Sugita, N., Ueta, T., Tamaki, Y., Tanimoto, K., Mitsuishi, M., A microsurgical robot to assist vitreoretinal surgery, International Journal of Computer Assisted Radiology and Surgery, 2011, in press.
・Sugita, N., Nakano, T., Abe, N., Fujiwara, K., Ozaki, T., Suzuki, M., Mitsuishi, M., Toolpath Strategy Based on Geometric Model for Multi-axis Medical Machine Tool, CIRP Annals, Vol.60, No.1, pp.419-424, 2011.

【Term of Project】 FY2011–2015

【Budget Allocation】 165,800 thousand yen

【Homepage Address and Other Contact Information】

http://www.nml.t.u-tokyo.ac.jp/
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Title of Project : Development of Highly-Functional Scanning Nonlinear Dielectric Microscopy and Its Application to Electronic Devices

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

Research Area : Engineering
Keyword : Scanning probe microscopy, Memory, Electronic device・IC, Dielectric

【Purpose and Background of the Research】

The researcher of this project has developed Scanning Nonlinear Dielectric Microscopy (SNDM). This microscopy technique has a world highest resolution and sensitivity in the ferroelectric domain observation and now it has an atomic resolution. In this study, we will develop SNDM with much higher resolution and extend its application area. Using this newly developed SNDM with high performance, we will observe and evaluate the surface of insulator material and also identify the electric dipole moment induced by the absorbed atom. Moreover, we will make the mechanism of atomic resolution appearance in dielectric measurement much clearer. Next, we will develop next generation high density ferroelectric data storage technique based on SNDM. We also study the visualization technique of charges stored in semiconductor electronic device using SNDM. Evolving this technique, we will make a failure analysis in semiconductor device possible, which has been believed to be impossible in capacitance measurement.

【Research Methods】

1. We will develop new SNDM based on the technique detecting higher order nonlinear dielectric constants. Using this newly developed high performance SNDM, we will try to identify atomic species of insulator material. 2. Next, we will develop high speed hard disk type SNDM ferroelectric data storage system with quite high memory density. To do so, we investigate the ferroelectric thin film for the recording medium with large nonlinear dielectric constants. 3. Finally, in the study on the visualization of charges stored in semiconductor device, using the above mentioned newly developed SNDM, we will resolve the electronic structure in the very small new generation semiconductor devices. And also we will apply the SNDM technique to evaluate next generation compound semiconductor device as well as Si devices.

【Expected Research Achievements and Scientific Significance】

The expected research achievements and scientific significance are summarized in Fig.1.

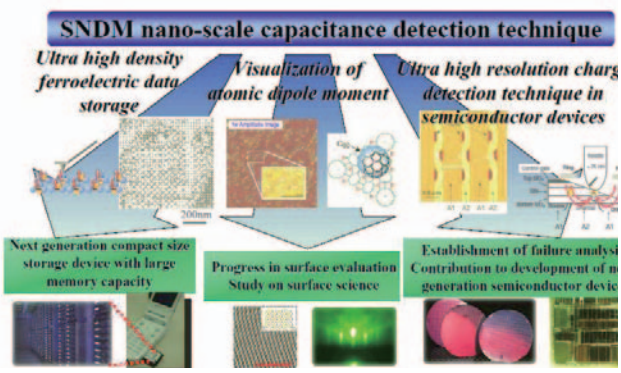

Fig.1 Future perspective -Creation of SNDM Nano Science & Technology-

【Publications Relevant to the Project】

・Yasuo Cho and Ryusuke Hirose: “Atomic Dipole Moment Distribution of Si Atoms on a Si(111)-(7 × 7) Surface Studied Using Noncontact Scanning Nonlinear Dielectric Microscopy”, Physical Review Letters, Vol.99, pp.186101-1-4 (2007).
・Kenkou Tanaka and Yasuo Cho, ”Actual information storage with a recording density of 4 Tbit/in.^{2} in a ferroelectric recording medium” Appl. Phys. Lett,Vol.97, pp.092901-1 -3 (2010).

【Term of Project】 FY2011-2015

【Budget Allocation】 161,800 Thousand Yen

【Homepage Address and Other Contact Information】

http:// www.d-nanodev.riec.tohoku.ac.jp/
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Title of Project : Development of dopant atom devices based on silicon nanostructures

Michiharu Tabe
(Shizuoka University, Research Institute of Electronics, Professor)

Research Area : Engineering
Keyword : electronic device/integrated circuit, silicon, dopant, atom device

【Purpose and Background of the Research】

Since the invention of the transistor, silicon technology has been developed using dopant impurity atoms. The statistical effect of many dopants has worked effectively until now, but recently device downscaling reached the point where the number of dopants and fluctuations in their arrangement significantly affect device characteristics. This is a fundamental problem related to the principle of operation of semiconductor devices and drastic solution is required. On the other hand, several groups, including ours, recently reported FETs with operation governed by individual dopants.

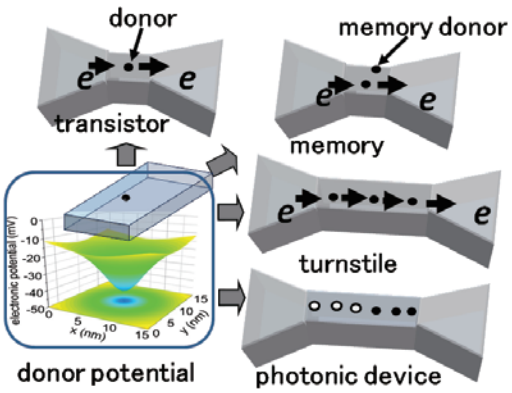
This research aims at the development of atom-level devices utilizing individual dopant atoms. A transistor using only one dopant atom is at the basis, and devices containing 2 or more dopant atoms can allow the development of memory, single-electron transfer, or photonic devices. In parallel, comprehensive research on single dopant implantation, detection technology, and first-principles calculations of nano-physical properties of dopants will form the grounds of dopant atom device engineering.

【Research Methods】

In this research project, significant advances will be pursued in dopant atom devices, high-accuracy dopant implantation, dopant position detection technology, and first-principles theoretical analysis. In particular, focus will be on single dopant atom transistors, although memory, single-electron transfer, and photon detection devices will also be studied for future integration.

【Expected Research Achievements and Scientific Significance】

The purpose of this research project is not the extension of technologies used so far, but the construction and study of a technical system for atomic devices. Some researchers in Australia, Europe and United States are working on quantum computers, utilizing the spin of phosphorus, but worldwide there are no other research projects similar to ours. The atomic devices produced from this research will produce a new group of extremely-small and low power devices, including single-electron FETs, single electron memory, single electron transfer devices, and photonic devices for optical information processing. Furthermore, we aim at room temperature operation of dopant atom devices for practical implementation. Thereafter, integration for industrial applications is expected with nanoelectronics and nanophotonics.



【Publications Relevant to the Project】

- M. Tabe, D. Moraru, M. Ligowski, M. Anwar, R. Jablonski, Y. Ono and T. Mizuno "Single-electron transport through single dopants in a dopant-rich environment", ***Phys. Rev. Lett.***, **105**, pp.016803-1-4 (2010).
- E. Hamid, D. Moraru, J. C. Tarido, S. Miki, T. Mizuno and M. Tabe, "Single-electron transfer between two donors in nanoscale thin silicon-on-insulator field-effect transistors", ***Appl. Phys. Lett.***, **97**, pp.262101-1-3 (2010).

【Term of Project】 FY2011-2015

【Budget Allocation】 161,100 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.rie.shizuoka.ac.jp/~nanohome
romtabe@rie.shizuoka.ac.jp

Title of Project : Advanced Micro Fluidic Engineering and Its Applications for High Sensitive Quantitative Measurements of Biomolecules

Shuichi Shoji
(Waseda University, Faculty of Science and Engineering, Professor)

Research Area : Instrumentation Technology
Keyword : Measurement System , MEMS・NEMS, Micro Bio System

【Purpose and Background of the Research】

Micro fluidic engineering have been developed with Micro Electro Mechanical Systems: MEMS technologies and nanotechnologies. The purpose of our research is to obtain high sensitive quantitative measurements of biomolecules by applying advanced micro fluidic engineering. In order to achieve this purpose, we develop micro fluidic devices/systems including on demand functional tools for optical measurements. The key issues of our research are to establish on demand high sensitive optical measurement methods and to develop precisely controlled sample preparation technologies in micro meter scale channels of the micro fluidic devices/systems. The precise time and positional control of micro droplets of sample and reagent obtains maximum optical signals. (Fig.1)

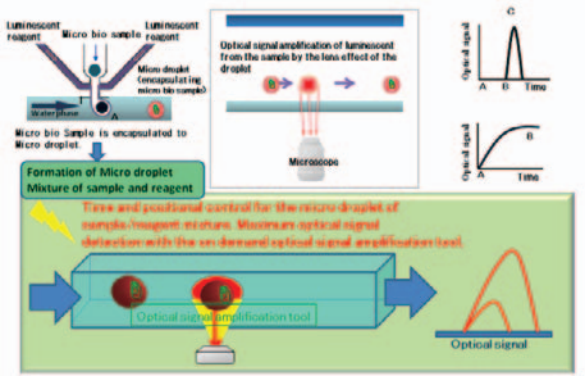


Fig.1: Principles of our research

【Research Methods】

To achieve high sensitive quantitative optical measurement we establish and integrate the following basic technologies. The fabrication and evaluation of functional micro fluidic devices and systems are also performed.

① Fabrication of high sensitive Optical Signal Amplification tools, e.g. ultra-flat glass surface, micro pillars, micro lens etc.
② Precise flow control technologies of specific three dimensional sheath flows and for ultra-fine droplet formation including nano/micro magnet beads.
③ Ultra-small volume sample preparation technologies to realize precise time controlled reaction for quantitative measurements.

【Expected Research Achievements and Scientific Significance】

The proposed micro fluidic engineering realizes precise time and position control of the ultra-small volume sample/reagent mixture in the micro channels. This is very important to obtain maximum signal at the optical detection point. Combination with on-demand Optical Signal Amplification tool makes remarkable improvements on sensitivity. The results of our researches will contribute on high sensitive quantitative analysis of a biological cell, a virus, an organelle, a DNA and a nano-particle. In the future, the advanced micro fluidic engineering enables functional on-site optical measurement to achieve efficient real-time analysis of ultra-small volume samples and to realize quantitative analysis of scarcity samples.

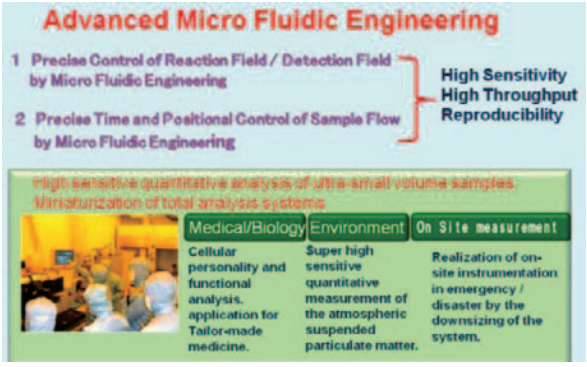


Fig.2: Expected contributions of our

【Publications Relevant to the Project】

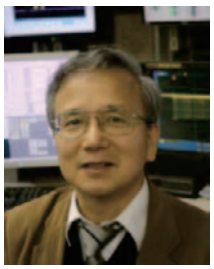
1. K. Ozaki, H. Sugino, T. Funatsu, S. Shoji, et. al., "Microfluidic Cell Sorter with Flow Switching Triggered by a Sol-Gel Transition of a Thermo-Reversible Gelation Polymer", Sensors and Actuators B 150 (2010) pp.449-455
2. T. Arakawa, Y. Shirasaki, T. Funatsu, S. Shoji, et. al., "Rapid Multi-Reagents Exchange TIRFM Microfluidic System for Single Biomolecular Imaging", Sensors and Actuators B 128, June 2007 (2007) pp.218-225

【Term of Project】 FY2011-2015

【Budget Allocation】 166, 100 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.shoji.comm.waseda.ac.jp/



Title of Project : Ultra-Compact Short Pulse and Coherent Teraherts (THz) Light Source Using Super-radiance

Junji Urakawa
(High Energy Accelerator Research Organization,
Accelerator Laboratory, Professor)

Research Area : Accelerator Physics, Applied Physics and Engineering Fundamentals
Keyword : RF Gun, Femtosecond(fs) Laser, Photo-Cathode, High Gradient Acceleration, FEL

【Purpose and Background of the Research】

The short pulse high-brightness coherent THz light source of ~0.3 to 10THz in the intermediate zone between radio and light waves gives a breakthrough in the rapidly expanding field of THz photon science. A photocathode is irradiated with a fs laser pulse train of ~10 pulses, and a fs electron bunch train (Comb beam) is accelerated by a radio-frequency(RF) accelerating field more than ~50MV/m. In this way, Comb beam is carried on a single RF accelerating field, enabling it to be accelerated to 5MeV in a 7.5cm RF gun. When the Comb beam is passed through a small wiggler (30cm), super-radiance in the THz region arises. The objective is to develop and apply an ultra compact high-brightness coherent THz light source, with short pulses of ~10MW, variable between 0.3 to 10THz, with radiation of ~10μJ/pulse.

Peak power of ~10MW is about 100 times that of earlier THz light sources, comparable to the intensity of THz light generated by 10m facility using advanced accelerator technologies, which are being developed around the world. With this light source, it is possible to substantially reduce THz time-domain spectroscopy (THz-TDS) measurement time, and greatly improve the accuracy of measurement. In addition, it enables fs timescale and multi-photon absorption nonlinear science phenomena to be captured with high precision. Applied experiments using the device developed(see the figure) will be carried out from 2014.

【Research Methods】

In order to maintain the time structure of the photoelectrons generated in the RF gun, it is necessary to engage them with the RF phase that overcomes Coulomb repulsion and in which bunch compression arises dynamically. The cathode end plate of the RF gun is fixed in the position where the high electric field of the cavity arises. If the accelerating field is an increasing phase(20 degrees) and the cathode is irradiated with 100 fs micro-pulses, the S-band(2856MHz) RF accelerating field (130MV/m) is changed from 44.46 to 44.68MV/m. The subsequent photoelectrons gain slightly larger acceleration and dynamic bunch compression while at the same time receiving rapid acceleration. By coming close to relativistic energy, Coulomb repulsion and Lorentz force reach equilibrium. The time difference between the beginning and end of the Comb beam is about 8ps. The accelerating field increases to 61.03 MV/m, therefore the 8ps bunch receives about 30% bunch compression at the RF gun exit. The electron micro-bunch structure predicted in the simulation is confirmed with CDR measurement.

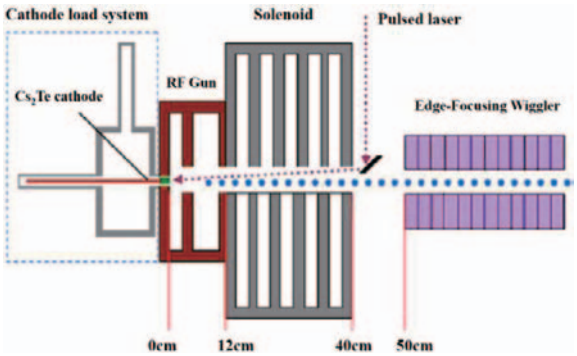


Table-Top Short Pulse and Coherent THz Light Source

【Expected Research Achievements and Scientific Significance】

By tuning the micro-bunch spacing to the THz wavelength, it is possible to generate a narrowband coherent THz wave. Depending on whether an ideal Comb beam can be formed in the RF gun by high gradient acceleration, super-radiance peak power from the small wiggler (30cm) reaches ~100MW. Innovative THz light source applications can be developed.

【Publications Relevant to the Project】

"Femtosecond pulse radiolysis and femtosecond electron diffraction", Jinfeng Yang et al., NIM, **A 637**, pp. S24-S27, 2011

"Experimental results of an rf gun and the generation of a multibunch beam", Abhay Deshpande et al., Phys. Rev. ST Accel. Beams, **14**, 063501-1-9, 2011

"Improvement of an S-band RF gun with a Cs_2Te photocathode for the KEK-ATF", N. Terunuma et al., Nuclear Instruments and Methods in Physics Research **A**, **613**, 1–8, 2010

【Term of Project】 FY2011-2015

【Budget Allocation】 154,700 Thousand Yen

【Homepage Address and Other Contact Information】

http://www-atf.kek.jp/thz/
junji.urakawa@kek.jp

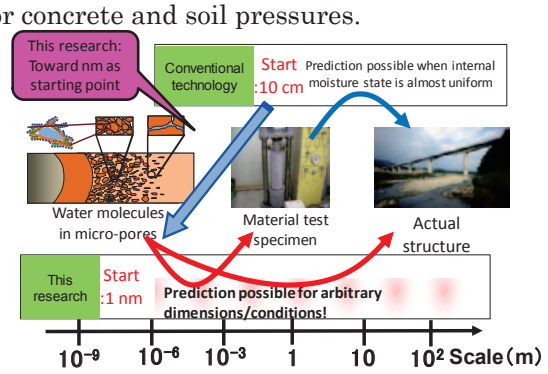
Title of Project : Long-Term Dynamic Simulation of Large-Scale RC-PC Infrastructures Based on Quasi Thermo-hygro Modeling

Koichi Maekawa
(The University of Tokyo, Graduate School of Engineering, Professor)

Research Area : Civil Engineering, Construction / Material / Management
Keyword : Concrete Engineering

【Purpose and Background of the Research】

The aim of this research is to develop a simulation technology for long-term kinematics of large-scale RC-PC infrastructures subjected to environmental actions and external loads, based on multi-scale analysis that satisfies the quasi-equilibrium states of moisture in micro-pores of cementitious composites and varying macroscopic momentum in time and 3D space. This research is directed at determining the leading causes of long-term excessive deflection of long-span bridge viaducts and the medium-term excessive deflection of shallow underground structures, which are risk issues of worldwide interest. Through this approach, it is aimed to rebuild the limit state design scheme for concrete and soil pressures.

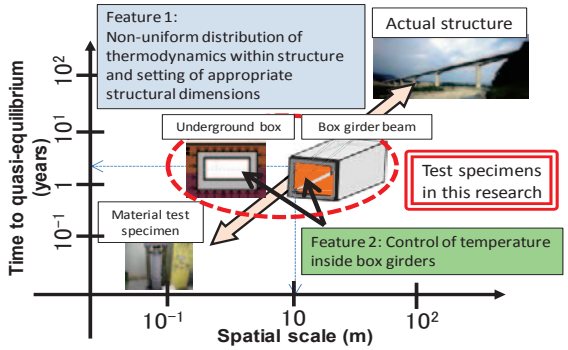


Framework of this research

【Research Methods】

The thermodynamic states of small-scale specimens, on which conventional creep analysis method is based, reach equilibrium with ambient states in a short period. However, in actual structures, non-uniform thermo-hygro states persist for a long time and this is likely to cause excessive deflection of long-span bridges. This research targets medium-scale structural concrete which may retain non-uniform thermo-hygro conditions but converge to the hygro-equilibrium within a couple of years.

Experimental verification of the multi-scale thermo-hygro analysis will be conducted by reproducing the high gradient of vapor pressure in micro-pores caused by fluctuating temperature and humidity inside the specimen.



Features of experimental method

The experimentally produced profile produced through the accelerated simulation and attainment of equilibrium states in specimens may allow prediction of excessive deformation phenomena that take place over hundreds of years in actual structures of large sizes.

【Expected Research Achievements and Scientific Significance】

Conventional methods may not adequately simulate the long-term kinematics of medium-scale structures because of the gap between assumption and reality of local moisture states. In this project, the strict thermo-dynamic multi-scale simulation is attempted in consideration of moisture migration and its state equilibrium for control of long-term deformation of large-scale concrete structures. These results will be applicable to maintenance in practice, risk assessment of existing structures, and preventive countermeasures.

【Publications Relevant to the Project】

- Maekawa, K., Ishida, T. and Kishi, T.: Multi-scale Modeling of Structural Concrete : Taylor & Francis, 2009
- Maekawa, K., Chijiwa, N. and Ishida, T. : Long-term deformational simulation of PC bridges based on the thermo-hygro model of micro-pores in cementitious composites, Cement and Concrete Research, 2011

【Term of Project】 FY2011-2015
【Budget Allocation】 172, 800 Thousand Yen

【Homepage Address and Other Contact Information】

http://concrete.t.u-tokyo.ac.jp

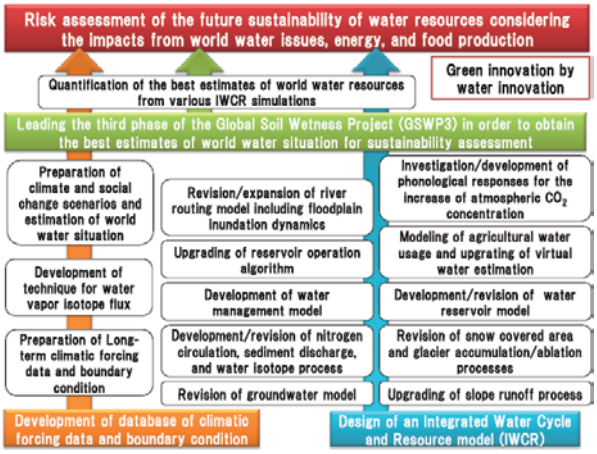
Title of Project : Leadership for Sustainability Assessment of World Water Resources using an Integrated Water Cycle and Resource Model

Taikan Oki
(The University of Tokyo, Institute of Industrial Science, Professor)

Research Area : Engineering
Keyword : Hydrology, global water cycle, climate change, human activities

【Purpose and Background of the Research】

An Integrated Water Cycle and Resource model (IWCR) is developed based on earth system science and coupled with human activities, crop growth, and environmental flow considerations derived from detailed process –level studies. Development of IWCR and its application to global water researches have been pioneered by our group and are currently utilized in various efforts throughout the world. In this project, we will revise IWCR for more precise and appropriate estimation of global hydrological cycles and organize the third phase of the Global Soil Wetness Project (GSWP3) to test and demonstrate improved real-world representation of the world water situation and world water resources.



【Research Methods】

The core of IWCR consists of a physically-based global water cycle model and an anthropogenic water intervention model. Both of them will be revised to simulate the real-world more precisely and realistically. Additional modules representing the phonological responses for the increase of atmospheric CO_2 concentration, the sediment discharge, and the water isotope processes, will be developed and coupled with the two main models. Long-term climatic forcing data, surface parameters, and climate and social change scenarios will be prepared based on the best available earth observational dataset. Furthermore, we will lead GSWP3, which seeks to provide best estimates of world water resources from an ensemble of IWCR simulations to be conducted under the GSWP3. Using these estimates, we will assess the future sustainability of water resources considering the impacts from drought and flood, water pollution, hydropower, and food production.

【Expected Research Achievements and Scientific Significance】

The best estimates of world water resources quantified under the framework of GSWP3 using various IWCR simulations will contribute to decision making and/or policy developments that seek to reduce the impacts of emerging global water issues. IWCR can is also expected to be a useful impact assessment tool for global water footprint, which has been discussed by International Organization for Standardization. Current understanding global water cycle is inadequate for many applications. This project, with international leadership from the Japanese community, will serve as a significant step toward illuminating the issues, and providing best science platform for discussing long-range variations of the global water cycles quantitatively.

【Publications Relevant to the Project】

Oki, T. and S. Kanae, 2006: Global Hydrological Cycles and World Water Resources, *Science*, Vol.313(5790), pp1068-1072.

Hanasaki, N., T. Inuzuka, S. Kanae, T. Oki, 2010: An estimation of global virtual water flow and sources of water withdrawal for major crops and livestock products using a global hydrological model, *Journal of Hydrology*, 384, pp232-244.

【Term of Project】 FY2011-2015

【Budget Allocation】 134,300 Thousand Yen

【Homepage Address and Other Contact Information】

http://hydro.iis.u-tokyo.ac.jp/

Title of Project : A Comparative Study on Water Cities from the Viewpoint of History and Environment

Hidenobu Jinnai
(Hosei University, Faculty of Engineering & Design, Professor)

Research Area : Urban and Architectural History
Keywords : Water City, Typology, Sustainability, Cultural Landscape

【Purpose and Background of the Research】

Throughout the world there exist many spectacular "water cities." Located in close proximity to the oceans and rivers, these cities flourished economically due to waterborne commerce, and boasted beautiful vistas and vibrant cultures centered on and around the water. However, during the 20th Century, with industrialization and the spread of the automobile, these spaces of water were the first to be sacrificed, becoming a distant memory for many of the cities citizens. Having come full circle, in a historical sense, the 21st Century now provides an ideal time for the peoples of the cities located along the rivers and oceans to regain what has been forgotten.

At Hosei University's Laboratory of Regional Design with Ecology we conduct research on the revitalization of the "water city." The past seven years have provided many research results, including the formation of an international network. Our research aims to make active use of this accumulated data, combining historical and environmental viewpoints in an original manner, which we further seek to develop and deepen over time. While doing so we hope to study the world's "water cities" in an interdisciplinary, moreover synthesized manner.

【Research Methods】

Our goal is to do comparative research from a global perspective on the different historical and environmental viewpoints held by the West (Europe and America) and East (Asia/Japan). This research also seeks to synthesize the fields of "history" and "environment" that have usually been treated as separate fields in the past, and will take a look at the formations and transformations of "water cities," and the sustainability of revitalization movements concerning them.

Target cities will be Venice, Suzhou, Bangkok, Amsterdam, and Tokyo/Osaka with their large water networks, which contrast with Middle and Early Modern cities such as Amalfi, Genova and Tomo which are located on inlets. Inland cities located along rivers like London, Paris, Firenze and Kyoto etc. and modern port cities like New York and Sydney will also be touched upon. Cities will be classified and studied, focusing on the role/function of water within them, and how the "meaning" of water and spatial structure changed historically.

【Expected Research Achievements and Scientific Significance】

In the past, the relationships between the fields of river engineering, water circulation/ source studies/ecology and architectural/urban history and urban design/construction etc. have been rather weak.

As a result of our research, "water" has come to play an intermediary of role of sorts, creating a bridge between the different disciplines.

Japanese cities such as Tokyo-Edo etc. exist(ed) as "eco cities" ; using the fruits of our historical and environmental research on this subject, our hope is to spread the conceptualization and methods behind the formation of the ideal 21 Century Japanese "water city" to countries outside our borders.

【Publications Relevant to the Project】

・H.Jinnai, "Urban Regeneration in Tokyo", *Places*, Vol.19, no.1, Berkeley, 2007. April, pp.62-67
・Laboratory of Regional Design with Ecology, Hosei University, *Regional Design based on History and Ecological Viewpoint*, Gakugei Shuppannsha,2004.
・H.Jinnai, *Tokyo: A Spatial Anthropology*, University of California Press, Berkeley, 1995

【Term of Project】 FY2011-2015

【Budget Allocation】 105, 500 Thousand Yen

【Homepage Address and Other Contact Information】

http : //suito.ws.hosei.ac.jp
http : //eco-history.ws.hosei.ac.jp/

Title of Project : Control of Dynamics of Quantized Vortices and Progressing to Materials Science

Kaname Matsumoto
(Kyushu Institute of Technology, Faculty of Engineering, Professor)

Research Area : Science and Engineering, Engineering, Material engineering, Inorganic materials/Physical properties
Keyword : (A) Crystal structure/Microstructure control

【Purpose and Background of the Research】

A nano-composite/hetero-epitaxial thin film that consists of two materials or more has a big possibility of inventing a new functionality material. There are a lot of promising targets; an efficient superconducting film approaching the theoretical limit of loss-less supercurrent; a multiferroic film interacting the magnetic phase and the ferroelectric phase in the same film; a quantum-dot solar cell film dramatically raising conversion efficiency. This technology enables to draw out the best interaction between a characteristic length/quantum effect and a material by producing an interface, a local strain, a steep change/pattern of electronic state, etc. in the crystal. In this research, the route to improve the loss-less supercurrent to the theoretical limit by using the nano-composite /hetero-epitaxial film technology is investigated. The obtained findings will be also progressed to variety of functionality materials.

【Research Methods】

Parameters defining the superconducting phase are a critical temperature T_c, an upper critical field B_{c2}, and a deparing current density J_0. The energizing of large current is necessary for the measurement of J_0 though T_c and B_{c2} are measured under a small current. But, it is very difficult to achieve a critical current density J_c that almost equals J_0 because the flux pinning of quantized vortices comes off by Lorentz force quickly before reaching J_0. In this research, exceeding the limit of J_c/J_0 = 1-10 %, a new physics of J_c/J_0 = 30-50 % is developed under large Lorenz force. An introduction of strong pinning centers is studied from the viewpoints of "optimized pinning structure", "thin film technology", and "microscopic characterization".

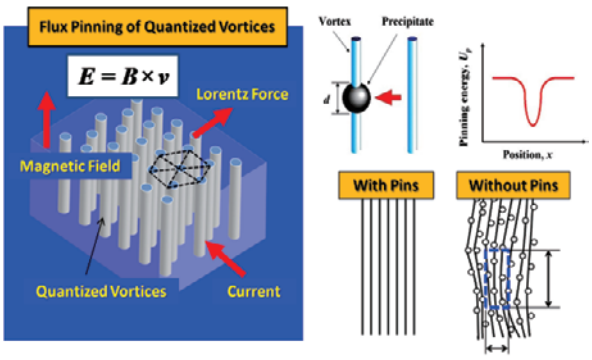


Fig.1 Flux pinning of quantized vortices.

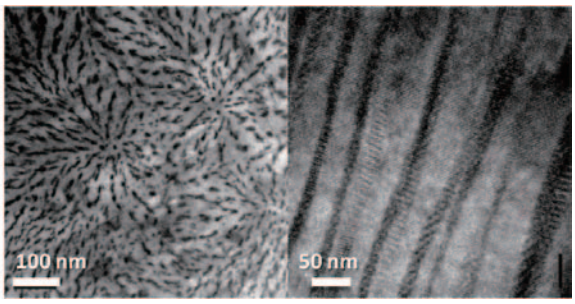


Fig. 2 Advanced flux pinning structure.

【Expected Research Achievements and Scientific Significance】

Showing the route that achieves J_c/J_0 = 30-50 % is the monument of the flux pinning technology. Acquiring the experiences of a nanostructure design, an evaluation from an atom/molecular level, and a large-scale calculation, etc. is effective for development of other functionality films.

【Publications Relevant to the Project】

K. Matsumoto, P. Mele, "Artificial pinning center technology to enhance vortex pinning in YBCO coated conductors", *Supercond. Sci. Technol.* **23**, pp. 014001－pp. 014013, 2010.
Tomoya Horide, Kaname Matsumoto *et al.*, "Control of the glass-liquid transition temperature in $YBa_2Cu_3O_{7-x}$ films", *Phys. Rev.* B **79**, pp. 092504－pp. 092507, 2009.

【Term of Project】 FY2011-2015

【Budget Allocation】 159, 600 Thousand Yen

【Homepage Address and Other Contact Information】

http://w3.matsc.kyutech.ac.jp/energy/index.html

Title of Project : Fuel Cell Electrocatalysts with Extended Durability

Kazunari Sasaki
(Kyushu University, Faculty of Engineering, Professor)

Research Area : Engineering
Keyword : Fuel cell materials

【Purpose and Background of the Research】

Fuel Cell, one of the most important solid state electrochemical devices and systems, is considered as a promising environmentally-compatible clean energy technology. Electrocatalysts are important materials determining the performance of polymer electrolyte fuel cells (PEFC). In order to ensure durability under practical operational conditions, sufficient stability is required during start-up, shut-down, idling, and voltage fluctuation associated with severe voltage changes. Pt electrocatalysts supported on carbon-based materials suffer from carbon corrosion especially on the cathode side. In order to ensure sufficient life time up to 10 or 20 years for fuel cell vehicles, break-thorough in electrocatalyst research is desired without using conventional carbon-based materials.

Our research group has succeeded to demonstrate an extended durability of alternative electrocatalysts using conductive oxides as catalyst support materials, up to 60,000 voltage cycles corresponding to the life time of fuel cell vehicles [1, 2]. In this project, fuel cells with the carbon-free electrocatalysts will be prepared and characterized under practical operational conditions in order to establish scientific materials design principles for these important electrochemical devices based on solid state electrochemistry, chemical thermodynamics, catalysis, materials process engineering, and mechanical engineering.

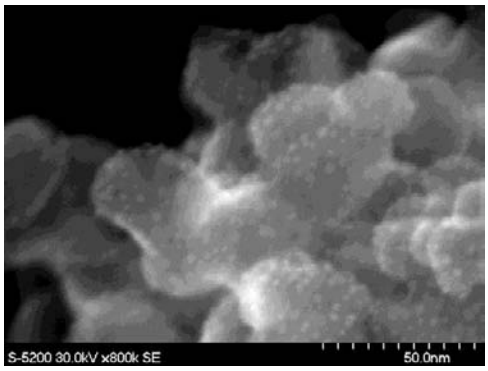


Figure: Scanning electron microscope micrograph of Pt/SnO_2 electrocatalysts.

【Research Methods】

Comprehensive research approach will be made on following research topics: (1) stability and dissolution kinetics in strongly-acidic environment, (2) electrocatalyst development with alternative support materials, (3) defect chemistry at catalyst/support interfaces, (4) device fabrication and characterization, (5) application to other related electrochemical devices. These research activities are carried out in collaboration with team members of the fuel cell research division of the World Premier International Research Center Initiative Program (WPI).

【Expected Research Achievements and Scientific Significance】

This research is of significance not only for fuel cell technologies but also for various electrochemical devices. Oxide catalyst support materials are important in the metal/semiconductor structure. Materials design principles established can contribute to realize an energy-efficient low-carbon society [3].

【Publications Relevant to the Project】

1) K. Sasaki, F. Takasaki Z. Noda, S. Hayashi, Y. Shiratori, K. Ito, "Alternative Electrocatalyst Support Materials for Polymer Electrolyte Fuel Cells.", *ECS Transactions*, **33** [1] 473-482(2010).
2) A. Masao, Z. Noda, F. Takasaki, K. Ito and K. Sasaki, "Carbon-Free Pt Electrocatalysts Supported on SnO_2 for Polymer Electrolyte Fuel Cells", *Electrochem. Solid-State Lett.*, **12** [9] B119-B122 (2009).
3) K. Sasaki, "Hydrogen Energy: Current Status and Future Perspectives", *J. Japan Soc. Mech. Eng.*, **114** [4] 265-267 (2011).

【Term of Project】 FY2011-2015
【Budget Allocation】 166,000 Thousand Yen
【Homepage Address and Other Contact Information】

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Title of Project : Development of Magnetotactic Bacteria Producing Useful Substances, through the Reconstruction of Organelles Synthesizing Magnetic Particles

Tadashi Matsunaga
(Tokyo University of Agriculture and Technology, President)

Research Area : Engineering, Process engineering, Biofunction・Bioprocess
Keyword : Applied microbiology, Genome, Cell・Tissue, Biofunction utilization, Biotechnology

【Purpose and Background of the Research】

Magnetotactic bacteria synthesize intracellular magnetic particles (magnetite; Fe_3O_4) of approximately a few dozens of nanometers to 100 nanometers in size. The particles are covered by a lipid bilayer on their surface, and by modifying molecules such as proteins or DNA, they can be used for bioanalysis and recovery of various substances. Previous researches have revealed that the magnetic particles were synthesized inside subcellular organelles (magnetosomes).

In this study, we will analyze the functions and localization of the proteins involved in the magnetosome formation, and will reconstruct magnetosomes by reorganizing the genome. In addition, we will develop a technology which will allow the synthesis of magnetic particles in an adjustable manner, using cells, by modifying the protein's functions and the regulation of its expression.

【Research Methods】

In this study, we will use two strains of magnetotactic bacteria whose genome sequences have been clarified: *Magnetospirillum magneticum* strain AMB-1 (Figure A) and *Desulfovibrio magneticus* strain RS-1 (Figure B). We will prepare various gene-deficient strains based on the information on their genomes and proteins; and will analyze the morphology of the magnetic particles, and intracellular structures. Furthermore, to understand the functions and structures of magnetosomes at the molecular level, we will conduct an analysis of the intracellular localization of magnetosome proteins, and an analysis of the expression of the genes encoding magnetosome proteins.

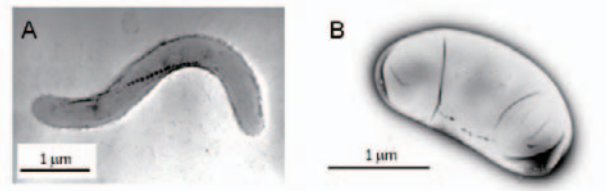

Figure Transmission electron micrographs of *Magnetospirillum magneticum* strain AMB-1 (A) and *Desulfovibrio magneticus* strain RS-1 (B).

Meanwhile, in previous studies, the deletion of a large gene region resulted in the obtention of mutant strains which lost the ability to form magnetosomes. We will reconstruct magnetosomes intracellularly by introducing genes involved in the formation of magnetosomes, into deletion mutants. In addition, we will modify the structure and functions of proteins by introducing mutations into their genes, will modulate the level and timing of protein expression, and will artificially control the functions of magnetosomes.

【Expected Research Achievements and Scientific Significance】

This study should provide guidance in the field of system biology and synthetic biology research. This study may also lead to the elucidation of the mechanism of biomineralization of iron oxide. Moreover, these basic researches are expected to lead to the expansion of the range of applications of microorganisms for industrial use, such as in the production of functional magnetic particles, or in the production of substances, using the magnetic recovery capability of the cells.

【Publications Relevant to the Project】

M. Tanaka, E. Mazuyama, A. Arakaki, and T. Matsunaga; "Mms6 protein regulates crystal morphology during nano-sized magnetite biomineralization *in vivo*." J. Biol. Chem., 286, 6386-6392 (2011).

H. Nakazawa, A. Arakaki, S. Narita-Yamada, I. Yashiro, K. Jinno, N. Aoki, A. Tsuruyama, Y. Okamura, S. Tanikawa, N. Fujita, H. Takeyama, and T. Matsunaga; "Whole genome sequence of *Desulfovibrio magneticus* strain RS-1 revealed common gene clusters in magnetotactic bacteria." Genome Res. 19, 1801-1808 (2009).

【Term of Project】 FY2011-2015

【Budget Allocation】 160,800 Thousand Yen

【Homepage Address and Other Contact Information】

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Title of Project : A New Spilled Oil and Gas Tracking Autonomous Buoy System and Application to Marine Disaster Prevention System

Naomi Kato
(Osaka University, Graduate School of Engineering, Professor)

Research Area : Integrated Engineering (Naval and Maritime Engineering)
Keyword : Undersea and subsea engineering, Environmental model, Reduction technology of environmental impact, Environmental safety and security

【Purpose and Background of the Research】

There have been many major sea oil spills in recent years. These spills damage not only the ocean environment but also regional economies. Once spilled oil washes ashore, it is difficult to effectively recover it. This results in a high residual amount of spilled oil and long-term damage to the environment as well as to marine and human life.

The objectives of this study are as follows:

(1)Autonomous tracking and monitoring of spilled plumes of oil and gas from subsea production facilities by an underwater buoy robot,

(2)Autonomous tracking of spilled oil on the sea surface and transmission of useful data to a land station through satellites in real time by multiple floating buoy robots,

(3)Improvement of the accuracy of simulations for predicting diffusion and drifting of spilled oil and gas by incorporating the real-time data from these robots.

【Research Methods】

This research project adopts the following methods to realize these objectives:

(1)An underwater buoy robot equipped with a buoyancy control device and two pairs of rotational fins for guidance and control, and sensors to detect dissolved gas and oil will be developed. It will be tested in areas in the Gulf of Mexico and off Niigata where methane gas is released.

(2)Multiple floating buoy robots equipped with sails—the orientation and size of which are adjustable—and sensors to detect oil slicks on the sea surface will be developed. They will be tested in Japan using artificial targets on the sea surface, and in Norway using real oil on the sea surface.

(3)A data fusion method incorporating real-time measured data from buoy robots in simulation models for not only gas and oil blowouts, but also spilled oil drifting on the sea surface will be developed.

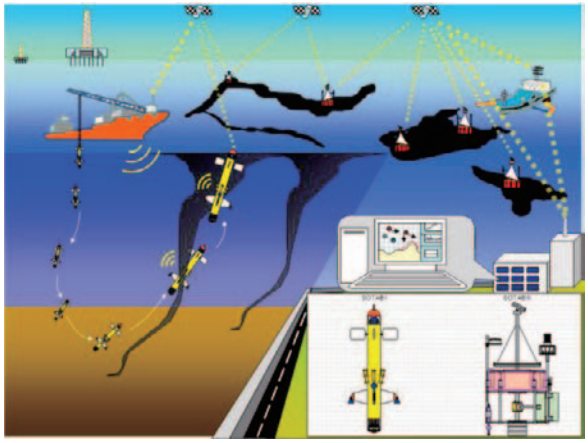

Fig.1 Concept of spilled oil and gas tracking autonomous buoy system

【Expected Research Achievements and Scientific Significance】

The system described above can be applied to regular environmental monitoring around subsea production facilities, the collection of spilled oil drifting on the sea surface, and the deployment of oil-recovery devices.

【Publications Relevant to the Project】

・H. Senga, N. Kato, M.Yoshie et al., Spilled Oil Tracking Autonomous Buoy System, J. of Advanced Robotics , Vol. 23 , pp.1103－1129 ,2009
・H. Senga, N. Kato, H. Suzuki, M. Yoshie, T. Tanaka et al., Development of a New Spilled Oil Tracking Autonomous Buoy, Marine Technology Society Journal, Vol.45, No. 2, pp.43-51, 2011

【Term of Project】 FY2011-2015

【Budget Allocation】 156,200 Thousand Yen

【Homepage Address and Other Contact Information】

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Title of Project : Imaging of Crystal Textural Structure and Physical Values of Materials and Fields by Pulsed Neutrons

Yoshiaki Kiyanagi
(Hokkaido University, Faculty of Engineering, Professor)

Research Area : Nuclear Engineering
Keyword : Radiation, Neutron, Imaging, Crystal texture structure, Magnetic field,

【Purpose and Background of the Research】

It has been revealed that energy resolved imaging using a pulsed neutron source can give information on strain, preferred orientation, crystallite size as well as elements, and also information on magnetic field and magnetic domain for a bulk material as a real space image. Only neutron can give such physical values in a nondestructive way. This method is expected to be very useful for evaluation and development of materials and to be applicable to various fields. In this project we intend to develop the technology components for advancing this method, and establish it as a practical method. After then, we promote advanced applications.

【Research Methods】

A pulsed neutron source produces various energy neutrons in pulsed nature. We can analyze neutron velocity (energy) by using the time-of-flight method, in which arrival time of the neutron is measured at a certain distance from the source. The interaction of the neutron with a material (neutron cross section) depends on the neutron energy. As shown in Fig. 1 at a high energy region resonance peaks appear, which are peculiar to an element. As in the finger print we can identify the name, evaluate the amount of the element in the material, and measure the temperature by analyzing the peak width. On the other hand at a low energy region knurlings appear which correspond to the crystal structure. Information on crystallite size, preferred orientation and strain is deduced from this. In the case of hydrogenous materials, the neutron cross section increases with velocity, and the gradient is larger for the weak bounded one. Furthermore, the neutron is a small magnet, interacts with magnetic field, and gives the information on the magnetic field.

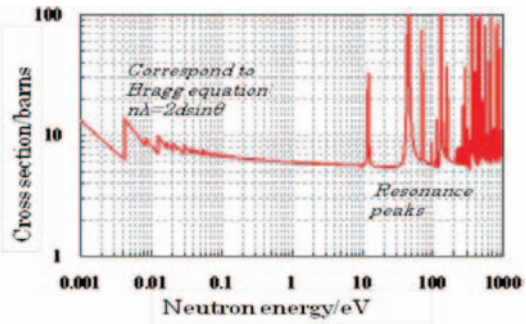

Fig. 1 Neutron cross section

In the pulsed neutron transmission coupled with the time-of-flight method, the energy dependent transmission can obtained for a wide area at once. By analyzing this kind of data we deduced, for example, the strain and the crystallite size as shown in Fig. 2.

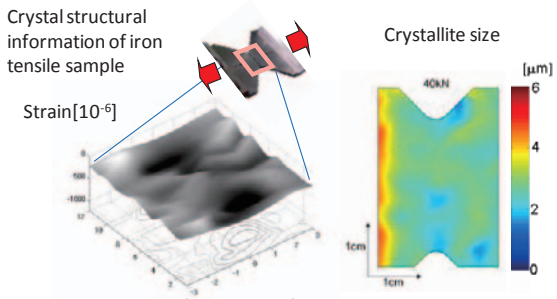

Fig. 2 Strain (left side) and crystallite size (right) in an iron tensile sample.

【Expected Research Achievements and Scientific Significance】

We will build up a nondestructive evaluation method for investigating the bulk material characteristics by expanding the applicability of the analysis code, developing the quantitative evaluation of the magnetic field and so on. Furthermore, we will apply this method to structural materials, hydrogen energy system, magnetic devices, antiques such as Japanese swords, which will contribute to highly reliable products, energy-saving society and culture.

【Publications Relevant to the Project】

H. Sato, T. Kamiyama and Y. Kiyanagi, A Rietveld-Type Analysis Code for a Pulsed Neutron Bragg-Edge Transmission Imaging and Quantitative Evaluation of Texture and Microstructure of a Welded Iron, *Materials Transactions*, **52,** 1294-1302(2011).

【Term of Project】 FY2011-2015

【Budget Allocation】 204, 400 Thousand Yen

【Homepage Address and Other Contact Information】

http://toybox.qe.eng.hokudai.ac.jp/about.html

Title of Project : All Solid State Superconducting System for Neutron Radiography with One Million Pixels and Submicron Resolution

Takekazu Ishida
(Osaka Prefecture University, Graduate School of Engineering, Professor)

Research Area : Superconductivity, Nanostructured superconductors
Keyword : neutron, radiography, MgB_2 superconductor, single flux quantum device

【Purpose and Background of the Research】

Neutron radiograph is an essential tool to lead progresses in science and industry in the 21st century. Two unique technologies will be applied to fulfill prerequisites (submicron resolution, one million pixels, high frame rate, and all solid-state system). A superconducting nanowire array of MgB_2 is used to recover a change in kinetic inductance ΔL_K of the nanowire induced by reaction heat between neutron and ^{10}B. This enables larger pixel size based on the achievement of submicron resolution and two-dimensional array of pixels. Maximum likelihood circuit of single flux quantum device (SFQ) plays a crucial role to detect ΔL_K at extreme sensitivity, and to process acquired data at high rate with ultra low power consumption.

【Research Methods】

High-quality MgB_2 epitaxial films, fabrication technique of MgB_2 nanowire, and a large-scale NxN array of superconducting nanowires will be developed. As shown in Fig. 1, two systems of linear arrays are installed at right angles. Nuclear reaction between neutron and ^{10}B yields alpha- and lithium-particle emissions in the opposite direction. Two particles are simultaneously counted by X-direction and Y-direction arrays. The principle to detect a signal is to see a change in kinetic inductance at 4 K. The 1-ns high speed of MgB_2 detector requires a 100-GHz SFQ circuit.

Ultimately, we intend to demonstrate our evolutional all-solid-state system by neutron irradiation at J-PARC or JRR-3M.

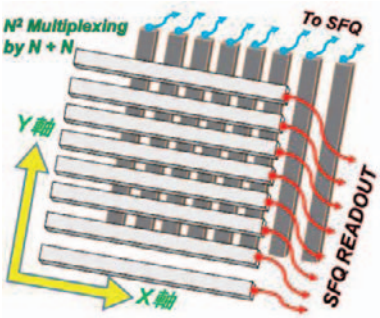

Fig. 1. Multiplexing of MgB_2 detectors consisting of 1D array of N detectors to X- and Y- directions for simultaneous counting of the event.

【Expected Research Achievements and Scientific Significance】

Neutron radiography is a powerful method for revealing the positions of light elements in materials and the observation of magnetic structures. A large number of pixels of submicron spatial resolution enable us to utilize a spintronics tool using spin-polarized neutrons. For example, dynamics of water as a byproduct of fuel cells can be observed as a fast animation with high spatial resolution. Our system will influence even other fields such as agriculture and biology.

【Publications Relevant to the Project】

1. T. Ishida, M. Nishikawa, Y. Fujita, S. Okayasu, M. Katagiri, K. Satoh, T. Yotsuya, H. Shimakage, S. Miki, Z. Wang, M. Machida, T. Kano, M. Kato, "Superconducting MgB_2 thin film detector for neutrons", J. Low Temp. Phys. **151**, 1074-1079 (2008).
2. M. Machida, T. Kano, T. Koyama, M. Kato, T. Ishida, "Direct numerical simulations for non-equilibrium superconducting dynamics at the transition edge: Simulation for MgB_2 neutron detectors", J. Low Temp. Phys., **152,** 58-63 (2008).
3. Y. Fujita, K. Arai, M. Nishikawa, K. Satoh, T. Yotsuya, H. Shimakage, S. Miki, Z. Wang, M. Machida, M. Kato, T. Ishida, "Nonequilibrium response of a meandered MgB_2 sensor by the irradiation of a pulsed laser", Physica C **468**, 1995-1997 (2008).
4. Y. Yamanashi, T. Kainuma, N. Yoshikawa, I. Kataeva, H. Akaike, A. Fujimaki, M. Tanaka, N. Takagi, S. Nagasawa, and M. Hidaka, "100 GHz Demonstrations Based on the Single-Flux-Quantum Cell Library for the 10 kA/cm² Nb Multi-Layer Process," IEICE Trans. Electron., **E93-C**, 440-444, (2010).

【Term of Project】 FY2011-2015

【Budget Allocation】 165,100 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.pe.osakafu-u.ac.jp/pe1/