Progress reports of groups

- Information (Storage) Group
- Information (Quantum Information) Group
- Energy Technology Group
- Medical Group
- Supramolecules and Self-Assembly Group
- Nanomaterials and Nanodevices Group
- Quantum Theory and Computation Group

Information Storage Group

Katsuji Nakagawa*, Akiyoshi Itoh, Arata Tsukamoto

1. Overview of the research plan in 2012

1) To succeed in fabricating magnetic domains on magnetic recording film by the effect of surface plasmon generated by femto-second laser, three issues will be performed: (1) a computational analysis of electro-magnetic field as well as thermal diffusion in magnetic film, (2) a structure design of surface plasmon antenna and antenna fabrication by electron beam lithography, and (3) magnetic recording test applying femto-second laser with surface plasmon antenna.
2) In the matter of a super fast phenomenon, optical, thermal, and magnetic response from femto-second laser light will be studied related to the issue 1).
3) The electro-magnetic field under the condition combining of dielectric optical waveguide and surface plasmon polariton will be studied by computational calculation.
4) Nano-meter structured FeCuPt magnetic film for high density recording will be fabricated, and stable magnetic domains will be studied by micro-magnetic computational calculation.

2. Advances and achievements in 2012

1) Thermally assisted magnetic recording with surface plasmon antenna has been succeeded by applying femto-second laser. Three issues are key points of this success: (1) a computational analysis of electro-magnetic field as well as thermal diffusion in magnetic film, (2) a structure design of surface plasmon antenna and antenna fabrication by electron beam lithography, and (3) magnetic recording test applying femto-second laser with surface plasmon antenna. The magnetic mark of 166 nm x 120 nm was written by this method. The written mark size has not reached the size of project goal: 77 nm x 77 nm. Our progress, however, is very big, and we still go forward to our goal in the final year.
2) We found experimentally a novel magnetization reversal phenomenon in a ferri-magnetic GdFeCo film driven by an ultrafast heating of the medium resulting from the absorption of a sub-picosecond laser pulse without the presence of a magnetic field. Also relevantly to technological applications, we have shown experimentally that switching can occur when the sample is at room temperature before laser excitation.
3) We found that the combination of dielectric optical waveguide and surface plasmon polariton is highly effective in optical energy transfer into small surface plasmon antenna. Besides, the combination structure can also create circularly polarized light in a small region.
4) A rapid thermal annealing is effective to obtain high Ku (uniaxial magnetic anisotropy) as well as small $L1_0$-FeCuPt grains. However, it revealed that each grain were mostly polycrystalline structure. We found that an application of adequate additional annealing makes grains into $L1_0$ single crystalline structures and grains kept almost similar size.

3. Collaborations and activities in 2012 as the group

A result about a nano-meter structured magnetic film with high uniaxial anisotropy was reported at an international conference (ICM2012, July 8-12, Pusan). At another international conference (ICAUMS2012, Oct. 1-5, 2012, Nara), six reports were also presented including femto-second laser thermally assisted magnetic recording, dynamics in first magnetic reversal, recording materials, and localized circularly polarized light. Some of these reports have been collaborated with Associate Prof. Ohnuki. We have kept an inner meeting at least once a month.

Quantum Information Group

Shuichiro Inoue*, Takeshi Kuwamoto, Hideomi Hashiba

1. Overview of the research plan in 2012

1) Evaluation of the entanglement swapping system
2) Fabrication of a single-photon emitter using CdSe colloidal quantum dot array
3) Observation of electromagnetically induced transparency of orthogonally polarized photon pairs and their storage in an atomic ensemble
4) Development of simple and reliable etching technique of Si on ICP

2. Advances and achievements in 2012

1) We performed fourfold coincidence measurements to investigate the indistinguishability between photons from the two independent photon-pair sources. The indistinguishability was measured to be 82 % by Hong-Ou-Mandel two-photon interference experiments. Then Bell-state measurements were performed with one photon from each pair, which projected the two remaining photons, formerly independent onto an entangled state. The obtained fidelity of the swapped entangled state was 86 % (world record at telecommunication wavelengths), high enough to infer a violation of a Bell-type inequality.
2) Fabrication technique of an array of colloidal quantum dots covered by silica has been developed. The diameters of the quantum dot and the silica shell are 5 nm and 30 nm, respectively. We attained a 55 nm wide, 1.5 μm long array of the quantum dots in sub one-dimensional shape using a trench made of ZEP on Si substrate as a template.
3) We studied absorption of orthogonally polarized photon pairs into rubidium (Rb) vapor. The photon pairs were filtered using several optical filters and two etalons so that they were resonant with Rb atoms. At Rb-vapor temperature of 95 ℃, the absorption ratio was reached approximately 97%. However, at the vapor temperature of 70 ℃, which was optimum one derived from classical-light (laser-light) storage experiments, the absorption ratio was 90 %. In future, we improve the ratio to 100% by removing the non-resonant frequency components of photon pairs.
4) Fabrication technique of Si waveguides has been furbished and Si waveguides (320 nm wide and more than 1 mm long) have been fabricated. The waveguides have small roughness of side-walls (less than 10 nm) and the optical loss due to the roughness is to be measured.

3. Collaborations and activities in 2012 as the group

We proposed a multichannel single-photon emitting device which is composed of CdSe colloidal quantum dot arrays and plasmonic waveguides. CdSe colloidal quantum dots were synthesized in Prof. Ohtsuki's lab and numerical calculations to design plasmonic waveguides were performed in Prof. Ohnuki's lab. We had three group meetings and discuss the direction of our final goal.

Energy Technology Group

Takuya Hashimoto,* Nobuyuki Nishimiya, Yasuo Asada, Sachiko Matsushita, Joe Otsuki

1. Overview of the research plan in 2012

The first object for solid oxide fuel cells (SOFC) is development of materials which construct SOFC, which can be operated as low as 600 °C. The next one is construction of SOFC which can work at 600 °C.

On dye-sensitized solar cells, employment of photonic crystals or new dyes is examined and their properties are clarified by various electrochemical and optical measurements. The targets of energy conversion efficiency of the solar cells employing organic dyes and precious metal based ones are more than 5% and around 10%, respectively.

Photonic to chemical energies transformation systems are to be developed through functionalizing metal hydrides and specializing active bio-species on one hand and through confirming the concept on the photo-assisted hydrogen absorption and adopting that to non-rare metallic combinations on the other hand.

Preparation and characterization of supramolecular non-precious metal photocatalysts are also targets.

2. Advances and achievements in 2012

The optimization of preparation and sintering conditions of $LaNi_{0.6}Fe_{0.4}O_{3-\delta}$, which attract much attention as Sr-free cathode material of SOFC, has been completed. For electrolyte material, optimization of preparation method and kinds of trivalent ion of $BaCe_{1-x}M_xO_{3-\delta}$ (M: trivalent ion) has been carried out. As trivalent ion, it has been revealed that Y is the most suitable since ionic radii of Y^{3+} is close to that of Ce^{4+}. Also it has been clarified that the valence changes to tetravalent by employing Nd as trivalent ion in order to adjust ionic radii for B-site, resulting in less oxide ion vacancy and proton conductivity. Examination apparatus for SOFC has been successfully constructed and fabrication of SOFC using above mentioned materials has started.

Using photonic crystals prepared by self-assembly methods, improvement of photon-to electron conversion efficiency of dye-sensitized solar cells has been confirmed. Also, lithographic technique of TiO_2, which is base material for solar cells, is established. Dyes with varied structures were prepared and tested as dyes for dye-sensitized solar cells. This year, however, has seen no improvement from previously reported our efficiency record of 3.1%. As for precious metal dyes, model complexes were prepared and characterized as a preceding step to the application to the dye-sensitized solar cells.

Bio-actively transferred hydrogen energy was successfully recovered by magnesium-based alloy composites and the entity of hydrogen fermentation was partly specialized through DNA abstraction from Yokohama National University's active mixtures. Non-rare metallic composites comprising boron, carbon and/or nitrogen provided with graphene-derived carbon nano-balls with high hydrogen capacity as well as layered carbon nitrides with high performance photo-assisted hydrogen absorption additives.

For supramolecular photocatalysts, the synthesis is ongoing. The major achievements of this year was that discovery of double helices made of chlrophyll derived molecules, which will constitute a basis for the design of artificial antenna systems and (ii) demonstration of lower temperature processing for the fabrication of thin films of reduced graphene oxide, which will be used as the substrate for organic photovoltaic

3. Collaborations and activities in 2012 as the group

Bio-activity transferred hydrogen is a collaborate work of Prof. Asada and Nishimiya. Patent of preparation via Pechini process by Prof. Hashimoto is under way with the advice of Prof. Nishimiya.

Medical Group

Members

ARISH: Fukuda N, Severe Disease G: Saito K, Igarashi J, Fujiwara K, Soma M, Radiology: Abe O, Ishibashi N, Urology Takahashi S, Pediatric Surgery: Koshinaga S, Bioresourse Science: Masuhiro Y, Kano K, Pharmacy: Matsumoto Y, Aoyama T, Chiba Cancer: Nagase H, Watanabe T

Progress and Production by Whole Medical Group in 2012

1. **Development of an E-box targeting Pyrrole-Imidazole polyamide to inhibit cell growth** (Fujiwara, Soma): PI polyamides targeting E-box consensus inhibited proliferation of the osteosarcoma cell line treated with Myc-6 showing reduced growth rate by WST8 assay and colony formation assay. In the wound-healing assay, Myc-6 inhibited cell migration activity dose-dependently. Intravenous injection of Myc-6 once a week for a month caused growth inhibition MG63 xenograft developed in Nude mouse without evidence of toxicity.

2. **Development of antitumor PI polyamides for pediatric cancer** (Koshinaga): PI polyamides（h-CCAAT1, h-CCAAT3）designed on the CAAT box in promoter reasion of LIT1 gene efficiently suppressed expression of LIT1 gene and proliferation of Hepatoblastoma cell line (HuH6 clone5, HepG2), and Wilm's tumor cell line (G401).

3. **Development of PI polyamide targeting human TGF-β1 -Preclinical study-** (Igarashi, Fukuda): We confirmed that GB1101 is strongest to inhibit the expression of TGF-β1 mRNA in human- and marmoset-derived fibroblasts. We checked the combination of components of soluble materials and solutions for PI polyamides and found that Macrogol Ointment was most effective substrate to delivery the PI polyamide into skin. We examined effects of PI polyamides targeting human TGF-β1 on development of skin finrotic scar created in common marmosets and confirmed acual inhibition of the skin scar.

4. **Development of the Nihon University original methodology inducing iPS cells using the PI polyamide targeting human TGF-β1** (Saito, Fukuda, Masuhiro)：We examined the iPS-producing method establishment using proteolysis resistant cell-permeable proteins and the iniciation factor, TGF-β1 inhibitor, PI polyamide targeting human TGF-β1, Apigenin, TGF-β1antagonist and Apigenin, and TGF-β1 and PI polyamide targeting human TGF-β1.

5. **Establishment of a breast cancer-inducing mouse model by the transplantation of DFAT** (Kano): We tried the creation of a breast cancer-inducing mouse model by the transplantation of DFAT-GFP transfected oncogene, which is transformed to epithelial cells.

6. **Histone acetylation of specific genomic region induced by PI polyamide-SAHA conjugate** (Nagase, Watanabe) : We made considerable advances in coupling of existing drug SAHA that is begin used as an HDAC inhibitor, to PI polyamides for targeting specific subsets of genes for reactivation in cancers (e.g. Cdkn2a / p16). Watanabe developed a method of simple synthesis with solid phase synthesis method using glutamic acid which is the usual amino acid. Six ring cyclic PI polyamide was synthesized.

7. **Pharmacokinetic/Pharmacodynamic Analysis of tumor-localizing photosensitizing compounds**

(Matsumoto, Aoyama): To describe the relationships between effects following photodynamic therapy, light dose, and plasma compound concentration, they developed a high-performance liquid chromatography (HPLC) method for the determination of plasma concentration and investigate the pharmacokinetics of novel compound CT101019a.

8. Development of plasma medicine for skin malignant melanoma (Saito, Fujiwara, Fukuda)**:** We started a project of the development of plasma medicine for skin malignant melanoma collaborating with the plasma team in College of Science and Technology. This plasma medicine targets the cancer stem cell with all trans retinoic acid to reduce the tolelance of radical oxygen species.

Activities of Medical Team in 2012

1) Meeting of N. Research team in every week.
2) Meetings four times in the collaborating institute Central Institute for Experimental Animals Common marmoset team for the development of PI polyamide targeting TGF-β1.
3) June: Meeting with the Drug Preparation Room in Nihon University School of Medicine Itabashi Hospital and Clinical Pharmacokinetics team in College of Pharamacy about the development of PI polyamide targeting TGF-β1.
4) October: Meeting with the team in College of Pharamacy about the GLP grade phamakokinetics study for PI polyamide targeting TGF-β1
5) November: Meeting for the development of plasma medicine for skin malignant melanoma collaborating with the plasma team in College of Science and Technology.
6) December: Presentation for the development of PI polyamide as practical medicine in College of Pharmacy.

Supramolecules and Self-Assembly Group

Hiroki Ikake*, Akiyoshi Itoh, Joe Otsuki, Arata Tsukamoto and Sachiko Matsushita

The goal of the supramolecules and self-assembly group is to develop advanced technologies on nanomaterials and nanostructures and to supply these technologies to the application-oriented groups, *i.e.*, the information, energy, and medical groups, thus strongly promoting networking among these groups on diverse fields. As follows, each groups theme in 2012.

· Itoh & Tsukamoto Group

We tried to prepare and utilize nano-structured substrates such as silica thin film having self-assembled nano-pores and self-assembled silica particle substrate. In 2012, we preformed additional annealing to above isolated FeCuPt grains by using same annealing chamber of rapid thermal annealing, for crystallizing those poly-crystal grains to form single crystalline grains. As a result, the grain consists of c-axis oriented single crystalline structure from complementary results of X-ray diffraction and electron beam diffraction. We found that an application of adequate additional annealing makes grains into $L1_0$ single crystalline structures and grains kept almost similar size.

· Otsuki Group

Self-assembly of appropriately designed molecules will afford a bottom-up method for producing nanostructures. This work aims at developing new molecular self-assembling systems, revealing self-assembled structures and dynamic behaviors at the molecular level, and searching for applications of self-assembly to energy, medical, and information technologies through the collaboration with researchers of the *N*. research project.

1. Self-Assembly of Molecules and Quantum Dots

2. New Dyes for Dye-Sensitized Solar Cells

· Matsushita Group

Two subjects related with self-assembly and self-organization were studied with perspective of the developments of unexplored scientific fields and new technology.

1. Dye-sensitized photonic crystal electrodes

We examined the fluorescence inhibition effect of a self-assembled photonic crystal using Chlorine e6 dye. Chlorine e6 is derived from chlorophyll and has a long excited electron lifetime.

2. Noble Planar and Symmetric Nanostructures in Prospective Plasmonic Devices

Noble planar and symmetric nanostructures, such as rod or spiny structures, were prepared by the combination of colloidal self-assembly, thermal sintering and chemical etching, which enables the tuning of both size of the particle and neck diameter. As a result, the rod structure showed the biggest SERS effect among our structures in spite of the smallest amount of Au coating.

· Ikake Group

In our group, the aim of development of poly(L-lactic acid) (PLLA) films as biopolymer with the high thermal- and mechanical- resistance. And then, the improved PLLA was submitted to new material field. In particular, we have discussed as follows theme in 2012.

1. Preparation of High Crystallinity and High Orientation Poly(L-lactic acid) Films under Electric Field

2. Morphological change of Poly(L-lactic acid) Films with Magnetic Irradiation

Nanomaterials and Nanodevices Group

Kaoru Suzuki*, Yoshiki Takano, Tomohiko Asai, Nobuyuki Iwata, Hideomi Hashiba, Ken Judai and Shigeru Chaen

1. Overview of the research plan in 2012

This group aims at fabrication of nanomaterials and nanodevices for high functional applications such as 1) Takano has a plan to prepare single phase samples of $Sr_{1-x}R_xFeAsF$(R=rare earth) and try to make thin films of $Sr_{1-x}Nd_xFeAsF$ with collaboration with Prof. K. Suzuki. Quantum dot single-photon terahertz detector by Fe-based superconductor films, 2) Magnetic probe of Scanning probe microscope by Ni, etc. encapsulated carbon nanotubes and semiconducting single-walled carbon nanotubes by controlling specific chirality for field effect transistor, 3) Photocatalytic La,Sr,Ca:TiO2 films for hydrogen generation, storage and oxygen (hydrogen) storage and release with metal oxides (metal hydrides) nanoparticles, 4) New photo-memory by highly-photoluminescent material (NiO-ZrO_2 solid solutions) and in-vitro single molecule imaging of these proteins by membrane receptors.

Asai has a plan to 1) Development of rapid generation method of alloy thin-film by using a MCPG
Thin-film formation method with a MCPG has been studied for practical applications; TiZrFeMn film, titanium oxide film and surface treatment of ceramic materials. 2) Medical application of LF plasma jet: Basic test device of LF plasma jet for a cancer treatment has been developed and an experimental study has been initiated. 3) Design study of new scenario of a muon-catalyzed nuclear fusion: Innovative scenario of a muon-catalyzed nuclear fusion has been proposed and basic design study has been performed. The concept is utilize the “pack-man method” in a translated field-reversed configuration to realize hydrogen solid hydrogen pellet in a warm plasma for an effective re-activation method for muon.

Hashiba plans in 2012 are as follows: Development of fabrication technics and Study of silicone wave guide devices with its third-order nonlinearities, development of fabrication technics and Study of two dimensional phonic crystals (PCs) of titanium oxide (TiO_2) of low refractive index to meet the needs of the advanced solar cells, and revealing higher order THz plasma excitations of quantum dots confined with shallow potential barriers.

2. Advances and achievements in 2012

Prof. K. Suzuki approached 1)Metal encapsulated carbon nanotube for magnetic force microscope probes:The diameter and length of the metal core is in the range of 10 – 80 nm and 100 – 800 nm with varying heating period and temperature, respectively. The walls consist of cylindrical graphene sheets with 3 -50 layer. 2)Creation of carbon nano-tube/fiber and diamond-like carbon circuit:synthesized phosphorus doped n-type carbon nano-tube/fiber by Joule heating on ethanol/Si surface, and diamond-like carbon films by ion beam plating method. Type of p-n junction diode and wiring were created by focused Ga+ ion beam injection. 3) Synthesize of photocatalytic SrxLa1-xTiO3 film for hydrogen generation on polymer films with visible area in solar light excitation by laser induced forward transfer method: try to deposit of TiO2 on polymer films by laser induced forward transfer method. 4)Synthesis of ZnO nano-films for light emitting device by infrared light excited pulsed laser deposition method: High quality crystalline of p-type ZnO nano-films were improved by pulsed YAG laser annealing below 532 nm of laser wavelength. 5)Bio-electronics:studied the sterilization of periodontal bacterium by atmosphere pressure low frequency jet plasma; fresh plasma, and splintering/regeneration of enchytraeus japonensis by irradiation of free electron laser. 6)Green technology:studied the evolution of controlled nano/micro bubble by laser/focused ion beam fabricated nozzle on piezoelectric vibrator for defecation of water.

Prof. Y. Takano has prepared $Sr_{1-x}Nd_xFeAsF$ and obtained the high T_c superconductivity previously reported in $Sr_{1-x}Sm_xFeAsF$. Although he has tried to prepare single phase samples, they have not been obtained. On the other hand, Takano has prepared F deficient $SrFeAsF_{1-y}$ and investigated their electrical properties. Although the

metallic conductivity is obtained, superconductivity is not observed above 3 K. However, he has found that the decrease of T_c by y in optimum doped $Sr_{1-x}R_xFeAsF_{1-y}$ is independent of R ions. Takano has also investigated the possibility of $Sr_{1-x}Nd_xFeAsF$ for the superconducting wire rod and obtained that the upper critical magnetic field of this sample is higher than that of MgB_2 that has the highest critical current density.

Asso. Prof. T. Asai has developed 1) Basic and applied study on a magnetized plasmoid has been performed in the project. In FY2012, the prospect of actually using a multi-pulsed magnetized plasmoid generation system for a rapid generation of alloy thin film has been emerged and applied for a patent. Also, the invented technique has started to be studied as an innovative surface treatment method for dental ceramics. 2) The feasibility of medical applications of an atmosphere pressure LF jet plasma has been performed. Based on the results, a test equipment of LF jet system has been developed. 3) For the basic study of self organization process of magnetized plasmoid, an experimental device for a super Alfvenic velocity FRC translation has been developed. The experiments on the newly developed device have been started in December 2012. The experimental facility has also been applied for a feasibility test of a muon-catalyzed nuclear fusion.

Asso. Prof. N. Iwata has studied the selective growth of single-walled carbon nanotubes (SWNTs) with specific chirality controlled by irradiating the FEL. The G/D ratio, which indicates quality of SWNT, was significantly improved from about 30 to over 400 by developing a new substrate heater system. $[ABO_3/REMO_3]$(A=Ca,La, B=Fe,Mn, RE=La,Bi, M=Fe,$Fe_{0.8}Mn_{0.2}$) superlattices were deposited on surface treated $SrTiO_3$(100) substrates by pulsed laser deposition method; 3 types of $CaFeO_3$(CFO)-series, 3 types of $CaMnO_3$(CMO)-series, 3 types of $LaMnO_3$(LMO)-series. In a 2θ-θ x-ray diffraction, satellite peaks and Laue oscillations were clearly observed. Those results indicate that the homogenous interface is created. From the results of reciprocal space mapping (RSM), all superlattices except for LMO/$BiFe_{0.8}Mn_{0.2}O_3$(BFMO), cubu-on-cube structure was observed with the film lattice fitted to the substrate lattice in-plain. Sheet resistance of the superlattices showed semiconducting behavior. The E_A of CMO and LMO single layer was 0.076 and 0.17eV at higher temperature. The E_A of the superlatatice was smaller than the value of single layers, indicating that the electron transfer, intermixing of cation at the interface, and modification of the band structure. At the T_C, magnetic transition is expected. The author did the organizer at the biggest joint symposium in this field (JSAP-MRS 2012 Spring Meeting). The author was invited to the OMTAT international conference hold at Kochi, India with the title of Oxides heterostructures for giant magnetoelectric effect. The research has been done with Prof. Hashimoto and IMS group of Univ. of Twente, Netherlands as a collaboration research. In addition, collaboration research with ETH Zűrich, Swiss about the observation of antiferromagnetic domain of Cr_2O_3 thin film using SHG technique was carried out. The domain with Néel temp. of 307K was clearly observed.

Asso. Prof. H. Hashiba has studied the 1)Research of silicone wave guide devices of this year has been focused on development of simple fabrication method of the waveguides and we attained to develop concrete fabrication method for a Si waveguide of 320 nm wide and more than 1 mm long. The waveguide has small roughness of side-walls of less than 10 nm and accuracy of shape of the waveguide is restricted by our EBL. 2)Our TiO_2 PCs are fabricated with standard electron beam resist mask and deposition techniques of Ag-O_2 mixture gas of 1:1.5 at 1 x 10^{-2} Torr. The patterned TiO_2 film is then baked at 550 degrees and transform amorphous to mixture of rutile and anatase. The observation of the layer under XRD measurement shows that some rutile turns into anatase at that temperature. 3)Plasma excitations of QDs formed on a GaAs hetero-structure arises with a formation of confinement potential barrier from the reservoir having resistances more than resistance quanta, and we revealed that appropriate shape of the barriers lowers dark counts by suppression of flow of hot electrons form the reservoir and reveals higher order excited states. The higher order excited states is expected to have the same plasma frequency of that of the first and shows a heat bath effect of the QD. This will promise high temperature operation of the THz detection.

Prof. S. Chaen and Prof. T. Tojo have succeeded in estimating ADP release rate from the displacement of fluorescent nucleotides bound to myosin heads in the *in vitro* motility assay system by flash photolysis of caged ATP. And they have developed a new wet cell system of Scanning Electron Microscopy to observe a living cell

in aqueous solution with at nanometer resolution.

Asso. Prof. K. Judai has studied the “self-assembled nano helix”. He found silver tolyl-acetylide molecules self-assemble into nano helical morphology, however, the x-ray crystal structure analysis could not be performed yet. He established also the method of the metallic cluster preparation for electrochemical analysis.

3. Collaborations and activities in 2012 as the group

Each crew has team meetings and offered the research sample, respectively. We obtained the several collaborations results such as superconductor films, nanotube device, hydrogen generation/storage/release nano-particles/films and single-moecule fluorescent imaging.

Hashiba has collaborative projects of “electric field dependence of polarity of molecular moters” with prof. Otsuki, and “single photon emission from CdSe quantum dots coupled with metal waveguide” with Prof. Inoue.

Quantum Theory and Computation Group

Hiroshi Ishida, Shinichiro Ohnuki, Tokuei Sako,* Tsuneki Yamasaki

1. Overview of the research plan in 2012

（1－1，Ishida）Electronic structure and conductivity of singe-molecular chain linked between metal electrodes are examined by the finite-temperature Green's function method.（1－2，Sako）Structure of conjugate Fermi holes in artificial atoms as well as natural atoms is examined and their relation with electronic properties is rationalized.（1－3a，Ohnuki）Aiming at designing an optimal plasmon antennas for the direct opto-magnetic recoding the localized field in the vicinity of plasmonic antennas of various shape is examined.（1－3b，Ohnuki）An efficient numerical method for solving coupled Maxwell and Schrödinger equation is established.（1－4，Yamasaki）An optimal structure of photonic crystal wave guide incorporating dielectric materials is examined.

2. Advances and achievements in 2012

（1－1，Ishida）We considered *N*-site Hubbard molecules linked between two metal electrodes and examined their equilibrium electronic structure at temperature in the zero-bias limit by calculating the finite-temperature Green's function. The integrated one-electron density of states (DOS) near the chemical potential of metal electrodes for different gate voltage was examined. The result indicates the formation the Kondo resonance at below the Kondo temperature (Phys. Rev. B, 2012). The present scheme is shown to be capable of describing the electronic structure of adsorbed molecules in the wide parameter range including the ballistic, Coulomb blockade, and Kondo regimes.

（1－2，Sako）Through the continuing research of this *N*. project we have found last year the existence of the so-called conjugate Fermi hole in the wave function of two electrons with antiparallel spins. This year we have focused on artificial atoms and have examined in detail the structure of the conjugate Fermi holes in the systems. As a consequence of the analysis, the origin of the first Hund rule in artificial atoms has been rationalized, and the difference in the mechanism operating in artificial atoms and in the corresponding He-like systems has been clarified（J. Phys. B, 2012）.

（1－3a，Ohnuki）We have designed plasmonic antennas to generate the localized circularly polarized light inside the bit-patterned media for realizing ultra-high density magnetic recording. Using the ADE-FDTD method, the generation time and the intensity of the localized circularly polarized light are clarified in terms of the combination of cross antennas.

（1－3b，Ohnuki）A nanoplate in laser fields is analyzed by the coupled Maxwell-Schrodinger scheme which is based upon the FDTD method. We investigate the current densities and electromagnetic fields near the nanoplate in terms of tunneling effects due to well structures. Advantages of our proposed method are clarified in comparison with conventional classical solvers.

（1－4，Yamasaki）We have analyzed the guiding problem by dielectric waveguides with defects composed of dielectric circular cylinders array and deformed rhombic dielectric structure in the middle layer and investigated the influence of energy flow for the defect area by using the propagation constants at the guided region. From the numerical results, it is shown that we can obtain the best efficiency by rhombic dielectric structure compared with deformed rhombic dielectric structures in the middle layer for both TE0 and TM0 modes.

3. Collaborations and activities in 2012 as the group

We have organized a meeting every month at Prof. Ohnuki's laboratory with Prof. Nakagawa and Dr. Ashizawa of Information Storage Group to study mainly theoretical methods for solving coupled Maxwell and Schrödinger equations.