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Invited

An Attempt for Industrial-Academic-Governmental Joint Research in the Basic Studies of Device, Material and Process —Research on Ultimate Manipulation of Atoms and Molecules at the National Institute for Advanced Interdisciplinary Research—

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SUMMARY

The present status and problems for the "Research and Development of Ultimate Technology for Manipulating Atoms and Molecules" will be presented, which has been carried out at the National Institute for Advanced Interdisciplinary Research (NAIR) as an innovative attempt for tripartite joint research project involving industrial, academic and governmental sectors. The project consists of four subfields: (1) chemical species identification and manipulation of atoms and molecules, (2) self-organization of nano-scale structures, (3) creation of innovative materials and properties, and (4) computer simulation (fundamental theory) of atomic process. While the effects of recruiting qualified scientists and intensive investment are appreciable in the above-mentioned joint research, some improvement may be desired in regard to more flexible handling of research fund.

1. Introduction

The industrial, academic and governmental (to be abbreviated hereinafter as I-A-G) joint research with personnel recruited broadly from all the three sectors and research fund intensively endowed, has recently been adopted in various areas, as a promising research paradigm for pursuing high quality strategic research and indispensable for creating new industries. I would like to portray here the present status and problems in the "Research and Development of Ultimate Technology for Manipulating Atoms and Molecules" being run at NAIR, as an example of I-A-G joint research in the field of device fundamentals study.

2. I-A-G Joint Research at NAIR-AIST

2.1 Significance of I-A-G Joint Research

The realization of information networks has promoted the information exchange in communities in accelerated manner, and been increasingly requesting internationally distinguished achievements on the part of basic research. In order to harvest expected results and to extend them to the creation of new industries under such an environment, it has been urgently needed to organize a comprehensive joint research covering industrial enterprises, universities, government and national institutes, to invest research fund intensively for attaining to the project goal, and to repeat far-reaching discussions from multifarious points of view among qualified scientists gathered overcoming institutional and disciplinary boundaries, for pursuing the target research in flexible manner.

In such a form of basic research, the government and national institutes are obliged to design and organize strategic research projects on themes of national needs and to appropriate ample governmental funds for the execution of research. The academic sector is requested to supply persons willing joint the project on the basis of deep scientific insight out of staff enjoying free studies, and also to train young researchers through such research activities. And finally, the industries are desired to join the project based on their productive activities, to support the growth of enterprises through R&D, and to contribute to the project by turning back some of their profit to the basic research. In this way, three sectors can joint the project on the basis of specific motivation and contribute to reaching their own goals.

2.2 National Institute for Advanced Interdisciplinary Research (NAIR-AIST)

NAIR-AIST-MITI was founded in January 1993 as a theater for I-A-G joint research. The basic policies of NAIR include exploiting new interdisciplinary field in industrial science and technology, implementing intensive joint research involving scientists recruited from I-A-G sectors, both domestic and overseas, and creating favorable environment for I-A-G and international joint research. The basic features of NAIR are open recruitment, flexible personnel exchange, international collaboration and objective evaluation by outside experts. The mission of the NAIR management is to provide an ideal environment for research works through implementing the basic policies and keeping the basic features.

Currently, four research projects are being run at NAIR: Ultimate Manipulation of Atoms and Molecules (for 10 years), Cluster Science (for 6 years), Bionic Design (for 6 years) and newly started Next Generation Optoelectronics Basic Research. NAIR has about 214 staff, including about 167 research staff. The latter consists of regular staff, concurrent assignments from AIST and STA (Science and Technology Agency) institutes and universities, scientists loaned from enterprises, fellows under various programs, postdoctorals and graduate students, including 34 foreigners. The joint research project encompasses 33 firms including 5 overseas enterprises.

As NAIR accepts a lot of concurrent assignments, it may be regarded as a common asset of national institutes and universities.

3. Research on Ultimate Manipulation of Atoms and Molecules

The largest of NAIR Projects is being carried out by the Joint Research Center of Atom Technology (JRCAT) composed of the Atom Technology Group of NAIR and Angstrom Technology Partnership (ATP). The project is characterized as a basic research aiming at the establishment of generic technology for future industries involving devices, materials and processes, and has the following subgoals:

(1) Chemical Species Identification and Manipulation of Atoms and Molecules.

The technology to identify, observe, measure and manipulate atoms, molecules and organic polymers such as DNA on surface or in space is developed by using mechanical probe, electron beam, laser and so on, aiming at creating nano-scale structures having innovative properties and functions.

(2) Self-Organization of Nano-Scale Structures.

The technology to align and grow nano-scale 3D structures autonomously is to be developed by using the tendency of heterogeneous clusters to grow immediately above areas of intensive strain, aiming at making foundation of structure formation for nano-scale electronics in the future.

(3) Creation of Innovative Materials and Properties.

Innovative materials and properties are to be developed by collectively controlling spatial configuration of electrons (spins), atoms and molecules. A typical example is materials exhibiting insulator-metal transition under magnetic field (colossal magnetoresistance effect).

(4) Computer Simulation (Fundamental Theory) of Atomic Process.

In order to control the material construction on the atomic scale for creating materials of desired function, behavior of atoms and molecules and microscopic mechanism of functional manifestation are to be elucidated theoretically. Innovative algorithms are to be developed in addition to *ab initio* calculation, molecular dynamics, Monte Carlo simulation, and so on.

A few examples of achievements in the Ultimate Manipulation of Atoms and Molecules are presented below:

1) Extraction of Silicon (Si) Atoms and Control of Surface Structure by Scanning Tunneling Microscope (STM)

The study performed as a part of "Chemical Species Identification and Manipulation of Atoms and Molecules" has explicitly demonstrated clearing surface atoms from a crystal. When a tungsten (W) probe biased at - 2 V, once brought in contact with silicon Si(111)-7x7 was withdrawn, atoms of uppermost two layers were extracted leaving a pit of about 0.3 nm depth, and neatly aligned arrays of atoms were observed as surface atomic layer at the bottom of pit. [*Appl. Phys. Lett.* **68** (24): 3482-3484, 1996]

2) Nano-Scale Wire Construction on Surface of Gallium (Ga)-Covered Silicon (Si) Formed by Using Scanning Tunneling Microscope (STM) Probe in Self-Organizing Manner

In this experiment, carried out as a part of "Self-Organization of Nano-Scale Structures", a surface of silicon (Si) crystal slightly tilted from the alignment face and covered with a monolayer of gallium (Ga) was approached with

an STM probe and high voltage was applied to the latter to remove gallium layer partly. When the specimen was heated to 560 ℃, the Ga-free area was extended as a band of a few nanometer width exposing Si atoms. Since the band can adsorb atoms of different species, this process will provide a basis for self-organizing construction of nano-scale wire structure. [*Appl. Phys. Lett.* **68** (6): 770-772, 1996]

3) Creation of Weak-Field, Colossal Magnetoresistance Effect Materials

The study was executed as a part of "Creation of Innovative Materials and Properties". In the conventional perovskite-type oxides of manganese, it was necessary to apply a magnetic field as high as a few tesla for implementing colossal magnetoresistance effects. With a new material, $(Nd,Sm)_{1/2}Sr_{1/2}MnO_3$, created by this study, the resistivity was changed by three orders of magnitude or more under a magnetic field as low as 0.2 tesla, though cryogenic atmosphere of 115 ℃K was needed. [*Science* **272** (5 April): 80-82, 1996]

4) Development of Cluster Capturing Device and Formation of Atomic Cluster in Space

With a quadrupole device to keep ions floating in space by use of electrostatic force, atomic clusters composed of silicon and hydrogen atoms was created, with certain structures preferred. [*Appl. Phys. Lett.* **67** (16): 2341-2343, 1996]

5) Photochromism of Sodium Cluster in Zeolite LTA

This study was carried out under the Cluster Science Project. It was found that when sodium clusters were fed into minute tubular spacings in zeolite crystal, photochromism was induced. [*Proc. Int. Symp. on Science and Technol. of Atomically Engineered Materials*, Richmond, Virginia, USA, 1995]

6) Theory of Initial Oxidation Stages on Silicon Si(001) Surfaces by Spin-Polarized Generalized Gradient Calculation

The research constitutes a part of "Computer Simulation (Fundamental Theory) of Atomic Process". The oxidation process of silicon surface, an unavoidable topic for the silicon device process was analyzed by use of supercomputing systems, and it was successfully demonstrated that oxygen molecule (O_2) was dissociated into two atoms at the Si(001) surface and combined with Si atoms of the substrate. [*Proc. MRS Symposium*, 1996 — to be published]

7) Direct Decoding of Base Sequence in Gene DNA

By using a high resolution atomic force microscope (AFM), the base sequence of DNA in bacteriophage FX175 infecting colon bacteria *Escherichia coli* was directly decoded. [*Extended Abstr. '96 JRCAT Symp. on Atom Technol.* 181-184, 1996]

4. Conclusion

An outline of the "Ultimate Manipulation of Atoms and Molecules" Project being carried out at NAIR has been presented, as an example of I-A-G joint research on the device fundamentals.

On the basis of our experience with the joint research at NAIR, the following features may be pointed out: It is natural that the personal issue is the key factor of the joint research, and it is essential that some qualified persons skillfully steers the project. The intensive investment of research fund for the project seems to have extensive merits, achieving successful recruit of competent scientists. Particularly, setting a duration as long as 10 years to the "Ultimate Manipulation of Atoms and Molecules" Project has a great significance for the scheme of NAIR projects, unique in the world, under which scientists have to leave the institute after the termination of the project. As an attractive merit to compensate certain sacrifices of leaving the original affiliation and relocating residence to join the project, 10-year project duration would be indispensable. Moreover, gathering talented staff of international caliber is essential, and the objective evaluation and straight advice by competent outside specialists will play a significant role for keeping the research atmosphere in high tension.

There are some problems to be solved immediately. The flexible use of research fund for personnel and travel costs has been strongly requested. Concerted tuning of thought among staff members of different backgrounds, provisions to be considered on the termination of existing projects and start-up of new projects are left unsolved. For successful execution of project requiring personal transfers, it is inevitable to invite warm understanding from surroundings. It is the task of NAIR management to overcome these problems and create friendly research environment. Advice and instructions from outsiders are cordially invited.