

Priority Area:

**2. Advanced Materials, including Polymers and
Nanomaterials**

Coordinators:

(Japanese)

Masao Doyama

Professor Emeritus

University of Tokyo

(Indian)

P. Rama Rao

Vice-Chancellor

University of Hyderabad

India-Japan Cooperative Science Programme
Activity Report in the Area: Advanced Materials, including Polymers and Nanomaterials

Overview and Future Plan

1.FY2001-2002 Overview

1.1 Joint Research Projects.

1.1.1 Materials Design by First Principles Computer Simulation

Coordinators: Prof. Yoshiyuki Kawazoe, Tohoku University and Prof. S. Yashonath (Indian Institute of Science), From April 1999 to March 2003.

Important results obtained are simulation of silicon fullerenes, water clathrates and carbon nanotubes using supercomputer system in the Institute for Materials Research. More than fifty papers have been published.

1.1.2. Investigation of the Optical and Electrical Properties of Tetrahedral Amorphous Carbon (ta-c) Film by Pulsed Laser Deposition

Coordinators: Prof. Masayoshi Umeno, Chubu University and R.M. Mehra University of Dalhi, South, from April 2000 to March 2003. The project has been completed with a great success.

n-type carbon (doped camphoric carbon) / p-type silicon heterojunction, p-type-carbon / n-type silicon heterojunction and n-type carbon / p-type carbon / p-type silicon heterojunction have been grown at Nagoya Institute of Technology and Chube University and were analyzed by determining their solar cell parameters.

1.1.3. Preparation and Characterization of Thin Films of Conjugated Polymers Suitable for Optoelectronic Devices

Coordinators: Prof. Mitsuyoshi Onoda (Himeji Institute of Technology) and Professor P.K.Batnagar (University of Delhi, South Campus, from April 2002 to March 2005.

Organic nano-materials with flexible structure is being investigated. The fundamental properties of devices are affected by interfacial properties.

1.1.4. Fabrication of Semiconductor Nanocrystals and Their Biosensor Application

Coordinators: Prof. Shinji Nozaki (The University of Electro-Communications) and Prof. Surendra Nath Sahu (Indian Institute of Physics), from April, 2002 to March 2005.

Electrical characteristics such as I-V and C-V of electrochemically deposited GaAs nanocrystals on ITO(indium tin oxide) coated glass substrates were measured. Gold or ITO contact were not ohmic. The research was just started and they are struggling to remove the contact

1.2. Seminars:

1.2.1. FY2001: Asia Science Seminar was held at Hyderabad so that other seminar on new materials was not held in FY2001.

1.2.2.FY2002: Two seminars were planned but both seminars were not held because the safety warning was by the Ministry of Foreign Affairs.

1.2.2a. Workshop on Advanced Magnetic and Magnetoelectric Materials and Devices, Hiroyuki Akinaga (National Institute of Advanced Industrial Science and Technology) and Prof. Sukumar Basu (Indian Institute of Technology, Kharagpur). First planned to be held in India but changed to Japan. Never be held.

1.2.2b. Materials Design by First Principles Computer Simulation

Planned by Prof. Yoshiyuki Kawazoe, Tohoku University and Prof. S. Yashonath (Indian Institute of Science), on the occasion of the completion of joint research project. Also not be held.

2.FY2003-2004 Future Plan

2.1. FY2003:

A large International Conference on Advanced Materials will be held at Yokohama, Japan (IUMRS-ICAM2003, International Union of Materials Research Societies-International Conference on Advanced Materials 2003).

Prof. CNR Rao (Founding President, MRS-I) is giving an invited talk on “Electronic Phase Separation in Solids” in Symposium B-8, Prof. P. Rama Rao is the Vice President of IUMRS. Prof. D. Chakravorty is the MRS-I (Materials Research Society of India) and Dean S. V. Subramanyam is the vice President of MRS-I. It is quite a rare occasion for such important Indian scientists to come to Japan together. Therefore a Japan-India Seminar on “Materials Education and Research Strategy and New Materials” is planned. The seminar on “Materials Education and Research Strategy” is joined with IUMRS-ICAM2003 and the seminar on “New Materials” is independent of IUMRS-ICAM2003.

The other seminar is “ India-Japan workshop on Advanced Molecular Electronics and Bionics”, organized by Prof. Keiichi Kaneto (Kyushu Institute of Technology) and Dr. B.D.Malhotra (National Physics Laboratory).

2.2. FY2004:

It is ideal to split into joint research, seminar and visiting scientists, so that the situation in FY2003 is an exception.

3.Summary

I feel the Programme on New materials is going very well, except FY2002 seminars. This was due to a political safety reason. It is ideal to split the budget into three categories, joint research, seminars, and individual visitors.

We receive many proposals for the Programme. We always have hard time to decide which should be selected.

Proposals well planned and well agreed between Indian side and Japan side bring good results.

Modes of Cooperation:

1. Joint Research Projects
2. Seminars
3. Visiting Scientists for Information Exchange

Report

1. Joint Research Projects

FY2001 – FY2002

Project No.1

Title: Material Design by First Principles Computer Simulation

Objectives:

To design new materials it is becoming more and more important to apply the advanced technology of computer simulation. Recent development of the state-of-art *ab initio* calculation has made it possible to design nanostructured materials without any experimental parameters. Therefore, it is important to establish an international collaboration between various countries. Accordingly, we have proposed a plan to establish a fundamental relation between researchers in India and Japan to achieve a system of materials design on the presently urgent nanostructured materials.

Project Coordinators:

(Japanese)

Yoshiyuki Kawazoe

Professor

Tohoku University

(Indian)

S. Yashonath

Professor

Solid State and Structural Chemistry Unit

Indian Institute of Science

Date of Commencement: 1 June 1999**Date of Completion:** 31 May 2002**Accomplishment Status:**

We have organized a group of researchers in India and Japan, and visited both countries frequently. Moreover, in the Kawazoe laboratory, Institute for Materials Research, Tohoku University, already 5 Indian researchers are working based on this program. We have also organized ACCMS (Asian Consortium on Computational Materials Science) based on this exchange program in 2001, and have published a conference report. Important subjects studied by this group are silicon fullerenes, water clathrates, carbon nanotubes, etc. and by using the supercomputer system in the Institute for Materials Research, Tohoku University to achieve very large scale computer simulations. Already more than 50 papers have been published based on this collaboration.

Future Plan:

This collaborative research program made it possible to collaborate strongly in materials design by computer simulation. Now it is planned to continue employment from India in the Institute for Materials Research and encourage this collaboration in the future. We plan to organize ACCMS-2 to meet again to discuss about mutual communication. The group work based on this program is really useful and we will keep good relation among all the contributors.

Exchange Visits Undertaken:**FY2001**Japan to India

<u>Name and Affiliation</u>	<u>Research Subject</u>	<u>Main Host</u>	<u>Period</u>
Vijay Kumar	First Conference of Asian Consortium for	Umesh Waghmare	26 Nov.2001-
Visiting Professor	Computational Materials Science	Professor	12 Dec.2001
Institute for Material Research	(ACCMS-1)	Jawaharlal Nehru Center for Advanced Research	(17 days)

Tohoku University

Yoshiyuki Kawazoe Professor Institute for Material Research Tohoku University	First Conference of Asian Consortium for Computational Materials Science (ACCMS-1)	Umesh Waghmare Professor Jawaharlal Nehru Center for Advanced Research	27 Nov.2001- 2 Dec.2001 (6 days)
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India to Japan

<u>Name and Affiliation</u>	<u>Research Subject</u>	<u>Main Host</u>	<u>Period</u>
Subramanian Yashonath Associate Professor Indian Institute of Science	Material Design by First Principles Computer Simulation	Akira Miyamoto Professor Tohoku University	18 Feb.2002- 18 Mar.2002 (29 days)

Project No.2

Title: Investigation of the Optical and Electrical Properties of Tetrahedral Amorphous Carbon (ta-c) Films by Pulsed Laser Deposition

Objectives:

- Growth of doped camphoric carbon (CC) films on Quartz, Glass and ITO substrates using XeCl excimer pulsed laser deposition and ion beam sputtering
- Optimization of deposition parameters to achieve the required optical band gap and resistivity
- Characterization of thin films for their structural, optical and electrical properties using XRD, FTIR Raman spectroscopy, SEM and AFM.
- Fabrication of hetro-structures & homo-structures (p-i-n) solar cells using the CC films
- Determination of solar cell parameters V_{oc} , I_{sc} , FF and efficiency
- Determination of the various solar cell parameters (Experimentally as well as Theoretically).
- Intensity and temperature variation study and estimation of the Series Resistance of the CC solar cell by using the family of curves of intensity variation.
- Study of the photo degradation of the solar cell parameters due to light soaking

Project Coordinators:

(Japanese)

Masayoshi Umeno

Professor

Department of Electronic Engineering

Chubu University

(Indian)

R.M.Mehra

Professor

Department of Electronic Science

University of Delhi, South Campus

Date of Commencement: 1 April 2000

Date of Completion: 31 March 2003

Accomplishment Status:

The CC films and their heterostructures namely; n-C/p-Si heterojunction, p-C/n-Si heterojunction and n-C/p-C/p-Si heterojunction have been grown at NIT, Nagoya, and Chubu University, Kasugai, Japan. The

heterostructures were analyzed by determining their solar cell parameters. From the study made at Department of Electronic Science, University of Delhi South Campus, New Delhi, India, and Chubu University, Kasugai, Japan, three joint research papers have been published in refereed journals and two has been presented (one Orally) in the International Conference on `PV in Europe` From Energy solution to PV technology, Rome, Italy from October 7-11, 2002. One paper has also been accepted in the WCPEC conference to be held in Osaka, Japan during May 12-16, 2003.

Future Plan:

Sufficient work on the fabrication and characterization of heterojunctions namely; n-C/p-Si heterojunction, p-C/n-Si heterojunction and n-C/p-C/p-Si heterojunction have been done during the tenure of the project. However, it is necessary to eliminate silicon in order to realize a real carbon solar cell. The fabrication of the herterostructures ITO/n-C/p-C/Au and ITO/n-C/i-C/p-C/Au (p-i-n) has been started during the recent visit and the structures being characterized. Therefore, it is requested that the project tenure may be extended for one year to make detail measurements and analysis as done for heterostructures.

Exchange Visits Undertaken:

FY2001

India to Japan

<u>Name and Affiliation</u>	<u>Research Subject</u>	<u>Main Host</u>	<u>Period</u>
Ram Mohan Mehra Professor University of Delhi, South Campus	Amorphous Carbon Solar Cells	Masayoshi Umeno Professor Department of Technology Chubu University	22 Dec.2001- 12 Jan.2002 (22 days)
Avinashi Kapoor Reader University of Delhi, South Campus	Amorphous Carbon Solar Cells	Masayoshi Umeno Professor Department of Technology Chubu University	22 Dec.2001- 12 Jan.2002 (22 days)

FY2002

India to Japan

<u>Name and Affiliation</u>	<u>Research Subject</u>	<u>Main Host</u>	<u>Period</u>
Ram Mohan Mehra Professor University of Delhi, South Campus	Investigation of the Optical and Electrical Properties of Tetrahedral a-C films by Pulsed Laser Deposition and Application to Photovoltaic Devices	Masayoshi Umeno Professor Department of Technology Chubu University	8 Mar.2003- 16 Mar.2003 (9 days)
Avinashi Kapoor Reader University of Delhi, South Campus	Investigation of the Optical and Electrical Properties of Tetrahedral a-C films by Pulsed Laser Deposition and Application to Photovoltaic Devices	Masayoshi Umeno Professor Department of Technology Chubu University	8 Mar.2003- 16 Mar.2003 (9 days)

Project No.3

Title: Preparation and Characterization of Thin Films of Conjugated Polymers Suitable for Optoelectronic Devices

Objectives:

The object of this project shall be to discuss basics and applications in terms of optoelectronic devices. Organic nano-materials with flexible structure, techniques for the evaluation of Tricky but intelligent ideas for the optoelectronic devices, *etc.* will be Investigated.

Project Coordinators:

(Japanese)	(India)
Mitsuyoshi Onoda	P.K.Batnagar
Professor	Professor
Himeji Institute of Technology	University of Delhi, South Campus

Date of Commencement: 1 April 2002

Date of Completion: 31 March 2005

Accomplishment Status:

The fundamental device properties are affected by interfacial properties. Accordingly, it is necessary to understand not only the properties of the conducting polymer itself, but also interfacial electronic phenomena and electronic states on a nanometer scale.

This time we had discussed how to measure the interfacial phenomena of the organic devices to Prof. Bhatnager's group during my stay in New Delhi.

Future Plan:

The operation of most optoelectronic device is fundamentally ruled by the interfaces of semiconductor and metal contacts. The device performances are strongly depends on the interfacial properties. Then it is of great importance to pursue so-called "KARAKURI (in Japanese)" for the fruition of highly functional devices, where intentionally introduced tricky-but-intelligent nano-interfacial phenomena play a dominant role beyond the specific function of molecules themselves.

Electronic and optically functional devices using organic nano-materials with flexible structure have been developing to the stage of practical use. To improve the performance and the function of such devices, the profound understanding of electronic phenomena at the interface is critically important. Accordingly, it is necessary to understand what the "KARAKURI" of interface systems is and use intentionally the "KARAKURI" for the better performance. Our goal is to realize not only thin film electronic devices, but also mono-molecular film electronic devices in its turn molecular electronic devices.

Exchange Visits Undertaken:

FY2002

Japan to India

<u>Name and Affiliation</u>	<u>Research Subject</u>	<u>Main Host</u>	<u>Period</u>
Mitsuyoshi Onoda Professor Himeji Institute of Technology	Preparation and Characterization of Thin Films of Conjugated Polymers Suitable for Optoelectronic Devices	P.K.Bhatnagar Professor University of Delhi, South Campus	15 Dec.2002- 20 Dec.2002 (6 days)

India to Japan India

<u>Name and Affiliation</u>	<u>Research Subject</u>	<u>Main Host</u>	<u>Period</u>
P.K.Bhatnagar Professor University of Delhi, South Campus	Preparation and Characterization of Thin Films of Conjugated Polymers Suitable for Optoelectronic Devices	Mitsuyoshi Onoda Professor Himeji Institute of Technology	22 Jul.2002- 5 Aug.2002 (15 days)
P.C. Mathur Professor Himeji Institute of Technology	Preparation and Characterization of Thin Films of Conjugated Polymers Suitable for Optoelectronic Devices	Mitsuyoshi Onoda Professor Himeji Institute of Technology	22 Jul.2002- 5 Aug.2002 (15 days)

Project No. 4

Title: Fabrication of Semiconductor Nanocrystals and Their Biosensor Application

Objectives:

- Develop a technique to control deposition of semiconductor nanocrystals with a good control of the size and positioning.
- Explore a potential application of the semiconductor nanocrystals to biosensors.

Project Coordinators:

(Japanese)
Shinji Nozaki
Associate Professor
Department of Electronic Engineering
The University of Electro-Communications

(Indian)
Surendra Nath Sahu
Associate Professor
Indian Institute of Physics

Date of Commencement: 1 April 2002
Date of Completion: 31 March 2005

Accomplishment Status:

(FY2002)

The Japanese team provided the Indian team with several large pieces of ITO (indium tin oxide)-coated glass substrates for their experiments. Professor Sahu and his co-workers electrochemically deposited GaAs nanocrystals on the ITO-coated glass substrates. Mr. Nayak brought some of the samples to Professor Nozaki's lab as the 1st visiting scientist from the Indian team in this project. He stayed from the 21st till the 29th of January in Professor Nozaki's lab at the University of Electro-Communications. During his stay, he measured the electrical characteristics such as I-V and C-V of GaAs nanocrystals on ITO-coated glass substrates and found that the gold or ITO contact to the nanocrystals was not ohmic. As pointed out by Professor Nozaki, the characteristics might not represent those of GaAs nanocrystals but the contacts. He suggested that Mr. Nayak should vary the gold contact size and the thickness of the nanocrystalline film in order to exclude the contribution from the contacts and obtain the electrical characteristics of the GaAs nanocrystalline film. Because of a trouble with the photoluminescence (PL) system in Professor Nozaki's lab, Mr. Nayak was not able to measure PL of the GaAs nanocrystals.

In the fiscal year of 2002, Professor Sahu was a visiting professor at Satellite Venture Business Laboratory of the University of Electro-Communications and proposed a setup of the gas evaporation apparatus with a supersonic jet nozzle in his lab. The apparatus was developed by Professor Nozaki and his co-workers to deposit semiconductor nanocrystals with a good size uniformity. Mr. Nayak is in charge of the setup of the apparatus in Professor Sahu's lab. During his stay, he carefully studied the detailed design of the apparatus and observed the experiments using the apparatus. After his stay, he now understands more the apparatus, and his stay will help him to set up the similar apparatus in the Professor Sahu's lab.

Professor Nozaki made a few pieces of the two-electrode pattern with a narrow gap by e-beam lithography and handed them to Mr. Nayak for deposition of the semiconductor nanocrystal in the gap to study coulomb blockade and single electron tunneling.

In summary, although the 1st visit from the Indian team was short, we were able to have significant discussion on the future plan of experiments.

Future Plan:

- (1) Japanese team will receive the chemically synthesized samples from the Indian team and characterize the optical and electrical properties. Some of the samples are "DNA-treated". The Japanese team will study a difference in the properties with and without the DNA treatment.
- (2) The Indian team will set up the gas-evaporation with a supersonic jet nozzle, and the Japanese team will characterize the size distribution of the nanocrystals by TEM.
- (3) A scholar visits the Indian team of IOP for a week.

A scholar visits the Japanese team of the University of Electro-Communications for a week.

Exchange Visits Undertaken:

FY2002

India to Japan

<u>Name and Affiliation</u>	<u>Research Subject</u>	<u>Main Host</u>	<u>Period</u>
Jhasaketan Nayak	Fabrication of Semiconductor Nanocrystals	Shinji Nozaki	21 Jan.2003-
Phd. Student		Associate Professor	29 Jan.2003
Institute of Physics		The University of	(9 days)
		Electro-Communications	

FY 2003

Project No. 1

Title: Preparation and Characterization of Thin Films of Conjugated Polymers Suitable for Optoelectronic Devices

Project Coordinators:

(Japanese)

Mitsuyoshi Onoda

Professor

Himeji Institute of Technology

(India)

P.K.Batnagar

Professor

University of Delhi, South Campus

List of Members of Research Team

Japanese Members

Name (LAST, First M.)	Mitsuyoshi Onoda	
Affiliation & Position	Position Department University/Institution	Professor Department of Electrical Engineering and Computer Himeji Institute of Technology
Name (LAST, First M.)	Kazuya Tada	
Affiliation & Position	Position Department University/Institution	Research Associate Department of Electrical Engineering and Computer Sciences Himeji Institute of Technology

Indian Members

Name (LAST, First M.)	Bhatnagar, Pramod Kumar	
Affiliation & Position	Position Department University/Institution	Professor Department of Electronic Science University of Delhi, South Campus
Name (LAST, First M.)	Mathur, Paramatma Chandra	
Affiliation & Position	Position Department University/Institution	Professor(now emeritus fellow in department) Department of Electronic Science University of Delhi, South Campus

2. Seminar

FY2001-2002

See attached Report about Asian Science Seminar in “7. Other Activities” for the seminar FY 2001

FY2003

Seminar No.1

Title: Japan-India Seminar on Materials Education, Research and Advanced Materials

Objectives:

Advanced or new materials are quite important for the development of industry. In the twentieth century of the development of new materials supported the industry and peoples life. However, we are facing a new big problem. In the twentieth century, we thought the materials having good physical and chemical properties are the best materials, but we have learned some effects are dangerous to human life. For example, PCB (PolyChloroBiphenyl) has best properties but once it deteriorate environments it is hard to clean it. Once it is taken into human body it affects human health. Organic mercury goes into fish and organic mercury suffer human health. In the twenty first century we have to consider how the products affect human body and environments. Process to produce new materials is also important. These are new problems we are facing in this new century. Up to fairly recently, we thought that the earth is infinite and the resources are infinite and oil or energies are infinite. Now we know these are limited and we have to share them and save them for the future. We have to know the way of solving these problem is also science or industry.

Another point is that young good people are not coming to the materials fields although we know materials field is quite important for the human life. Here at the Japan-India seminar we discuss how we attract young people to study materials field for future development of materials

Fortunately, IUMRS (International Union of Materials Research Societies and the Materials Research Society is having an international Conference on Advanced Materials at Pacifico Yokohama from October 8 to 13, 2003. Many materials experts are gathering to this conference so we have a part of Japan-India Seminar on Materials Education and Research with the IUMRS-ICAM2003 on October 9 and the other part on Advanced Materials is also held at Pacifico Yokohama on October 12. In this way, we can discuss materials experts from the world.

Seminar Coordinators:

(Japanese)

Prof. Masao Doyama

Professor Emeritus

Teikyo University of Science & Technology

(India)

Prof. Pallerama R. Rao

Professor

International Advanced Research Centre for Powder Metallurgy and New Materials

Period: 9-12 October 2003

Place: Japan

Seminar No.2

Title: India-Japan Workshop on Advanced Molecular Electronics and Bionics

Objectives:

The aims of workshop are that active researchers from both countries present and exchange their recent outstanding results on Advanced Molecular Electronics and Bionics and related topics, and to contribute the promotion of science and technology in Asian countries.

The development of science and technology is accelerated in these years, especially electronics and nano-technology. New materials for next generation of the electronic devices are demanded. Organic molecules and bio and biomimetic materials are excellent candidates and have been intensively studied for the future electronics materials. The topics are one of important future technologies, which reduce the energy consume and environmental pollution, and develop bio based devices to perform the high efficient energy conversion as well as bio mimetic sensing and information processing.

Seminar Coordinators:

(Japanese)

Prof. Kenichi Kaneto

Professor

Kyushu institute of Technology

(India)

Dr. Bansi D. Malhotra

Scientist E II

National Physical Laboratory

Period: 11-13 December 2003

Place: Japan

3. Visiting Scientists for Information Exchange

FY2001

Japan to India

<u>Name and Affiliation</u>	<u>Research Subject</u>	<u>Main Host</u>	<u>Period</u>
Mitsumasa Iwamoto Professor Tokyo Institute of Technology	Asian Science Seminar	Dr.P. Rama Rao Vice-Chancellor University of Hyderabad	9 Dec..2001- 17 Dec..2001 (9 days)
Mitsuyoshi Onoda Professor Himeji Institute of Technology	Asian Science Seminar	Dr.P. Rama Rao Vice-Chancellor University of Hyderabad	9 Dec..2001- 17 Dec..2001 (9 days)
Keiichi Kaneto Professor Kyushu Institute of Technology	Asian Science Seminar	Dr.P. Rama Rao Vice-Chancellor University of Hyderabad	9 Dec..2001- 17 Dec..2001 (9 days)
Tamio Endo Associate Professor Mie University	Asian Science Seminar	Dr.P. Rama Rao Vice-Chancellor University of Hyderabad	11 Dec.2001- 28 Dec..2001 (18 days)

India to Japan

<u>Name and Affiliation</u>	<u>Research Subject</u>	<u>Main Host</u>	<u>Period</u>
Shreekari Tantry	A study on High Temperature Mechanical	Toyohiko Yano	1 Jul..2001-
Professor	Properties of Mosi2 Based Materials	Associate Professor	12 Aug..2001
National		Tokyo Institute of	(43 days)
Aerospace		Technology	
Laboratories			
