

Program

Innovative Nanoscale Approach to Dynamic Studies of Materials

9 - 14 January 2006
Okinawa, Japan

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Japan Atomic Energy Research Institute, Japan

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Monday, January 9, 2006

16:00 – 18:00	Registration (<i>Laguna Garden Hotel Okinawa</i>)
18:00 - 19:00	Welcome reception (<i>Laguna Garden Hotel Okinawa</i>)
19:00	Dinner (<i>Laguna Garden Hotel Okinawa</i>)

NOTES FOR CONFERENCE PARTICIPANTS

Participants should observe no smoking at ECI technical and social events.

During technical sessions please keep cell phones on vibrate or shut off. Take any telephone conversations out of the session room.

Presenters should leave time at the end of their talks for discussion.

Tuesday, January 10, 2006

08:00 – 09:00	Breakfast
09:30	Ceremonial Session & Opening Lecture [<i>Okinawa Convention Center</i>]
09:30 – 09:40	Greeting from the Chair (Masatoshi Arai)
09:40 – 10:40	Opening Lecture (Chairperson: Nghi Q. Lam) Akira Tonomura, Hitachi, Ltd., RIKEN, OIST, Japan THE QUANTUM WORLD UNVEILED BY ELECTRON WAVES
10:40 – 11:00	Coffee Break
11:00	<u>Session I: Slow dynamics of soft matter, glass transition and nonlinear dynamics</u> Session Chairs: Toshiji Kanaya, Marie-Louise Saboungi
11:00 – 11:50	Invited Talk C. Austen Angell, Arizona State University, USA COOPERATIVE PROCESSES: NEARLY IDEAL GLASS TRANSITIONS, LIQUID-LIQUID TRANSITIONS, AND FOLDING TRANSITIONS, AND ENERGY LANDSCAPE DISTINCTIONS
11:50 – 12:30	Invited Talk Michio Tokuyama, Tohoku University, Japan MEAN-FIELD THEORY OF GLASS TRANSITIONS
12:30 – 14:00	Lunch
14:00 – 16:30	<i>ad hoc</i> discussions / Free time
16:30 – 17:30	Keynote Lecture H. W. Spiess, Max Planck Institute for Polymer Research, Germany DYNAMICS IN NANOSTRUCTURED MATERIALS PROBED BY NMR SPECTROSCOPY
17:30 – 18:10	Invited Talk B. X. Liu, Tsinghua University, China MULTISCALE MODELING OF CRYSTAL-TO-AMORPHOUS TRANSITION IN THE EQUILIBRIUM MISCIBLE/IMMISCIBLE BINARY METAL
18:10 – 18:30	Coffee Break

Tuesday, January 10, 2006 (continued)

- 18:30 – 18:55 Invited Talk
Junji Saida, Tohoku University, Japan
LOCAL STRUCTURE STUDY IN Zr-BASED METALLIC GLASSES
- 20:00 Dinner

Wednesday, January 11, 2006

- 07:00 – 08:30 Breakfast
- 09:00 **Session II: Constrained water and liquids**
Session Chairs: Shuit-Tong Lee, Michio Tokuyama
- 09:00 - 09:50 Keynote lecture
Nick Quirke, Imperial College, UK
DYNAMICS OF FLUIDS INTERACTING WITH NANOTUBES
- 09:50 – 10:30 Invited Talk
Yoshio Bando, NIMS, Japan
DYNAMIC BEHAVIOR OF LIQUID GALLIUM IN NANOTUBES AS
NANOTHERMOMETER
- 10:30 – 10:55 Alexander Kolesnikov, IPNS, Argonne National Laboratory, USA
WATER IN CARBON NANOTUBES: NEUTRON SPECTROSCOPY
AND MD SIMULATIONS
- 10:55 – 11:20 Coffee Break
- 11:20 – 12:00 Invited Talk
Iwao Ohmine, Nagoya University, Japan
WATER DYNAMICS: POTENTIAL ENERGY LANDSCAPE AND
FLUCTUATION
- 12:00 – 12:25 Chung-Yuan Mou, National Taiwan University
FRAGILE-TO-STRONG TRANSITION TEMPERATURE IN
DEEPLY SUPERCOOLED CONFINED WATER
- 12:25 – 12:50 Esko I. Kauppinen, Helsinki University of Technology, Finland
NOVEL HYBRID NANOMATERIAL:
FULLERENE-FUNCTIONALISED CARBON NANOTUBES
- 13:00 – 14:00 Lunch

Wednesday, January 11, 2006 (continued)

14:30 – 16:30

Poster Session

Session Chairs: Haruo Niki, Seiichi Watanabe

[P-1] *AB-INITIO* STUDY OF HYPERFINE PARAMETERS USING ALL ELECTRON MIXED-BASIS METHOD:
AN APPROACH TO FIND OUT THE SPIN POLARIZATION MECHANISM OF CORE LEVELS

Mohammad Saeed Bahramy, Institute for Materials Research (IMR), Tohoku University, Japan

[P-2] DYNAMICS OF AMORPHOUS TRANSITION OF GRAPHITE UNDER IRRADIATION

Keisuke Niwase, Hyogo University of Teacher Education, Japan

[P-3] HIGHLY GRAPHITIZED GIANT CARBON HOLLOW SPHERES GENERATED FROM C₆₀ FULLERENE
BY SHOCK COMPRESSION

K. Niwase, Hyogo University of Teacher Education, Japan

[P-4] ATOMIC-SCALE STRUCTURE OF POLYMORPH FeOOH

S. Suzuki, Tohoku University, IMRAM, Japan

[P-5] PHASE-FIELD SIMULATION OF SELF-ASSEMBLY OF FACETED SiGe/Si QUANTUM DOTS

Tomohiro Takaki, Kobe University, Japan

[P-6] MOLECULAR DYNAMICS SIMULATION ON DEFORMATION BEHAVIOR OF CRYSTAL/AMORPHOUS
POLYETHYLENE UNDER NANOINDENTATION

Kisaragi Yashiro, Kobe University

[P-7] SPATIAL DISTRIBUTION CONTROL OF GOLD NANO PARTICLES SUPPORTED BY NANOPOROUS
SURFACES

Masafumi Tsunekane, Graduate Student, Dept. of Environmental Studies, Tohoku University, Japan

[P-8] PREPARATION OF SELF-ALIGNED FE NANOPARTICLES FOR SPIN-DEPENDENT TRANSPORT
MEASUREMENTS

Franck ERNULT, Institute for Materials Research, Japan

[P-9] ULTRA FINE-GRAINED FE-32%NI ALLOY PRODUCED BY SEVERE PLASTIC DEFORMATION AT
LOW TEMPERATURE

Baojun Han, Key Laboratory for High Temperature Materials and Tests of Ministry of Education,
Shanghai Jiaotong University, China

[P-10] POINT DEFECTS FORMATION AND NANO-STRUCTURE IN FAR-FROM-EQUILIBRIUM SYSTEMS

Kosuke Nishikawa, Hokkaido University, Japan

[P-11] DIRECT PYROLYTIC DECOMPOSITION OF WATER MOLECULE INDUCED BY PLASMA
ELECTROLYSIS

Yu Toriyabe, Division of Quantum Science and Engineering, Graduate School of Engineering, Hokkaido
University, Japan

Wednesday, January 11, 2006 (continued)

[P-12] LOCAL STRUCTURE OF FERRIC OXIDES CONVERTED FROM $\text{Fe}(\text{OH})_3$ GEL
Shigeru Suzuki, Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Japan

[P-13] DIELECTRIC CONSTANT OF NANOPOROUS MATERIAL FILLED WITH LIQUID AND APPLICATION TO POROSIMETRY
Insuk Yu, School of Physics and Nano-Systems Institute (NSI-NCRC), Seoul National University, Korea

[P-14] KINETICS OF ORDERED DOMAIN FORMATION AND COARSENING IN BINARY ALLOYS OF $L1_2$ TYPE ORDER
Ryuichiro Oguma, Department of Applied Physics, Fukuoka University, Japan

[P-15] NMR STUDIES OF INTERMETALLIC COMPOUND ERCO_3
Haruo Niki, Department of Physics, Faculty of Science, University of the Ryukyus, Japan

[P-16] CHARACTERIZATION OF SILVER-SATURATED Ge-Te CHALCOGENIDE THIN FILMS FOR NONVOLATILE RANDOM ACCESS MEMORY
Soon-Gil Yoon, Chungnam National University, Korea

[P-17] MAGNETOTRANSPORT PROPERTIES OF ANNEALED AMORPHOUS $\text{Ge}_{0.97}\text{Mn}_{0.03}$ SEMICONDUCTOR THIN FILMS
Sang Soo Yu, Chungnam National University, Korea

[P-18] STRUCTURE AND DYNAMICS OF A FORSTERITE COMPOSITION GLASS
Kentaro Suzuya, Japan Atomic Energy Agency, Japan

[P-19] MULTISCALE MODELING OF DENDRITE PATTERN FORMATION DURING SOLIDIFICATION
Kenichi Ohsasa, Hokkaido University, Japan

[P-20] LOW-ENERGY DYNAMICS OF TYPICAL NETWORK GLASS AND SUPERIONIC CONDUCTING GLASS
Mitsutaka Nakamura, Japan Atomic Energy Agency, Japan

[P-21] MAGNETIC PROPERTIES OF MBE-GROWN $\text{Si}_{1-x}\text{Mn}_x$ EPILAYERS
Tran Thi Lan Anh, Chungnam National University, Korea

[P-22] NANOSCALE STRUCTURE AND DYNAMICS OF POLY (VINYL ALCOHOL) GELS
Nabuaki Takahashi, Japan Atomic Energy Agency, Japan

Thursday, January 12, 2006

07:00 – 08:30	Breakfast
09:00	<u>Session IV: Quantum effect and nanomaterials</u> Session Chairs: Akira Suzuki, Jongbae Hong
09:00 – 09:50	Keynote Lecture Miki Wadati, University of Tokyo, Japan BOSE-EINSTEIN CONDENSATION OF ULTRACOLD NEUTRAL ATOMS
09:50 – 10:20	Coffee Break
10:20 – 11:00	Invited Talk S. S. Saxena, University of Cambridge, UK SUPERCONDUCTIVITY NEAR A QUANTUM CRITICAL POINT AND BEYOND
11:00 – 11:40	Invited Talk Nguyen Van Lien, Vietnamese Academy of Science and Technology, Vietnam SHOT NOISE IN COULOMB BLOCKADE DOUBLE METALLIC QUANTUM DOT DEVICES
12:00 – 12:50	Lunch
13:00	Excursion
20:00	Traditional Dinner

Friday, January 13, 2006

- 07:00 – 08:30 Breakfast
- 09:00 **Session V: Nanomaterials and nanodynamics**
Session Chairs: Robert Sinclair, Toyohiko Konno
- 09:00 – 09:40 Invited Talk
F. J. Bermejo, University of Basque Country, Spain
NANOMETER-SIZED DYNAMIC CORRELATIONS IN DISORDERED MATTER
- 09:40 – 10:20 Invited Talk
Masahiro Kitajima, NIMS, Japan
FEMTOSECOND DYNAMICS IN MATERIALS BY MEANS OF LASER PULSE
- 10:20 – 10:45 K. Cho, Stanford University, USA
MULTISCALE MODELING OF SILICON NANOWIRES
- 10:45 – 11:10 Coffee Break
- 11:10 – 11:50 Invited Talk
Robert Sinclair, Stanford University, USA
IN SITU HIGH-RESOLUTION ELECTRON MICROSCOPY OF MATERIALS
- 11:50 – 12:30 Invited Talk
S.T. Lee, City University of Hong Kong, China
CHEMICAL, BIOSENSING AND PHOTOCONDUCTIVE PROPERTIES OF SEMICONDUCTOR NANOWIRES
- 12:30 – 12:55 Jens-Boie Suck, University of Technology Chemnitz, Germany
ATOMIC DYNAMICS OF NANOCRYSTALLINE MATERIALS PRIOR AND AFTER GRAIN BOUNDARY RELAXATION
- 13:00 – 14:00 Lunch
- 14:00 – 16:30 *ad hoc* discussions / Free time
- 16:30 **Session VI: Biomolecule dynamics**
Session Chairs: Tomohisa Ogawa, Douglas Tobias
- 16:30 - 17:20 Keynote Lecture
Douglas Tobias, University of California, Irvine, USA
STRUCTURE AND DYNAMICS AT BIOMOLECULAR INTERFACES

Friday, January 13, 2006

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| 17:20 – 18:00 | Invited Talk
Carolyn Larabell, University of California, San Francisco, USA
X-RAY NANOTOMOGRAPHY OF BIOLOGICAL CELLS |
| 18:00 – 18:20 | Coffee Break |
| 18:20 – 19:00 | Invited Talk
Marie-Louise Saboungi. UMR CNRS-Université d'Orléans,
France
DYNAMICS OF NANOCOMPOSITES: FROM POLYMERS TO
BIOMATERIALS |
| 19:00 – 19:25 | Tomohisa Ogawa, Tohoku University, Japan
MICROSTRUCTURE OF ARAGONITE CRYSTALS AND PROTEINS
IN BIOMINERALIZATION MECHANISMS OF PTERIA PENGUIN
NACRE |
| 20:00 | Conference Banquet |

Saturday, January 14, 2006

07:00 – 08:00	Breakfast
09:00	<u>Session VII: Nanopatterning and self-organization in nonequilibrium open systems</u> Session Chairs: Nicolas Quirke, Kyosuke Yoshimi, Michel Van Hove
09:00 - 09:40	Invited Talk Michel Van Hove, City University of Hong Kong, Hong Kong SAR MONTE CARLO SIMULATIONS OF SURFACE SEGREGATION IN BIMETALLIC CATALYST NANOPARTICLES
09:40 – 10:05	Kyosuke Yoshimi, Tohoku University, Japan NANOSCALED SURFACE SELF-PATTERNING IN B2-TYPE INTERMETALLICS BY VACANCY ENGINEERING
10:05 - 10:20	Coffee Break
10:20 - 10:45	Jongbae Hong, Seoul National University, Korea A NONPERTURBATIVE DYNAMICAL THEORY FOR NONEQUILIBRIUM TRANSPORT
10:45 - 11:10	K. Niwase, Hyogo University of Teacher Education, Japan SELF-ORGANIZED NANOPATTERN APPEARED ON METAL SURFACES UNDER LOW-TEMPERATURE ELECTRON IRRADIATION
11:10 – 11:25	Break
11:25 – 11:50	M. Kohyama, National Institute of Advanced Industrial Science and Technology, Japan FIRST-PRINCIPLES STUDY OF THE ADHESIVE AND MECHANICAL PROPERTIES OF MATERIALS INTERFACES
11:50 - 12:15	Hideo Kaburaki, Japan Atomic Energy Agency MESOSCALE APPROACHES TO THE SIMULATION OF THE MICROSTRUCTURE FORMATION OBSERVED AT HIGH-BURNUP UO ₂ FUEL
13:00	Closing remarks and departure