

Program

Nonstoichiometric Compounds

**March 8-13, 2009
Jeju Island, Korea**

Conference Chairs

Professor Han-III Yoo
Seoul National University, Korea

Professor Shu Yamaguchi
The University of Tokyo, Japan

Professor Juergen Janek
Justus-Liebig-University, Germany

Professor Sossina M. Haile
California Institute of Technology, U.S.A.



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Sunday, March 8, 2009

16:00 - 18:00	Registration
18:00 – 20:00	Welcome Party/Dinner

NOTES

- Audiotaping, videotaping and photography of presentations are strictly prohibited.
- Speakers – Please leave at least 5 minutes for questions and discussion.
- Please do not smoke at any conference functions.
- Turn your cellular telephones to vibrate or off during technical sessions.
- Wednesday dinner is on your own. A list of restaurants in the area will be provided.
- Wednesday's excursion is optional. Information will be at the registration desk.
- Be sure to make any corrections to your name/contact information on the Master Participant List or confirm that the listing is correct. A corrected copy will be sent to all participants after the conference.

Monday, March 9, 2009

07:30 – 08:20 Breakfast

08:20 – 08:30 **Opening Remarks**

Session I: Basics/Defects/ Defect Driven Phenomena

Session Chairs: S. Yamaguchi & X. Guo

08:30 - 09:00 DEFECT INTERACTIONS IN SrTiO₃ IN THE TEMPERATURE RANGE OF 25^o TO 250^o C

Xin Guo, Institute of Solid State Research, Research Jülich, Germany

09:00 - 09:20 THE OXYGEN RELEASE BEHAVIOR OF CaF₂-TYPE (Pr_{0.75}ZrR_{0.25})O_{2-γ} PHASE WITH WIDE OXYGEN NONSTOICHIOMETRY

Shinya Otsuka-Yao-Matsuo, Osaka University, Japan

09:20 - 09:40 DEFECT STRUCTURE AND DEFECT-INDUCED EXPANSION OF ADVANCED OXIDE MATERIALS

Zuev Andrey, Ural State University, Russia

09:40 - 10:00 DEFECT MODEL OF LIQUID APPLIED TO IONIC CONDUCTIVITY OF GLASS

Junichi Kawamura, IMRAM, Tohoku University, Japan

10:00 - 10:20 DISORDER, LATTICE DYNAMICS AND IONIC CONDUCTION IN SUPERIONIC COPPER CHALCOGENIDES

Sergey A. Danilkin, ANSTO, Australia

10:20 - 10:50 Coffee break

10:50 - 11:20 ON THE ORIGIN OF ANOMALOUS V_{TH} SHIFT IN HIGH-K MOSFETS

Akira Toriumi, The University of Tokyo, Japan

11:20 - 11:40 DIRECT OBSERVATION OF REVERSIBLE OXIDATION AND REDUCTION AT BURIED OXIDE/METAL INTERFACES

Andreas Klein, Technical University Darmstadt, Germany

11:40 - 12:00 STRUCTURAL FEATURES OF BaTiO₃ NANO-POWDERS AND NANO-GRAINED CERAMICS

Nam-Hee Cho, Inha University, Korea

12:00 - 12:20 DEFECT COMPLEX AND DIELECTRIC PROPERTIES OF ACCEPTOR AND MNO-DOPED BaTiO₃

Young Ho Han, Sungkyunkwan University, Korea

12:20 - 14:00 Lunch

Session II: Ferroelectrics

Session Chairs: H-I. Yoo & P. McIntyre

14:00 - 14:30 THE DEVELOPMENT TREND IN BME-MLCC : MATERIAL ASPECTS

Kang-Heon Hur, Samsung Electro-Mechanics Co., Korea

14:30 - 14:50 DIFFUSION PROCESSES IN MULTI-LAYER CERAMIC CAPACITORS

Markus Kessel, Institute of Physical Chemistry, RWTH Aachen University, Germany

Monday, March 9, 2009 (continued)

- 14:50 – 15:10 STUDY ON THE EFFECTS OF BaTi₄O₉ CONTENT ON RELATIVE PERMITTIVITY OF POLYETHERIMIDE/BaTi₄O₉ COMPOSITE
Chia-Ching Wu, National Sun Yat-Sen University, Taiwan
- 15:10 - 15:30 ROLE OF ELECTRON EMISSION FROM THE RARE-EARTH METAL OXIDES IN DISPLAY DEVICE
Ki-Woong Whang, Seoul National University, Korea
- 15:30 – 16:00 Coffee break
- 16:00 – 16:30 BULK AND INTERFACIAL OXYGEN DEFECTS IN HAFNIA DIELECTRIC STACKS: A CRITICAL ASSESSMENT
Paul C. McIntyre, Stanford University, USA
- 16:30 – 16:50 ATOMIC-RESOLUTION STRUCTURAL ANALYSIS OF LA_{2/3-x}LI_{3x}TiO₃ BY HIGH RESOLUTION ELECTRON MICROSCOPY
Takao Tsurui, Tohoku University, Japan
- 16:50 - 17:10 TRANSMISSION ELECTRON MICROSCOPY STUDY OF AN ELECTRON-BEAM-INDUCED ORDER TO DISORDER TRANSFORMATION OF NONSTOICHIOMETRIC NIOBIUM NITRIDE
Jonghan Won, Los Alamos National Laboratory, USA
- 17:10 – 18:00 **Poster Session I**
- 18:00 – 19:30 Dinner
- 19:30 – 20:30 **Poster Session I (continued) and Social Hour**

Tuesday, March 10, 2009

07:30 – 08:30 Breakfast

Session III: Thermoelectric, Energy Conversion/Storage

Session Chairs: K. Koumoto & M. Schroeder

- 08:30 - 09:00 NANOSTRUCTURED STRONTIUM TITANATE-BASED OXIDES FOR THERMOELECTRICS
Kunihito Koumoto, Nagoya University, Japan
- 09:00 - 09:20 THERMOELECTRIC PROPERTIES OF NONSTOICHIOMETRIC CHALCOGENIDE COMPOUNDS: THEORETICAL AND EXPERIMENTAL STUDIES
Min Wook Oh, Korea Electrotechnology Research Institute, Korea
- 09:20 - 09:40 COPPER INDIUM DISELENIDE AND DISULFIDE SEMICONDUCTOR NANOCRYSTALS; SYNTHESSES AND THEIR DEFECT RELATED OPTICAL PROPERTIES
Takahisa Omata, Osaka University, Japan
- 09:40- 10:00 NANO-ORDERED BACK CONTACT IN THIN-FILM SOLAR CELLS
A. Khodin, Korea Institute of Science and Technology, Korea
- 10:00 - 10:20 WORK FUNCTIONS OF TRANSPARENT CONDUCTING OXIDES
Andreas Klein, Technical University Darmstadt, Germany
- 10:20 - 10:50 Coffee break
- 10:50 - 11:20 KEY PROPERTIES OF INORGANIC MEMBRANES FOR PARTIAL OXIDATION AND ENERGY CONVERSION PROCESSES
Michael Schroeder, RWTH Aachen University, Germany
- 11:20 - 11:40 DISORDER AND DIFFUSION IN VARIOUSLY DOPED MAYENITES
Hans Boysen, LMU, Germany
- 11:40 - 12:00 CHEMICAL ROUTE FROM A SOLID ELECTROLYTE TO AN ELECTRIDE - DEFECT CHEMISTRY OF MAYENITE ($C_{12}A_7$)
D. K. Lee, Justus-Liebig-University Giessen, Germany
- 12:00 - 12:20 DEFECT STRUCTURE AND TRANSPORT PROPERTIES OF MG-Y-BASED HYDRIDES PREPARED UNDER HIGH PRESSURE
Hitoshi Takamura, Tohoku University, Japan
- 12:20 - 14:00 Lunch
- Session IV: Wuensch Symposium**
Session Chairs: Sossina Haile & Manfred Martin
- 14:00 - 14:30 A CHEMICALLY DRIVEN INSULATOR-METAL TRANSITION IN AMORPHOUS AND NON-STOICHIOMETRIC GALLIUM OXIDE
Manfred Martin, RWTH Aachen University, Germany
- 14:30 - 15:00 DISCOVERY AND PROGRESS OF IRON-BASED SUPERCONDUCTORS
Hideo Hosono, Tokyo Institute of Technology, Japan
- 15:00 - 15:30 LOW-TEMPERATURE PROTONIC CONDUCTION IN NANOCRYSTALLINE FLUORITE-STRUCTURED OXIDES: CONDUCTION MECHANISM
Sangtae Kim, University of California, Davis, USA

Tuesday, March 10, 2009 (continued)

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| 15:30 - 16:00 | Coffee break |
| 16:00 - 16:30 | THE NANO-GRAIN COMPOSITE MODEL (N-GCM): AN ALTERNATIVE TO THE BRICK LAYER MODEL FOR ANALYZING NANOCERAMICS
Thomas O. Mason, Northwestern University, USA |
| 16:30 - 17:10 | CRYSTAL CHEMISTRY AND STRUCTURE FOR ANION-DEFICIENT FLUORITE PHASES
Bernhardt J. Wuensch, Massachusetts Institute of Technology, USA |
| 17:10 - 18:00 | Poster Session II |
| 18:00 - 19:30 | Dinner |
| 19:30 - 20:30 | Poster Session II (continued) and Social Hour |

Wednesday, March 11, 2009

07:30 - 08:30 Breakfast

Session V: Magnetic Materials

Session Chairs: W. Bensch & K.-D. Becker

08:30 - 09:00 THE DEVELOPMENT OF A-SITE ORDERED MANGANITES UTILIZING OXYGEN NONSTOICHIOMETRY
Yutaka Ueda, University of Tokyo, Japan

09:00 - 09:20 NONSTOICHIOMETRY AND PHYSICAL PROPERTIES OF δ -PHASE $\text{Ag}_x\text{V}_2\text{O}_5$ ($0.65 < X < 0.90$)
Masahiko Isobe, University of Tokyo, Japan

09:20 - 09:40 STRUCTURE ANALYSIS OF COBALT OXIDE SUPERCONDUCTORS BASED ON COMPOSITE CRYSTAL MODELS
Kazunori Takada, National Institute for Materials Science, Japan

09:40 - 10:00 DEFECT-CHEMICAL PROPERTIES AND ELECTRONIC STRUCTURE OF DOPED BaPrO_3
Shogo Miyoshi, The University of Tokyo, Japan

10:00 - 10:20 AVERAGE AND LOCAL STRUCTURE INVESTIGATION OF ION CONDUCTORS BY MEANS OF TOTAL NEUTRON SCATTERING
Lorenzo Malavasi, University of Pavia, Italy

10:20 - 10:50 Coffee break

10:50 - 11:20 A HIGH-TEMPERATURE MÖSSBAUER STUDY INTO THE STRUCTURE, DISORDER, AND FORMATION KINETICS OF IRON NITRIDES
Klaus Becker, Technical University Braunschweig, Germany

11:20 - 11:40 SURFACE MODIFICATION OF $(\text{La},\text{Sr})\text{CoO}_3$ FOR HIGH PERFORMANCE SOFC CATHODE
Koji Amezawa, Tohoku University, Japan

11:40 - 12:00 MICROSTRUCTURAL EVOLUTION IN PEROVSKITES BY OXYGEN PARTIAL PRESSURE CHANGE AND DONOR DOPING
Suk-Joong L. Kang, KAIST, Korea

12:00 - 14:00 Lunch

14:00 Excursion (optional)

Dinner on your own

Thursday, March 12, 2009

07:30 – 08:30

Breakfast

Session VI: Mixed Conductors

Session Chairs: H. Tuller & J. Mizusaki

08:30 - 09:00

INVESTIGATION OF CATHODE BEHAVIOR OF MODEL THIN FILM $\text{SrTi}_{1-x}\text{Fe}_x\text{O}_{3-\delta}$
MIXED IONIC-ELECTRONIC CONDUCTING ELECTRODES AND CORRELATION
WITH DEFECT PROPERTIES

Harry Tuller, Massachusetts Institute of Technology, USA

09:00 - 09:20

OXIDATION STATES OF THE TRANSITION METAL CATIONS IN THE HIGHLY
NONSTOICHIOMETRIC PEROVSKITE-TYPE OXIDE $\text{Ba}_{0.1}\text{Sr}_{0.9}\text{Co}_{0.8}\text{Fe}_{0.2}\text{O}_{3-\text{DELTA}}$

David N. Mueller, RWTH Aachen, Germany

09:20 - 09:40

DEFECT STRUCTURE AND RELATED PROPERTIES OF DOUBLE PEROVSKITE
 $\text{GdBaCo}_2\text{O}_{5.5\pm\delta}$

Dmitry Tsvetkov, Ural State University, Russia

09:40 - 10:00

OXYGEN NONSTOICHIOMETRY IN MIXED CONDUCTORS FROM
ELECTROCHEMICAL IMPEDANCE SPECTROSCOPY IN A THIN FILM GEOMETRY

Sossina M. Haile, California Institute of Technology, USA

10:00 - 10:20

ANALYSIS OF STRUCTURAL PHASE TRANSITION OF $\text{BaCe}_{1-x}\text{Y}_x\text{O}_{3-f\text{A}}$ BY
THERMAL ANALYSES AND X-RAY DIFFRACTION AT HIGH TEMPERATURES

Takuya Hashimoto, Nihon University, Japan

10:20 - 10:50

Coffee break

10:50 - 11:20

B-SITE CATION MIXING EFFECTS ON CHEMICAL STABILITY AND DEFECT
EQUILIBRIUM OF LaCrO_3 BASED PEROVSKITE-TYPE OXIDE ELECTRONIC
CONDUCTORS

Junichiro Mizusaki, Tohoku University, Japan

11:20 - 11:40

PHASE STABILITY AND PROTON CONDUCTIVITY OF BARIUM CERATES DOPED
BY TRIVALENT CATIONS HAVING DIFFERENT IONIC RADII

Byung-Kook Kim, Korea Institute of Science and Technology, Korea

11:40 - 12:00

OXYGEN TRANSPORT KINETICS IN PBCF DOUBLE PEROVSKITE MEMBRANE

Ji Haeng Yu, Korea Institute of Energy Research, Korea

12:00 - 12:20

MONITORING OF CHEMICAL POTENTIAL OF OXYGEN ON THE SURFACE OF
GROWING OXIDE SCALES IN HIGH TEMPERATURE OXIDATION OF METALS AND
ALLOYS

Toshio Maruyama, Tokyo Institute of Technology, Japan

12:20 - 14:00

Lunch

Session VII: Interface/Composite/Nanosize Effects

Session Chairs: S-T. Kim & R. A. De Souza

14:00 - 14:30

STRUCTURE-PROPERTY RELATIONSHIPS FOR TILT GRAIN BOUNDARIES IN
STRONTIUM TITANATE

Roger A. De Souza, RWTH Aachen University, Germany

Thursday, March 12, 2009 (continued)

- 14:30 - 14:50 ELASTIC STRAIN IN INTERFACES AND ITS INFLUENCE ON THE INTERFACIAL IONIC TRANSPORT – EXPERIMENTAL STUDIES AND FORMAL CONSIDERATIONS
Nicole Schichtel, Justus-Liebig-Universität Gießen, Germany
- 14:50 - 15:10 NANOSCALE CONTROL OF ELECTRODE MATERIALS FOR LI-ION BATTERY AND FUEL CELL
Byungwoo Park, Seoul National University, Korea
- 15:10 - 15:30 OXYGEN PERMEATION PROPERTIES OF GDBACO₂O_{5+δ}-CE_{0.8}GD_{0.2}O₂ COMPOSITE MEMBRANE
Sun-Ju Song, Chonnam National University, Korea
- 15:30 – 16:00 Coffee break
- 16:00 – 16:30 STOICHIOMETRY AND PROPERTIES OF COMPLEX OXIDE THIN FILMS
Susanne Stemmer, University of California, Santa Barbara, USA
- 16:30 – 16:50 RELATIONSHIP BETWEEN STRUCTURAL AND ELECTRICAL PROPERTIES ON PROTON CONDUCTING BaZrO₃ THIN FILM
Hiroo Yugami, Tohoku University, Japan
- 16:50 - 17:10 A COMPREHENSIVE ELECTRICAL CHARACTERIZATION OF ACCEPTOR DOPED BaTiO₃ IN QUENCHED STATE
Jong-Sook Lee, Chonnam National University, Korea
- 17:10 – 17:50 Poster Discussion
- 18:30 – 20:30 Conference Banquet

Friday, March 13, 2009

- 07:30 – 08:30 Breakfast
- Session VIII: Solid State Devices**
Session Chairs: T. Hasegawa & J. Janek
- 08:30 - 09:00 THREE-TERMINAL ATOMIC SWITCH USING Ta₂O₅
Tsuyoshi Hasegawa, National Institute for Materials Science, Japan
- 09:00 - 09:20 NONSTOICHIOMETRIC OXIDES AND THEIR APPLICATION TO RESISTIVE
SWITCHING MEMORY DEVICES
Jinha Hwang, Hongik University, Korea
- 09:20 - 09:40 CONTROL OF LOCAL ION TRANSPORT TO DEVELOP UNIQUE FUNCTIONAL
NANOIONICS DEVICES
Kazuya Terabe, National Institute for Materials Science, Japan
- 09:40- 10:00 MIXED CONDUCTING SILVER(I) POLYCHALCOGENIDE HALIDES, COMPOUNDS
WITH UNEXPECTED SWITCHING PROPERTIES
Tom Nilges, University of Muenster, Germany
- 10:00 - 10:20 AB INITIO STUDY ON THE ELECTRONIC CONDUCTION PATHS IN SOLID
ELECTROLYTE ATOMIC SWITCHES
Satoshi Watanabe, The University of Tokyo, Japan
- 10:20 - 10:50 Coffee break
- 10:50 - 11:20 DEFECT CHEMISTRY AND TRANSPORT PROPERTIES OF NITROGEN-DOPED
YSZ
Juergen Janek, Justus-Liebig-University Giessen, Germany
- 11:20 – 11:40 FABRICATION AND CHARACTERIZATION OF THE NANO-STRUCTURED THIN
FILM ELECTROLYTE
Jong-Ho Lee, Korea Institute of Science and Technology, Korea
- 11:40 - 12:00 THERMAL ATOMIC OXYGEN EMISSION FROM ZIRCONIA
Katsuro Hayashi, Tokyo Institute of Technology, Japan
- 12:00 – 12:10 Closing Remarks
- 12:15 Lunch and Departures

LIST OF POSTER PRESENTATIONS

Poster Session 1 (Monday)

<01> REDOX REACTION AND ELECTROCHEMICAL CHARACTERISTIC OF PT-(CE,GD)O₂ MIXED SYSTEM
Kenji Yoshimura, Department of Materials Engineering The University of Tokyo, Japan

<03> IONIC/ELECTRONIC TRANSPORT PROPERTIES AND DEFECT/ELECTRONIC STRUCTURE OF Ba(Zr,Pr)O₃
Mao Tamaru, Department of Materials Engineering, The University of Tokyo, Japan

<05> CONCENTRATION-DEPENDENT DIFFUSION OF DONORS IN ZINC OXIDE
Tsubasa Nakagawa, National Institute for Materials Science, Japan

<07> ELECTROCHEMICAL PROPERTIES OF ELECTRODE-SUPPORTED La_{0.75}Sr_{0.25}Ga_{0.8}Mg_{0.16}Fe_{0.04}O_{3-D} SOLID OXIDE FUEL CELLS
Ji Haeng Yu, Korea Institute of Energy Research, Korea

<09> QUANTITATIVE ESTIMATION OF VOLUME FRACTION OF VOID AT METAL/SCALE INTERFACE AND AT THE INTERFACE OF DUPLEX SCALE FORMED DURING HIGH TEMPERATURE OXIDATION OF METALS AND ALLOY
Mitsutoshi Ueda, Tokyo Institute of Technology, Japan

<11> TRANSPORT PROPERTIES OF La_{0.1}Sr_{0.9}Co_{0.8}Fe_{0.2}O_{3-δ} MEMBRANE
Moon-Bong Choi, Alternative Energy Materials Research Laboratory, School of Materials Science and Engineering, Chonnam National University, Korea

<13> ELECTRICAL PROPERTY OF BaCe_{0.85}XZrY_{0.15}O_{3-δ} (0 ≤ X ≤ 0.85) PROTON-CONDUCTORS
Cheol-Jae Park, Alternative Energy Materials Research Laboratory, School of Materials Science and Engineering Chonnam National University, Korea

<15> FIRST PRINCIPLES SIMULATION OF STOICHIOMETRY AND INTERFACE/SURFACE EFFECTS ON IONIC CONDUCTIVITY OF YTTRIA-STABILIZED ZIRCONIA
Shusuke Kasamatsu, Department of Materials Engineering, The University of Tokyo, Japan

<17> PREPARATION AND CHARACTERIZATION OF COMPLEX OXIDES FOR WATER PHOTOLYSIS
Eui-Chol Shin, Chonnam National University, Korea

<19> SYNTHESIS AND STRUCTURE OF NONSTOICHIOMETRIC COMPOUND V₄O₉ AS A MISSING LINK OF WADSWORTH PHASES
Satoshi Yamazaki, Institute for Solid State Physics, University of Tokyo, Japan

<21> EFFECT OF OXYGEN NON-STOICHIOMETRY ON THE MAGNETIC PROPERTIES OF TiO₂ THIN FILMS
Lorenzo Malavasi, University of Pavia, Italy

<23> NANOSTRUCTURED/AMORPHOUS FILMS - BASED HIGH-MELTING POINT NONSTOICHIOMETRIC COMPOUNDS
Rostislav A. Andrievskiy, Institute of Problems of Chemical Physics, Russian Academy of Sciences, Russia

Poster Session 2 (Tuesday)

<02> LOCAL STRUCTURE AND SIZE-DEPENDENT PROPERTIES OF MECHANOCHEMICALLY PREPARED NANOOXIDES

V. Sepelak, Institute of Physical and Theoretical Chemistry, Braunschweig University of Technology, Germany

<04> THE MAGNETORESISTANCE OF METAL-RICH Ag_{2+x}Se - A PROTOTYPE NANOSCALE METAL/SEMICONDUCTOR DISPERSION

Juergen Janek, Justus-Liebig-University Giessen, Institute of Physical Chemistry, Germany

<06> MOCVD GROWTH OF DOPED CERIA THIN FILMS

Tae-Sik Oh, California Institute of Technology, USA

<08> SYNTHESIS AND PHYSICAL CHARACTERIZATION OF NANO-GRAINED BaTiO_3 CERAMICS

S.-M. Moon, Inha University, Korea

<10> STRUCTURE OF Ti_4O_7 PREPARED BY MECHANOCHEMICAL SYNTHESIS

Kosuke O. Hara, Graduate School of Energy Science, Kyoto University, Japan

<12> EFFECT OF SM AND W CO-DOPING ON PROPERTIES OF FAST OXYGEN ION

Moon-Bong Choi, Alternative Energy Materials Research Laboratory, School of Materials Science and Engineering, Chonnam National University, Korea

<14> FIRST PRINCIPLES STUDY ON THE ELECTRONIC STRUCTURE AND REACTIVITY OF $\text{Ni}/\text{H}/\text{ZrO}_2$ TRIPLE PHASE BOUNDARY IN SOLID OXIDE FUEL CELL

Tomofumi Tada, Department of Materials Engineering, The University of Tokyo, Japan

<16> ROLES OF OXYGEN VACANCY AND INTERSTITIAL CU IN ATOMIC SWITCH OF Ta_2O_5 : AN AB INITIO STUDY

Tingkun Gu, Department of Materials Engineering, The University of Tokyo, Japan

<18> ACCEPTOR CENTERS IN Ga_2O_3

Detlev M. Hofmann, Physics Institute, University of Giessen, Germany

<20> EFFECTS OF EXCESS IRON ON THE MAGNETIC PROPERTIES OF A HIGH PERMEABILITY Ni-Zn FERRITE

Rosidah Alias, Microelectronic & Nanotechnology Program, Malaysia

<22> MAGNETIC/ANODIC DIELECTRIC NANOSTRUCTURES

E.A. Outkina, Belarussian State University of Information and Radioelectronics, Belarus

<24> THE CORRELATION BETWEEN THE PHYSICO-CHEMICAL CHARACTERISTICS AND CATALYTIC ACTIVITY OF COO(I), COO(II) AND COO(I,II)..

Virendra Goswami, Indian Institute of Technology Kharagpur (now, Aravli College of Engineering and Management), India