Program

Nonstoichiometric Compounds

March 8-13, 2009
Jeju Island, Korea

Conference Chairs

Professor Han-Il 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

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 TO 250 °C
Xin Guo, Institute of Solid State Research, Germany

09:00 - 09:20   THE OXYGEN RELEASE BEHAVIOR OF CAF₂-TYPE (PR₀.₇₅Zr₀.₂₅)O₂₋ₓ PHASE WITH WIDE OXYGEN NONSTOICHIOMETRY
Shinya Otsuka-Yao-Matsuo, Osaka University, Japan

09:20 - 09:40   MICROSTRUCTURAL EVOLUTION IN PEROVSKITES BY OXYGEN PARTIAL PRESSURE CHANGE AND DONOR DOPING
Suk-Joong L. Kang, KAIST, Korea

09:40 - 10:00   DISORDER, LATTICE DYNAMICS AND IONIC CONDUCTION IN SUPERIONIC COPPER CHALCOGENIDES
S.A. Danilkin, ANSTO, Australia

10:00 - 10:30   Coffee break

10:30 - 11:00   ON THE ORIGIN OF ANOMALOUS V_TH SHIFT IN HIGH-K MOSFETS
Akira Toriumi, The University of Tokyo, Japan

11:00 - 11:20   DIRECT OBSERVATION OF REVERSIBLE OXIDATION AND REDUCTION AT BURIED OXIDE/METAL INTERFACES
Andreas Klein, Technische Universität Darmstadt, Germany

11:20 - 11:40   STRUCTURAL FEATURES OF BATIO3 NANO-POWDERS AND NANO-GRAINED CERAMICS
N.-H. Cho, Inha University, Korea

11:40 - 12:00   DEFECT COMPLEX AND DIELECTRIC PROPERTIES OF ACCEPTOR AND MNO-DOPED BATIO3
Young Ho Han, Sungkyunkwan University, Korea
12:00 - 14:00  
**Lunch**

**Session II: Ferroelectrics**  
Session Chairs: H-I. Yoo & P. McIntyre

14:00 - 14:30  
Effect of Acceptor (Mg) Concentration on the Resistance Degradation Behavior in BaTiO$_3$ Model Dielectrics: Impedance Spectroscopy and TSDC (Thermally Stimulated Depolarization Current) Analysis  
Seok-Hyun Yoon, 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

14:50 - 15:10  
ROLE OF ELECTRON EMISSION FROM THE RARE-EARTH METAL OXIDES IN DISPLAY DEVICE  
Ki-Woong Whang, Seoul National University, Korea

15:10 – 15:40  
Coffee break

15:40 – 16:10  
BULK AND INTERFACIAL OXYGEN DEFECTS IN HAFNIA DIELECTRIC STACKS: A CRITICAL ASSESSMENT  
Paul C. McIntyre, Stanford University, USA

16:10 – 16:30  
ATOMIC-RESOLUTION STRUCTURAL ANALYSIS OF LA$_{2/3-x}$Li$_3$TiO$_3$ BY HIGH RESOLUTION ELECTRON MICROSCOPY  
Takao Tsurui, Tohoku University, Japan

16:30 - 16:50  
TRANSMISSION ELECTRON MICROSCOPY STUDY OF AN ELECTRON-BEAM-INDUCED ORDER TO DISORDER TRANSFORMATION OF NONSTOICHIOMETRIC NIOBIUM NITRIDE  
Jonghan Won, Los Alamos National Laboratory, USA

16:50 – 17:40  
**Short Presentation for Poster Session I (Odd number)**

18:00 – 19:30  
**Dinner**

19:30 – 20:30  
**Poster Session I and Social Hour**
Tuesday, March 10, 2009

07:30 – 08:30  Breakfast

Session III: Thermoelectric, Energy conv/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  AVERAGE AND LOCAL STRUCTURE INVESTIGATION OF ION CONDUCTORS BY MEANS OF TOTAL NEUTRON SCATTERING
Lorenzo Malavasi, University of Pavia, Italy

10:00 - 10:20  WORK FUNCTIONS OF TRANSPARENT CONDUCTING OXIDES
Andreas Klein, Technical University of 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  DEFECT MODEL OF LIQUID APPLIED TO IONIC CONDUCTIVITY OF GLASS
Junichi Kawamura, IMRAM, Tohoku University, Japan

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 & Tom Mason

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

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  Short Presentation for Poster Session II (Even numbers)

18:00 - 19:30  Dinner

19:30 - 20:30  Poster Session II and Social Hour
Wednesday, March 11, 2009

07:30 - 08:30  Breakfast

Session V: Magnetic Materials
Session Chairs: Manfred Martin & Klaus 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 ?-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 $\text{BAPRO}_3$
Shogo Miyoshi, The University of Tokyo, Japan

10:00 - 10:30  Coffee break

10:30 - 11:00  A HIGH-TEMPERATURE MöSSBAUER STUDY INTO THE STRUCTURE, DISORDER, AND FORMATION KINETICS OF IRON NITRIDES
K.-D. Becker, Technical University of Braunschweig, Germany

11:00 - 11:20  SURFACE MODIFICATION OF (La,Sr)$_3$CoO$_5$ FOR HIGH PERFORMANCE SOFC CATHODE
Koji Amezawa, Tohoku University, Japan

11:20 - 11:40  CHEMICAL ROUTE FROM A SOLID ELECTROLYTE TO AN ELECTRIDE - DEFECT CHEMISTRY OF MAYENITE ($\text{C}_{12}\text{A}_{7}$)
Juergen Janek, Justus-Liebig-University Giessen, Germany

12:00 - 13:00  Lunch

13:00  Optional excursions

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 SrTi_{1-x}Fe_xO_3-D 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 Ba_{0.1}Sr_{0.9}Co_{0.8}Fe_{0.2}O_3-Delta
David N. Mueller, RWTH Aachen, Germany

09:20 - 09:40  OXYGEN NONSTOICHIOMETRY IN MIXED CONDUCTORS FROM ELECTROCHEMICAL IMPEDANCE SPECTROSCOPY IN A THIN FILM GEOMETRY
Sossina M. Haile, California Institute of Technology, USA

09:40 - 10:00  ANALYSIS OF STRUCTURAL PHASE TRANSITION OF BaCe_{1-x}Y_xO_3 by THERMAL ANALYSES AND X-RAY DIFFRACTION AT HIGH TEMPERATURES
Takuya Hashimoto, Nihon University, Japan

10:00 - 10:30  Coffee break

10:30 - 11:00  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

11:00 - 11:20  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

11:20 - 11:40  OXYGEN TRANSPORT KINETICS IN PBCF DOUBLE PEROVSKITE MEMBRANE
Ji Haeng Yu, Korea Institute of Energy Research, Korea

11:40 - 12:00  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

12:00 - 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

14:30 - 14:50 ELASTIC STRAIN IN INTERFACES AND ITS INFLUENCE ON THE INTERFACIAL IONIC TRANSPORT – EXPERIMENTAL STUDIES AND FORMAL CONSIDERATIONS
N. Schichtel, Justus-Liebig-University 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 GdBaCO_{5+d}Ce_{0.8}Gd_{0.2}O_{2}
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
Jun Woo Son, University of California, Santa Barbara, USA

16:30 – 16:50 RELATIONSHIP BETWEEN STRUCTURAL AND ELECTRICAL PROPERTIES ON PROTON CONDUCTING BaZrO_{3} THIN FILM
Hiroo Yugami, Tohoku University, Japan

16:50 - 17:10 A COMPREHENSIVE ELECTRICAL CHARACTERIZATION OF ACCEPTOR DOPED BaTiO_{3} IN QUENCHED STATE
Jong-Sook Lee, Chonnam National University, Korea

17:10 – 17:50 Poster Discussion

18:30 – 20:30 Conference Banquet with entertainment
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

12:10 Lunch and Departures
List of Posters

Poster Session 1 (Monday)

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

<03> IONIC/ELECTRONIC TRANSPORT PROPERTIES AND DEFECT/ELECTRONIC STRUCTURE OF
Ba(ZRr,Pr)O3
Mao Tamaru, Department of Materials Engineering, 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 LA0.75SR0.25Ga0.9Fe0.04O3-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 La0.1Sr0.9Co0.8Fe0.2O3-δ MEMBRANE
Moon-Bong Choi, Alternative Energy Materials Research Laboratory, School of Materials Science and
Engineering, Chonnam National University, Korea

<13> ELECTRICAL PROPERTY OF BaCe0.85-XZrXY0.15O3-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, 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 WASLEY PHASES
Satoshi Yamazaki, Institute for Solid State Physics, University of Tokyo, Japan
Poster Session 2 (Tuesday)

<02> EFFECT OF OXYGEN NON-STOICHIOMETRY ON THE MAGNETIC PROPERTIES OF TiO$_2$ THIN FILMS  
Lorenzo Malavasi, University of Pavia, Italy

<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 BATIO3 CERAMICS  
S.-M. Moon, Inha University, Korea

<10> STRUCTURE OF Ti$_6$O$_7$ 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 Ni/H/ZrO$_2$ TRIPLE PHASE BOUNDARY IN SOLID OXIDE FUEL CELL  
Tomofumi Tada, Department of Materials Engineering, University of Tokyo, Japan

<16> ROLES OF OXYGEN VACANCY AND INTERSTITIAL Cu IN ATOMIC SWITCH OF Ta$_2$O$_5$: AN AB INITIO STUDY  
Tingkun Gu, Department of Materials Engineering, University of Tokyo, Japan

<18> ACCEPTOR CENTERS IN Ga$_2$O$_3$  
Detlev M. Hofmann, Physics Institute, University of Giessen, Germany