Program

Nonstoichiometric Compounds

Sheraton Kauai Resort Hotel
2440 Hoonani Road, Koloa, Kauai, HI 96756
Tel: 808-742-1661 Fax: 808-742-9777

April 3-8, 2005

Conference Chairs

Manfred Martin
RWTH Aachen University

Thomas O. Mason
Northwestern University

Junichiro Mizusaki
Tohoku University

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**Sunday, April 3, 2005**

16:00 – 18:00  Registration

17:00 – 18:00  Meeting of Organizing Committee, Session Chairs and Keynote Speakers

18:00 – 19:00  Opening Reception

19:00 – 21:00  Dinner (BeachLawn)

**Notes**

- Please observe “No Smoking” at ECI technical sessions, meals and social hours.
- Speakers should allow time at the end of their presentation for questions and discussion.
- Please silence your cell phone during sessions.
- Posters will remain on display throughout the conference.
- All General Sessions will be held at the Poipu Ballroom.
- All Socials and Poster Sessions will be held at Lawai
Monday, April 04, 2005

07:30 - 08:15   Breakfast Buffet (Shells)
08:15 - 08:25   Welcome and Opening Remarks
                Manfred Martin, Conference Chair
                Jules Routbort, Conference Liaison

**Session 1: Transport**
Session Chair: Thomas O. Mason

08:25 - 09:05   **OXYGEN TRANSPORT IN NON-STOICHIOMETRIC OXIDES** (keynote)
                J.A. Kilner, Imperial College, London

09:05 - 09:30   **QUANTITATIVE PREDICTION OF VOID FORMATION IN A GROWING SCALE IN HIGH TEMPERATURE OXIDATION OF METALS** (invited)
                Toshio Maruyama, Tokyo Institute of Technology

09:30 - 09:55   **IONIC TRANSPORT AND NEARLY CONSTANT LOSS IN Na_{1.70}Li_{0.32}Al_{0.66}O_{17}** (invited)
                Klaus Funke, University of Münster

09:55 - 10:20   **SYNTHESIS AND CHARACTERISATION OF POTENTIAL SULPHIDE ION CONDUCTORS**
                K. Hellgardt, Loughborough University

10:20 - 10:45   **NONSTOICHIOMETRICAL EFFECTS ON THE DIFFUSION OF GROUP I ELEMENTS IN II-VI SEMICONDUCTORS**
                Thomas Wichert, Universität des Saarlandes

10:45 - 11:05   Coffee Break

**Session II: Transport**
Session Chair: Junichiro Mizusaki

11:05 - 11:45   **BULK CATION DIFFUSION IN IONIC MATERIALS** (keynote)
                Rüdiger Dieckmann, Cornell University

11:45 - 12:10   **CREEP AND DIFFUSION IN NANO-YTTRIA TETRAGONAL ZIRCONIA POLYCRYSTALS (NANO-YTZP)** (invited)
                Diego Gómez-García, Universidad de Sevilla

12:10 - 12:35   **CATION DIFFUSION IN LITHIUM NI OBATE**
                H. Haneda, National Institute for Materials Science, Tsukuba

12:35 - 13:00   **DIFFUSION IN THE HIGH-TEMPERATURE MATERIAL MOLYBDENUM DISILICIDE**
                Helmut Mehrer, University of Münster

13:00 - 14:30   Lunch (Shells)
14:30 - 16:30   Ad hoc sessions / free time
16:30 - 17:00   Afternoon Coffee
Monday, April 04, 2005

Session III: Transport
Session Chair: Helmut Mehrer

17:00 – 17:40
CHEMICAL DIFFUSION IN COMPLEX OXIDES (keynote)
H.-I. Yoo, Seoul National University

17:40 – 18:05
OXYGEN NON-STOICHIOMETRY AND ASSOCIATED DIELECTRIC EVOLUTION OF BaTiO$_3$ BASE-METAL ELECTRODE MULTILAYER CERAMIC CAPACITORS
G.Y. Yang, The Pennsylvania State University

18:05 – 18:30
HOST CATION TRANSPORT AND SURFACE RECONSTRUCTION OF UNDOPED AND DONOR DOPED STRONTIUM TITANATE AT HIGH TEMPERATURES
Karsten Gömann, Technical University of Clausthal

18:30 – 18:55
ANION DIFFUSION IN Y- AND N-DOPED ZIRCONIA
Hans Boysen, LMU München

18:55 – 19:20
DEFECT CHEMISTRY AND TRANSPORT PROPERTIES OF NONSTOICHIOMETRIC LANTHANUM NICKEL OXIDES
Michael Schroeder, RWTH Aachen University

19:30 – 21:00
Dinner (BeachLawn)

21:00 – 22:30
Poster Session and Social Hour (Lawai)
Tuesday, April 05, 2005

07:30 – 08:30  Breakfast Buffet (Shells)

**Session IV: Bulk Properties**
Session Chair: Neil Allan

08:30 – 09:10  THERMOCHEMICAL STUDIES OF FLUORITE-BASED OXIDES: ENERGETICS OF DEFECTS IN YTTRIA-STABILIZED ZIRCONIA, HAFNIA, AND CERIA AND OF SOME RELATED NANOMATERIALS (keynote)
Alexandra Navrotsky, University of California at Davis

09:10 – 09:50  SPECTROSCOPIC STUDIES OF HIGH-TEMPERATURE SOLID STATE PROCESSES (keynote)
K.D. Becker, Technical University of Braunschweig

09:50 – 10:15  ELECTRICAL PROPERTIES OF SUBSTITUTED Ca$_2$Fe$_2$O$_5$ (invited)
Tim Armstrong, Oak Ridge National Laboratory

10:15 – 10:40  NONSTOICHIOMETRY, CONDUCTIVITY AND DEFECT CHEMISTRY OF (La$_x$Ca$_{1-x}$)(Cr$_{1-x}$Al$_x$)O$_3$
Junichiro Mizusaki, Tohoku University

10:40 – 11:10  Coffee Break

**Session V: Bulk Properties**
Session Chair: Toshio Maruyama

11:10 – 11:50  HYDROGEN IN OXIDES (keynote)
Truls Norby, University of Oslo

11:50 – 12:30  LOCAL ELECTRONIC STRUCTURE OF NONSTOICHIOMETRIC OXIDES BY ELECTRON SPECTROSCOPY (keynote)
Shu Yamaguchi, The University of Tokyo

12:30 – 12:55  SOLUTION HARDENING AND SOFTENING IN NON-STOICHIOMETRIC CERAMICS AND INTERMETALLICS (invited)
Terence E. Mitchell, Los Alamos National Laboratory

13:00 – 14:30  Lunch Buffet (Shells)

14:30 – 18:00  Ad hoc sessions / free time

18:30 – 20:00  Dinner (Beachlawn)
**Tuesday, April 05, 2005**

**Session VI: Transparent Conducting Oxides**
Session Chair: Tim Armstrong

20:00 – 20:40 **TRANSPARENT OXIDE SEMICONDUCTORS** (keynote)
Hideo Hosono, Tokyo Institute of Technology

20:40 – 21:05 **TRANSPORT AND DEFECT MECHANISM IN P-TYPE TCO MATERIALS**
Brian J. Ingram, Northwestern University

21:05 – 21:20 Break

21:20 – 21:45 **IN SITU AND EX SITU HIGH-TEMPERATURE STUDIES ON INDIUM-TIN OXIDE**
G.B. González, European Synchrotron Radiation Facility

21:45 – 22:10 **USE OF JONKER PLOTS TO CHARACTERIZE THE TRANSPORT PROPERTIES OF TRANSPARENT OXIDE SEMICONDUCTORS**
Thomas O. Mason, Northwestern University

22:10 – 23:00 Poster Session and Social Hour (Lawai)
Wednesday, April 06, 2005

07:30 – 08:30  Breakfast Buffet (Shells)

**Session VII: Surfaces, Interfaces**
Session Chair: Bernhardt J. Wuensch

08:30 – 09:10  **SIZE EFFECTS IN CERAMIC NANO-MATERIALS: TRANSPORT, REACTIVITY AND STORAGE** (keynote)
Joachim Maier, Max Planck Institute for Solid State Research

09:10 – 09:50  **NON-STOICHIOMETRY AND ELECTRONIC PROPERTIES OF INTERFACES** (keynote)
Andreas Klein, Darmstadt University of Technology

09:50 – 10:15  **TWO STEP MECHANISM OF GRAIN BOUNDARY POTENTIAL BARRIER FORMATION IN DONOR-DOPED PEROVSKITES**
Rene Meyer, Research Centre Jülich

10:15 – 10:40  **STRUCTURE-PROPERTY RELATIONSHIPS FOR GRAIN BOUNDARIES IN ACCEPTOR-DOPED SrTiO₃**
Roger A. De Souza, RWTH Aachen University

10:40 – 11:10  Coffee Break

**Session VIII: Surfaces, Interfaces**
Session Chair: Klaus Funke

11:10 – 11:50  **NITROGEN-DOPED ZIRCONIA – PREPARATION, SURFACE REACTIONS AND TRANSPORT PROPERTIES** (keynote)
Jürgen Janek, Justus-Liebig-University Giessen

11:50 – 12:30  **CHARACTERIZATION OF HIGH TEMPERATURE ELECTRODES UNDER OPERATION** (keynote)
Tatsuya Kawada, Tohoku University

12:30 – 12:55  **OXYGEN INCORPORATION INTO “ELECTRON-RICH” AND “ELECTRON-POOR” OXIDES: MECHANISTIC STUDIES ON Sr(FeₓTi₁₋ₓ)O₃₋ₓ**
Rotraut Merkle, Max Planck Institute for Solid State Research

13:00 – 14:30  Lunch Buffet (Shells)

14:30 – 19:30  Ad hoc discussions / free time

19:30 – 21:00  Dinner (Beachlawn)

After dinner speech
**AN HISTORICAL PERSPECTIVE OF INSIGHT INTO STRUCTURE-PROPERTY CONNECTIONS FOR FAST-ION CONDUCTORS**
Bernhardt J. Wuensch, Massachusetts Institute of Technology

Poster Session and Social Hour (Lawai)
Thursday, April 07, 2005

07:30 - 08:30  Breakfast Buffet (Shells)

Session IX: Theory
Session Chair: Manfred Martin

08:30 - 09:10  ATOMIC SCALE MODELS FOR DEFECT STRUCTURE AND TRANSPORT PREDICTIONS (keynote)
Robin W. Grimes, Imperial College London

09:10 - 09:35  SIMULATION OF OXIDE SOLID SOLUTIONS (invited)
Neil L. Allan, University of Bristol

09:35 - 10:00  ELECTRONIC STRUCTURE, PHASE STABILITY AND CHEMICAL BONDING OF TRANSITION-METAL OXYNITRIDES FROM FIRST-PRINCIPLES THEORY
Richard Dronskowski, RWTH Aachen University

10:00 - 10:25  NANOSCALE ORDERING IN SCANDIUM DOPED ZIRCONIA
A.N. Cormack, Alfred University

10:25 - 10:50  Coffee Break

10:50 - 11:15  LAYERED ATOM PATTERNS IN FLUORITE-STRUCTURED OXIDES
Kurt E. Sickafus, Los Alamos National Laboratory

11:15 – 11:40  AB INITIO BASED MODELLING OF SUBSTOICHIOMETRIC TITANIUM OXY-CARBONITRIDES
D.A. Andersson, P.A. Korzhavyi, B. Johansson, Royal Institute of Technology

Session X: Fuel Cells
Session Chair: Jules Routbort

11:40 - 12:05  INVESTIGATION OF THE INTERFACIAL STABILITY BETWEEN ELECTRODE AND ELECTROLYTE LAYER OF LSGM-BASED SOFCS (invited)
Jong-Ho Lee, Korea Institute of Science and Technology

12:05 - 12:30  HIGH ELECTRIC CONVERSION EFFICIENCY AND IMPURITY-POISONING OF SOLID OXIDE FUEL CELLS (invited)
Yoshio Matsuzaki, Tokyo Gas Co., Ltd

12:30 - 12:55  SUBSTOICHIOMETRIC PEROVSKITES AS CATHODES OR CATALYSTS IN SOLID OXIDE FUEL CELLS (invited)
Michael Krumpelt, Argonne National Laboratory

13:00 - 14:30  Lunch Buffet (Shells)

14:30 - 18:30  Ad hoc discussions / free time

18:30  Conference Banquet
Friday, April 08, 2005

07:30 – 08:30  Breakfast Buffet (Shells)

Session XI: Intermetallics
Session Chair: Klaus Hilpert

08:30 – 08:55  A HIGH-RESOLUTION AND IN SITU ELECTRON MICROSCOPE STUDY OF DISLOCATION CLIMB AND STRUCTURAL CHANGES IN TWO-PHASE TITANIUM ALUMINIUM ALLOYS
Fritz Appel, GKSS Research Centre

08:55 – 09:20  NONSTOICHEMETRY IN LINE COMPOUNDS
Gary S. Collins, Washington State University

09:20 – 09:45  SYNTHESIS OF AL BASED INTERMETALLIC COMPOUNDS WITH NONSTOICHEOMETRIC COMPOSITION BY MEAN OF ION IMPLANTATION OF Ni AND Ti
Heishichiro Takahashi, Hokkaido University

9:45 – 10:10  Coffee Break

Session XII: Transition Metal Compounds
Session Chair: R. Dieckmann

09:45 – 10:10  DEFECT FORMATION AND MECHANICAL STABILITY OF PEROVSKITES ON THE BASIS OF LaCrO$_3$
K. Hilpert, Research Center Jülich

10:10 – 10:35  ROLE OF CATION VACANCY DISTRIBUTION ON THE PROPERTIES OF CMR MANGANITES
Lorenzo Malavasi, Università di Pavia

11:00 – 11:25  OXYGEN PARTIAL PRESSURE CONTROL DURING SINTERING OF Mn-Zn-FERRITES
Jörg Töpfer, Fachhochschule Jena

11:25 – 11:50  MODELING OF THE DEFECT STRUCTURE OF COPPER-DOPED LANTHANUM COBALTITES
A. Yu. Zuev, Ural State University

11:50 – 12:15  Concluding Remarks

12:30 – 14:00  Lunch (Shells)
Departure
POSTER PRESENTATIONS

1. **DIFFUSION OF Al AND Fe IN IRON-ALUMINIDES**  
   Helmut Mehrer, University of Münster

2. **DIFFUSION OF Ni AND Mn IN NICKEL-MANGANESE ALLOYS**  
   Helmut Mehrer, University of Münster

3. **TUNEABLE CONDUCTIVITY AND CONDUCTION MECHANISM IN A UV LIGHT ACTIVATED ELECTRONIC CONDUCTOR**  

4. **OXYGEN CONTENT VARIATION IN THE DOUBLE-LAYERED MANGANITES: EFFECT ON THE STRUCTURAL, TRANSPORT AND MAGNETIC PROPERTIES**  
   Lorenzo Malavasi, Elena di Tullio, Christina Tealdi, Giorgio Flor, Maria Cristina Mozzati, Carlo B. Azzoni, Università di Pavia

5. **JOINING ADVANCED MATERIALS BY PLASTIC FLOW**  

6. **THE STRUCTURE RELATED PROPERTIES OF MIXED-CONDUCTING La-Sr CUPRATES**  
   G.N. Mazo, S.N. Savvin, Moscow State University

7. **NONSTOICHIOMETRY AND SOLID SOLUTION FORMATION IN UN, ZrN AND TiN**  
   Nicholas J. Ashley, Robin W. Grimes, Jonathan Ball, Imperial College London, Ken McClellan, Los Alamos National Laboratory

8. **DEFECT STRUCTURE AND CHARGE TRANSFER IN DOPED LANTHANUM COBALTITES AND MANGANITES**  

9. **ELEMENTARY MECHANISMS IN SOLID STATE REACTIONS**  
   Francoise Valdivieso, Michèle Pijolat, Michel Soustelle, Ecole Nationale Superieure des Mines de Saint-Etienne

10. **DEFECT INTERACTIONS VIA PAIRWISE DECONVOLUTION**  
    Jonathan A. Ball, Robin W. Grimes, Imperial College

11. **NEUTRON Rietveld REFINEMENT OF THE STRUCTURE OF OXYGEN-CONDUCTING PHASES IN THE Nd$_2$O$_3$-Yb$_2$O$_3$ SYSTEM: A SEARCH FOR POSSIBLE PYROCHLOR-LIKE CATION ORDERING IN NdYb$_2$O$_6$**  
    Emily B. Walton, Bernhardt J. Wuensch, Massachusetts Institute of Technology

12. **INTERACTION BETWEEN OXYGEN, WATER VAPOUR AND LSM IN SOFC SCREEN-PRINTED CATHODES**  
    Michele Pijolat, Ecole Nationale Superieure des Mines de Saint-Etienne

13. **THERMOCHROMIC PROPERTIES OF DOPED AND UNDOPED VO$_2$ FILMS**  
    Bruno K. Meyer, Ganhua Fu, Angelika Polity, Justus-Liebig-Universität Giessen
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<td>DEGRADATION OF YTTRIA-STABILIZED ZIRCONIA IN AN ELECTRIC FIELD</td>
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<td>DEFECT CHEMISTRY AND REDOX PROPERTIES OF NdCoO_3 PEROVSKITE-TYPE OXIDE</td>
<td>Cristina Tealdi, Lorenzo Malavasi, Giorgio Flor, Universita degli Studi di Pavia</td>
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<td>EFFECT OF NITROGEN DOPING ON IONIC CONDUCTIVITY OF ZIRCONIA</td>
<td>Joachim Maier, Jong-Sook Lee, Max Planck Institute for Solid State Research, Martin Lerch, Technische Universität Berlin</td>
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<td>OXIDATION KINETICS OF ZIRCONIUM AT HIGH TEMPERATURES STUDIED BY IN SITU X-RAY DIFFRACTION</td>
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<td>INVESTIGATIONS OF THE OXYGEN REDUCTION KINETICS IN SOLID OXIDE FUEL CELLS BY MEANS OF THIN FILM MICROELECTRODES</td>
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