

ISSM-SOFC 2013 Program

Monday 11th Mar.	
9:00	Registration
9:30	Opening
Session I	
Chair: Tatsuya Kawada	
9:40 - 10:25 (I-1)	Invited Talk Subhash C. Singhal (Pacific Northwest National Laboratory) Present status of SOFC research and development
Chair: Michihisa Koyama	
10:25 - 10:55 (O-1)	Tatsuya Kawada (Tohoku University) Engineering SOFC electrodes based on <i>in situ</i> characterizations
10:55 - 11:15 (O-2)	Shin-ichi Hashimoto (Tohoku University) Non-stoichiometry and phase stability of $\text{La}_{0.6}\text{Sr}_{0.4}\text{Co}_{0.2}\text{Fe}_{0.8}\text{O}_{3-\delta}$ cathode
11:15 - 11:35 (O-3)	Jun Kubota (University of Tokyo) Infrared Spectroscopic Approach for the Understanding of the Catalysis of Ni on YSZ and GDC
11:35 - 11:55 (O-4)	Hiroki Muroyama (Kyoto University) In-situ analysis of chemical state and crystalline structure of samaria-doped ceria in high-temperature reducing atmospheres
11:55 - 12:15 (O-5)	Haruo Kishimoto (AIST) Effect of the Oxide Substrate on the Property of Nickel Surface
12:15-13:30	Lunch
Session II	
Chair: Michihisa Koyama	
13:30 - 14:15 (I-2)	Invited Talk Kunal Karan (University of Calgary) Modeling Sulfur poisoning of SOFC Ni anodes: Insights and Issues
Chair: Koji Amezawa	
14:15 - 14:45 (O-6)	Dayadeep Monder (IIT Hyderabad) An atomistic model for sulfur poisoning of SOFC anodes
14:45 - 15:15 (O-7)	Michihisa Koyama (Kyushu University) Application of Computational Chemistry to Practical Issues in Solid Oxide Fuel Cells
15:15 - 15:35 (O-8)	Tepei Ogura (Kyushu University) Computational analyses for sulfur and carbon degradation mechanisms in an SOFC nickel
15:35 - 15:55 (O-9)	Tomofumi Tada (Tokyo Institute of Technology) First principles calculations and kinetic Monte Carlo simulations for chemical reaction analysis at the Ni/H ₂ /YSZ triple phase boundary
15:55 - 18:00	Poster with coffee
18:00 - 20:00	Banquet

Tuesday 12th Mar.

9:00 **Registration**

Session III

Chair: Naoki Shikazono

9:30 - 10:15 (I-3) **Invited Talk**

Paul Shearing (University College London)

Understanding the Role of Microstructure in SOFC Performance

Chair: Tatsuya Kawada

10:15 - 10:45 (O-10) Naoki Shikazono (University of Tokyo)

Three Dimensional Numerical Modeling of Ni-YSZ Anode

10:45 - 11:05 (O-11) Zhenjun Jiao (University of Tokyo)

Simulation of Solid Oxide Fuel Cell Anode Microstructure Evolution by Using the Phase Field Method

11:05 - 11:25 (O-12) Shotaro Hara (University of Tokyo)

Monte Carlo Modeling on Microstructural Evolution in Solid Oxide Fuel Cell Cermet Anode

11:25 - 11:45 (O-13) Yoshitaka Umeno (University of Tokyo)

Atomistic modeling of yttria-stabilized zirconia: Interatomic potential development and ab initio calculations

11:45 - 12:05 (O-14) Moon Young Yang (University of Tsukuba)

Theoretical Investigation for Designing High Quality ReRAM

12:05-13:30 **Lunch**

Session IV

Chair: Koji Amezawa

13:30 - 14:15 (I-4) **Invited Talk**

Jürgen Janek (Justus-Liebig-Universität Giessen)

Electrode processes on YSZ studied by in situ XPS, SPEM, and ToF-SIMS

Chair: Tomofumi Tada

14:15 - 14:45 (O-15) Koji Amezawa (Tohoku University)

In Situ X-Ray Absorption Spectroscopy for Analysis of SOFC Reactions and Materials

14:45 - 15:05 (O-16) Keiji Yashiro (Tohoku University)

Oxygen reduction reaction at hetero-interface electrode of perovskite-related oxides

15:05 - 15:25 (O-17) Shogo Miyoshi (University of Tokyo)

High surface reactivity of La/Sr-Co perovskite-based cathode with cation nonstoichiometry

15:25 - 15:45 (O-18) Bin Feng (University of Tokyo)

Oxygen nonstoichiometry in CeO₂ grain boundaries: a combined atomic resolution STEM and ab initio study

15:45 **Closing**

Poster presentations (Monday 11th Mar., 15:55-18:00)

Poster Session

- P1 Shixue Liu, Takayoshi Ishimoto, Haruhiko Kohno and Michihisa Koyama
Analysis of oxygen potential effect on the anodic reactions of solid oxide fuel cell based on first-principles calculations
- P2 Haruhiko Kohno, Shixue Liu, Teppei Ogura, Takayoshi Ishimoto and Michihisa Koyama
Toward a new numerical scheme for the analysis of the triple phase boundary region in solid oxide fuel cell anode
- P3 Leton C. Saha, Kazuhide Nakao, Takayoshi Ishimoto and Michihisa Koyama
Reactive molecular dynamics studies of CH₄ reactivity with/without CO and H coverage on solid oxide fuel cell anode
- P4 Kazuhide Nakao, Haruhiko Kohno, Takayoshi Ishimoto and Michihisa Koyama
Nickel sintering property analysis by using molecular dynamics
- P5 David S. Rivera Rocabado, Takayoshi Ishimoto and Michihisa Koyama
Density functional theory study on the catalytic properties of BaTiO₃ as solid oxide fuel cell anode
- P6 Junya Oishi, Junichiro Otomo, Yoshito Oshima and Michihisa Koyama
The effects of minor components in LSCF cathode on oxygen reduction reaction
- P7 Shu-Sheng Liu, Michihisa Koyama, Shoichi Toh, Takeshi Daio and Syo Matsumura
Microstructure observation of Ni/YSZ interface
- P8 Takaaki Shimura and Naoki Shikazono
Quantitative Analysis of SOFC Anode Microstructure Change During Redox Cycles
- P9 Xiaojun Sun, Yosuke Hasegawa and Naoki Shikazono
Calculation of contact angles at triple phase boundary in SOFC anode using Level Set Method
- P10 Albert M. Iskandarov, Atsushi Kubo and Yoshitaka Umeno
Many-body potential for molecular dynamics simulation of Yttria-stabilized zirconia
- P11 Shotaro Hara, Satoshi Izumi and Shinsuke Sakai
Atomistic study on Self-diffusion Properties of Cation in Yttria-stabilized Zirconia
- P12 Yu Sun and Shotaro Hara
Atomistic study on surface segregation and diffusion of cation in YSZ
- P13 Dhruba Panthi and Atsushi Tsutsumi
Computational fluid dynamics study of a hollow fiber-based micro-tubular solid oxide fuel cell
- P14 Hauk Metelmann, Andreas Laufer, Daniel Reppin, Swen Graubner, Angelika Polity, Bruno K. Meyer, Sebastian Geburt and Carsten Ronning
Quantification of Impurities in Metal Oxides
- P15 Rolas Timbul Doloksaribu, Shogo Miyoshi and Shu Yamaguchi
Proton conductivity in nano-grained yttria-doped zirconia
- P16 Joon Young Yoon, Dong Young Kim, Shogo Miyoshi and Shu Yamaguchi
Variation of local structure in doped BaZrO₃

Poster presentations (Monday 11th Mar., 15:55-18:00)

Poster Session

P17	<u>Yuta Kimura</u> , Julian Tolchard, Mari-Ann Einarsrud, Tor Grande, Koji Amezawa, Shin-ichi Hashimoto and Tatsuya Kawada Young's modulus and ferroelasticity of $\text{La}_{0.6}\text{Sr}_{0.4}\text{Co}_{1-y}\text{Fe}_y\text{O}_{3-\delta}$ at high temperatures
P18	<u>Yuki Gono</u> , Shin-ichi Hashimoto Hashimoto and Tatsuya Kawada Effect of mechanical stress on oxygen non-stoichiometry of $\text{La}_{0.6}\text{Sr}_{0.4}\text{CoO}_{3-\delta}$
P19	<u>Takashi Nakamura</u> , Keiji Yashiro, Kazuhisa Sato, K. Amezawa and Junichiro Mizusaki Oxygen defects and crystal structure of layered perovskite oxides
P20	<u>Mina Nishi</u> , Harumi Yokokawa, Katsuhiko Yamaji, Haruo Kishimoto and Teruhisa Horita Oxygen partial pressure dependence of oxide ionic diffusion in $\text{LaNi}_{0.6}\text{Fe}_{0.4}\text{O}_3$
P21	<u>Shiho Torashima</u> and Jun Kubota Infrared Study on Support Effect of Ni/GDC
P22	Adibah Hani TBA