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Institute for Materials Research, Tohoku University
Collaborative Research Center on Energy Materials (E-IMR)

E-IMR International Workshop 2024

2024.11.26 (Tue)

12:55 – 17:30

Program & Abstracts

Maximization of solar energy utilization and innovative materials
for heat, electricity, and hydrogen storages

Venue

Institute for Materials
Research, Tohoku
University Auditorium,
Bldg. 2(Online)

Free of charge

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E-mail: e-imr*grp.tohoku.ac.jp Please change * to @.

E-IMR International Workshop 2024 11.26 Thu. 12:55-17:30	
Hours	Content & Speakers
12:40	opening
12:55 - 13:05	Opening Remarks Tetsu Ichitsubo [Center Director, E-IMR Center]
【research publication】	
13:05 – 13:20	「On the dynamics of magnets and ferroelectrics」 Bauer Gerritt E.W [Solar Energy Conversion Materials Research Unit / Advanced Institute for Materials Research Professor]
13:20 – 13:45	「Recent Progresses in Skyrmionic Materials and Devices」 Wanjun Jiang [Tsinghua University Professor]
13:45 – 14:00	「Dissociative Oxygen Adsorption and Incorporation in Co ₃ O ₄ -Dispersed PCFC Cathodes」 Hitoshi Takamura [Energy Storage Materials Research Unit / School of Engineering Tohoku University Professor]
14:00 – 14:25	「Revealing the Surface Termination Effect of Perovskite for Oxygen Exchange Reaction」 Di Chen [Tsinghua University Associate Professor]
14:25 – 14:50	「Mobility and clustering of O and anion vacancies in perovskites as energy materials」 Francesco Cordero [CNR-ISM Istituto di Struttura della Materia Primo Ricercatore]
14:50 – 15:00	Break (10 minutes)
15:00 – 15:15	「Nanostructure and chemical state imaging of energy materials by coherent X-ray diffraction」 Yukio Takahashi [Materials Evaluation and Analysis Research Unit / International Center for Synchrotron Radiation Innovation Smart Professor]
15:15 – 15:30	「Layered Manganese Dioxide as a Heat-Storage Material Utilizing Environmental Water Vapor」 Norihiro Okamoto [Solar Energy Conversion Materials Research Unit / Institute for Materials Research Associate Professor]
15:30 – 15:45	「A new AB ₃ -based alloy with reversible hydrogen absorption and desorption reactions and less degradation」 Toyoto Sato [Energy Storage Materials Research Unit / Institute for Materials Research Associate Professor]
15:45 – 16:00	「Interface Design for Room-Temperature Rechargeable Magnesium Batteries with Transition Metal Oxide Cathodes」 Hongyi Li [Energy Storage Materials Research Unit/ Institute for Materials Research Project Assistant Professor]
16:00 – 16:10	Break (10 minutes)
16:10 – 16:35	「Recent advances of silicon crystal for solar cells」 Deren Yang [Zhejiang University Professor]
16:35 – 17:00	「Probing the Multipolar Structure of Berry Curvature in Magnetization Space by the In-plane Anomalous Hall Effect」 Dazhi Hou [University of Science and Technology of China Professor]
17:00 – 17:25	「Formation Rate as a Key Factor in Enhancing the Stability of Anode-Less Lithium Metal Batteries」 Michael De Volder [University of Cambridge Professor]
17:25 – 17:30	Closing Remarks Tetsu Ichitsubo [Center Director, E-IMR Center]

Opening address

As a satellite of the international conference “Summit of Materials Science” (SMS: <https://www.sms2024.imr.tohoku.ac.jp/>) to be held at Institute for Materials Research (IMR), Tohoku University on 27th and 28th November 2024, the Collaborative Research Centre on Energy Materials, IMR (called “E-IMR” Centre) is going to hold the “E-IMR International Workshop 2024 (E-IMR IWS 2024)” on the 26th November, the day before SMS.

The recent issues of energy and global warming/climate change have increased the importance of solving these problems, and the research and development of mechanisms for securing new energy sources, energy conversion and storage materials have become urgent tasks. The development of new materials for energy has become an essential issue and is currently a priority area of focus in IMR.

The activities of IMR, which was established in April 2015, will enter its ninth year in FY2024, and from FY2022, when the “Fourth Medium-Term Goals and Plans” of MEXT began, the E-IMR Centre was reorganized, expanded and strengthened as the second phase of its mission. The E-IMR centre was reorganized into four research units: 1. Solar Energy Conversion Materials Research Unit, 2. Energy Storage Materials Research Unit, 3. Materials Evaluation and Analysis Research Unit, and 4. Novel materials unit towards social implantation. In particular, Materials Evaluation and Analysis Research Unit has been newly established, with a team structure that can carry out quantum beam analysis using synchrotron radiation and neutrons, first-principles calculations, as well as materials evaluation and prediction using materials informatics (MI).

Each research unit, which is composed of researchers from the fields of science and engineering, promotes world-class materials research by exploring the research frontiers in the field of energy materials, and employs three specially appointed assistant professors to foster young researchers with advanced research skills in interdisciplinary fields. In addition, we are promoting research in areas not completely covered by IMR, with the participation of faculty members and researchers from research organizations not only inside but also outside IMR, including the Graduate School of Engineering, the Advanced Institute for Materials Research (AIMR), and the International Center for Synchrotron Radiation Innovation Smart (SRIS).

Our mission is to establish innovative energy materials and composite module creation that contributes to maximizing solar energy utilization and the three storages of “heat, electricity, and hydrogen”. Through these research topics, we intend to contribute to the construction of a green energy society using solar energy towards carbon neutrality.

Head, E-IMR Centre

Institute for Materials Research, Tohoku University

Professor Dr. Tetsu ICHITSUBO



Research Strategy Office

Solar Energy Conversion Materials Research Unit

Prof. (Concurrent)

Kozo FUJIWARA

Crystal growth



Prof. (Concurrent)

Takeshi SEKI

Magnetic thin films
Nanostructure
Spintronics



Prof. (Concurrent)

Atsushi TSUKAZAKI

Topological material science



Prof. (Concurrent)

Bauer, Gerrit E.W.

Theoretical condensed matter physics
Spintronics (AIMR)



Asst.Prof. (Concurrent)

Norihiko L. OKAMOTO

Transmission electron microscopy
Thermoelectrics



Assist. Prof. (Concurrent)

Kensaku MAEDA

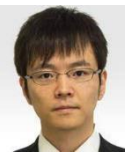
Crystal growth
Polycrystalline silicon



Assist. Prof. (Concurrent)

Keita ITO

Magnetic nitrides
Ordered alloys
Spintronics



Specially Appointed Assistant Professor

Jun NOZAWA

Colloidal science
Crystal growth



Energy Storage Materials Research Unit

Prof. (Concurrent)

Hitoshi MIYASAKA

Redox-active MOFs
Multi-functional frameworks
Function-synergistic LIB



Prof. (Concurrent)

Shin-ichi ORIMO

High-density hydrogen storage materials
Superionic conductors
Next generation batteries (AIMR)



Prof.(Concurrent)

Hitoshi TAKAMURA

Solid oxide cells
Proton Conductors
Hydrogen production (Graduate School of Engineering)



Asst.Prof. (Concurrent)

Toyoto SATO

Hydrogen storage materials
Hydrogen related materials



Specially Appointed Assistant Professor

Hongyi LI

Dual-cation batteries
Metal and alloy anodes



Materials Evaluation and Analysis Research Unit

Prof. (Concurrent)

Masaki FUJITA

Quantum beams
Strongly correlated electron systems
Crystal growth



Prof. (Concurrent)

Yu KUMAGAI

Computational material science
Materials informatics
Ceramics



Prof. (Concurrent)

Yukio TAKAHASHI

Coherent diffraction imaging
Nanostructure and chemical state analysis (International Center for Synchrotron Radiation Innovation Smart)



Asst. Prof.

Belosludov, Rodion V.

functional nanoporous materials; gas storage and separation



Asst. Prof. (Concurrent)

Tomoya KAWAGUCHI

Cathode materials for Li/multivalent rechargeable batteries, synchrotron X-ray scattering/spectroscopy



Composite Module and Social Implementation Research Unit

Prof. (Concurrent)

Hidemi KATO

Nanoporous metals of base and half metal elements
Amorphous alloys and metallic glasses



Prof./Center Director

Tetsu ICHITSUBO

Novel storage battery
Phase transformation and structure control
Statistical thermodynamics and microstructure formation theory



Specially Appointed Assistant Professor

Ruirui SONG

Dealloying
Porous metal/alloy
Catalyst



On the dynamics of magnets and ferroelectrics

G.E.W. Bauer^{1,2}

¹Tohoku University, ²UCAS

Keywords : magnetism, ferroelectricity



The duality between electric and magnetic dipoles in electromagnetism only partly applies to condensed matter. In particular, the elementary excitations of the magnetic and ferroelectric orders, namely magnons and ferrons, respectively, have received asymmetric attention from the condensed matter community in the past [1]. I will introduce and summarize the current state of magnonics and the budding field of “ferronics.” The introduction of dipole-carrying elementary excitations allows the modeling of many observables and potentially leads to applications in thermal, information, and communication technologies.

[1] G.E.W. Bauer, P. Tang, R. Iguchi, J. Xiao, K. Shen, Z. Zhong, T. Yu, S.M. Rezende, J.P. Heremans, and K. Uchida, Perspective: Polarization transport in ferroelectrics, *Phys. Rev. Applied* **20**, 050501 (1-7) (2023).

Towards functional skyrmion racetrack memory

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Key Words: (skyrmions, magnetic multilayers, spin torques, racetrack memory)

Magnetic skyrmions are topological spin textures that exhibit many exciting properties for emerging topological physics and functional spintronic devices [1-2]. In this talk, I will first review the most recent progress stabilizing magnetic skyrmions at room temperature in the interfacially asymmetric multilayers, I will particularly show how the skyrmion Hall effect [3-4] can be used for implementing novel device applications. Second, I will introduce a “bottom-up” method for stabilizing square and triangular skyrmion lattices by using topographically modified Si/SiO₂ substrate. Based on which, an experimental realization of skyrmion shift register will be presented [5]. Lastly, through integrating skyrmions with magnetic tunnel junction (MTJ), we will demonstrate the electrical detection of mobile skyrmions by using 100% tunneling magnetoresistance (TMR) effect [6]. In the end, a few promising directions towards skyrmion racetrack memory will be discussed.

References:

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- [4] L. Zhao, et al., *Phys. Rev. Letts.* **125**, 027206 (2020).
- [5] C. Song, et al., *Nano Letters* **22**, 9836 (2022).
- [6] L. Zhao, et al., *Science Bulletin* **69**, 2370 (2024)
- [7] M. Zhao, et al., *npj Quantum Materials* **9**, 50 (2024).

Dissociative Oxygen Adsorption and Incorporation in Co_3O_4 -dispersed $\text{BaZr}_{0.9}\text{Sc}_{0.1}\text{O}_{2.95}$ for a PCFC Cathode

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Department of Materials Science, Graduate School of Engineering, Tohoku University

Keywords : Surface exchange kinetics, spinel-type oxides, pulse isotope exchange

Proton-conducting fuel cells (PCFCs), which operate at lower temperatures than conventional solid oxide fuel cells (SOFCs) that use an oxide-ion conductor, have attracted considerable attention owing to their high energy-conversion efficiency. Even with mobile protons, oxygen reduction reactions at the cathode limit the performance of the PCFCs. To improve their cathode properties, a variety of functional oxides, including the so-called triple conductors, which have mobile oxide ions, protons, and holes, have been developed. Our group has focused on the excellent catalytic activity of Co_3O_4 for the dissociative adsorption of oxygen at elevated temperatures, which is comparable to that of Co-containing mixed conductors with perovskite-type structures [1,2]. In this study, Co_3O_4 -dispersed proton-conducting oxides, $\text{BaZr}_{0.9}\text{Sc}_{0.1}\text{O}_{2.95}$, were prepared for use as composite-type cathodes and their surface oxygen exchange behavior was investigated using the pulse isotopic exchange (PIE) technique.

$\text{BaZr}_{0.9}\text{Sc}_{0.1}\text{O}_{2.95}$ (BZS10) was prepared using a solid-state reaction method by sintering at 1300 °C for 10 h. To prepare the composite powders, BZS10 powders were ball-milled with x vol% Co_3O_4 ($x = 1, 3, 5, 10$, and 50). Prior to PIE, their specific surface area was determined by a BET method for the sample powder heat-treated at 630 °C and 880 °C, which is slightly higher than the highest PIE temperature to avoid morphological and compositional change during PIE. The PIE was performed at 800–200 °C under a 10% O_2 atmosphere.

Based on the almost constant lattice constants, regardless of the Co_3O_4 volume fraction, the composites heat-treated at 630 °C were successfully prepared in a dual-phase state, unlike Co-doped BZS10 prepared at 1225 °C, which showed a decrease in the lattice constant [3]. At 500 °C, the surface oxygen exchange rate R_0 of BZS10 without Co_3O_4 particles was approximately 4×10^{-6} mol/m²·s. R_0 was surprisingly enhanced by an order of magnitude with the addition of only 1 vol% Co_3O_4 . Further addition of Co_3O_4 exceeding 10 vol% reduced R_0 . This trend indicates that the optimum amount of Co_3O_4 provided sufficient dissociated oxygen on BZS10, which was readily incorporated into BZS10. Their electrochemical properties and detailed microstructural analyses are also discussed.

References

- [1] Y. Tomura *et al.*, J. Mater. Chem. A, **8** (2022) 21634–21641.
- [2] A. Ishii *et al.*, ACS Appl. Mater. Interfaces, **15** (2023) 34809–34817.
- [3] H. Uehara *et al.*, Int. J. Hydrogen Energy, **47** (2022) 5577–5584.

Revealing the Surface Termination Effect of Perovskite for Oxygen Exchange Reaction

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Key Words: electroceramics; surface termination; SOFCs; oxygen exchange; high-temperature electrochemistry

Surface atomic structure plays a critical role in the activity and reaction mechanism of SOFC electrode. However, precise control of uniform single termination for electrochemical solid/gas interface remains challenging. In this study, we developed an atomically flat epitaxial (La,Sr)FeO_{3-x} thin film (Figure 1) to understand how a single atomic termination influences oxygen exchange activity and the corresponding reaction mechanism.

Specially, the oxygen exchange activity exhibited a typical volcano-shaped relationship with surface termination. A single terminated LSF demonstrated the highest activity compared to other counterparts under both equilibrium and polarization conditions, showing up to more than 30-fold enhancement. A framework combining experimental micro-kinetic analysis through electrochemical and operando spectroscopic measurements with density functional theory calculation reveals that single termination induces a switch in the rate-determining step from a sole oxygen dissociation step to two comparable steps by significantly reducing the energy barriers for oxygen dissociation.

This study emphasizes the critical role of the top surface termination in regulating oxygen exchange kinetics and reaction mechanisms. Furthermore, this work provides a new framework applicable to extensive structure-activity studies on diverse solid/gas interface reaction systems.

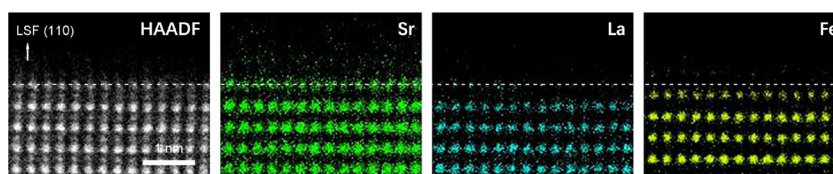


Figure 1 – Atomic-resolution EDX mapping of the surface region of SrO terminated LSF. Along the dashed line representing the top layer of the surface.

Mobility and clustering of O and anion vacancies in perovskites as energy materials

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Keywords : perovskites, anion vacancies, clustering

Perovskites ABX_3 exhibit the full range of electric, ferroelectric, magnetic, and ion conducting properties, depending on the choice of the constituents. In particular, they may be ionic conductors, through anion vacancies (V_X) or intercalation of small cations, finding application in fuel cells and as electrodes or catalysts in supercapacitors and batteries [1]. This talk presents results, partly published in [2-4], on the mobility and clustering of O vacancies in $(Ba,Sr,Ca)(Ti,Zr)O_{3-\delta}$ and halide vacancies in metal-organic halides, obtained by measuring the complex Young's modulus as a function of temperature and frequency. The ionic mobility is generally measured with methods that average the microscopic mechanisms of free diffusion, trapping and clustering. However, these processes can be selectively investigated through anelastic spectroscopy, which is the mechanical analogue of dielectric spectroscopy, since the V_X in perovskites lack electric dipoles but possess elastic dipoles. The anelastic spectra can reveal Debye relaxations corresponding to different types of vacancy jumps—whether they are isolated, paired, or trapped by other defects or dopants—allowing for the measurement of their respective activation energies (see figure).

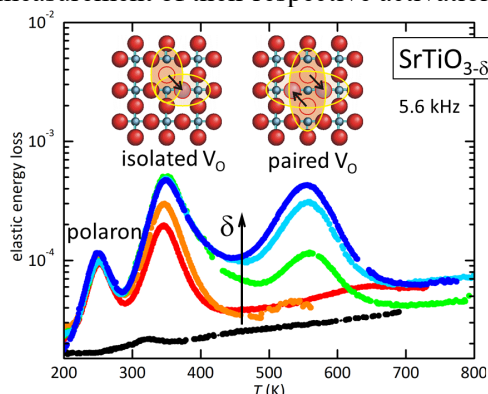


Fig. 1 Elastic energy loss coefficient $Q^{-1} = E''/E'$ of the dynamic Young's modulus E of $SrTiO_{3-\delta}$ measured at $f = 5.6$ kHz. When increasing the O deficiency δ , peaks due to hopping of isolated and paired V_O develop. The insets show the reorientations of the corresponding elastic dipoles. The peaks are centred at the temperatures where the conditions $2\pi f\tau(T) \cong 1$ are met, so allowing the mean hopping times τ and their activation energies to be measured by varying f .

Titanate perovskites are generally used as ferroelectric or dielectric materials rather than ion conductors, but the results presented here should be relevant also to the ion conducting compositions. It is shown that even at very low concentrations of V_O , $\delta < 0.01$, and in the absence of other defects, the V_O in $(Ba,Sr)TiO_{3-\delta}$ form linear V_O —Ti— V_O pairs and longer chains, relatively stable up to >600 K, and the same occurs in $(Ba,Ca)(Ti,Zr)O_{3-\delta}$, with much larger lattice disorder. The isolated V_O are quite mobile, with activation energy $E \sim 0.6$ — 0.7 eV, while the reorientation rate of the pairs requires $E \sim 0.9$ — 1.4 eV. The overall mobility is limited by the fraction of slow pairs and this explains why macroscopic methods generally find $E \sim 1$ eV in perovskite titanates.

It is also shown that the clustering of the V_O strongly affects the electronic properties through the localization of two electrons in the Ti^{2+} ions belonging to the pairs or chains. This fact is probed in the present experiments through the dependence of the Curie temperature on aging and thermal history, which affects the fraction of isolated and aggregated V_O .

Similar phenomena are expected to play a role also in perovskites used as electrodes or catalysts in supercapacitors and batteries, both when the V_O determine the mobility of the anionic carrier and when they modulate the lattice volume and hence affect the mobility of the intercalated cations.

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Nanostructure and Chemical State Imaging of Energy Materials by Coherent X-ray Diffraction

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⁴ *RIKEN SPring-8 Center*

Keywords : Synchrotron radiation, Coherent X-ray diffraction imaging, Energy materials

Coherent X-ray diffraction imaging (CXDI) is a lensless imaging technique based on the measurement of coherent diffraction patterns and phase retrieval calculation, which can realize high spatial resolution beyond the limitation of lens-based X-ray microscopy. In particular, scanning CXDI, also known as X-ray ptychography, is a technique that is rapidly gaining popularity in synchrotron radiation facilities, allowing micrometer-sized objects to be observed with nanoscale resolution. So far, we have developed a high-resolution and high-sensitivity X-ray ptychography apparatus at SPring-8 [1], and have applied it to nanoscale structural imaging of various samples. X-ray ptychography using multiple energies including the absorption edge of a specific element, which is often referred to as X-ray spectroscopic ptychography, enables us to visualize not only nanoscale structures but also chemical states. So far, we have applied it to the observation of catalysts [2] and battery [3, 4] materials. The 3 GeV high-brilliance synchrotron radiation facility NanoTerasu, which commenced operations in April 2024, provides higher brilliance synchrotron radiation than SPring-8 in both the soft X-ray and tender X-ray regions. We have performed the first experiment of tender X-ray ptychography at NanoTerasu. The coherent diffraction patterns from a micrometer-sized particle of sulfurized polymer were collected, and then the phase image was reconstructed with resolutions of sub-50 nm [5]. In the near future, tender X-ray ptychography with sub-10 nm resolution is anticipated to potentially revolutionize the visualization of nanoscale structures and chemical states in various energy materials composed of light elements.

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Layered Manganese Dioxide as a Heat-Storage Material Utilizing Environmental Water Vapor

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Keywords : water intercalation, heat of hydration, interlayer cation

The significance of heat storage technologies has been increasing in terms of the efficient utilization of low-grade waste heat (100–200°C) occupying more than 60% of the industrial waste heat for the realization of a carbon-neutral society. Heat storage materials, which can store heat energy and release it as needed, have several different types, including sensible heat, phase-change, chemical reaction, and chemisorption. Although chemical-reaction and chemisorption types that utilize oxidation/hydration reactions have a high heat storage energy density, their heat-storing (i.e., charging) temperature is too high and, furthermore, they lack cyclability and reversibility due to large structural/volumetric changes. Phase-change materials using sensible heat or latent heat show excellent reversibility of heat absorption/release but have low heat storage energy density and difficulty in maintaining the heat-stored (high enthalpy) state. Therefore, a new material with a new heat storage mechanism that has all the properties required for heat storage materials (high energy density, relatively low charging temperature, fast charge/discharge capability, reversibility, resourcefulness, environmental compatibility, etc.) is desired.

The birnessite-type layered manganese dioxide (δ -type MnO_2), one of polymorphs of manganese dioxide possessing a layered structure with MnO_2 layers stacked in the c -axis direction, is generally known to accommodate alkaline metal cations (K, Na, etc.) as well as H_2O molecules in the interlayer space for phase stabilization [1]. Our research group has found that these accommodated H_2O molecules (0.5 mol- H_2O per mol- $\text{K}_{0.33}\text{MnO}_2$) can be reversibly extracted/inserted from/into the interlayer of MnO_2 layers at 100–140°C under ambient atmosphere via a water (de)intercalation mechanism with small structural/volumetric changes (see Figure 1) [2]. We have demonstrated that this K-containing layered MnO_2 exhibits a volumetric heat energy density of $\sim 1000 \text{ MJ m}^{-3}$ with high charge/discharge rate, cyclability, and stability. This material can store heat at a relatively low temperature of 100–140°C, which is equivalent to low-grade waste heat, and can release heat by absorbing the environmental moisture, making it suitable for various heat storage applications.

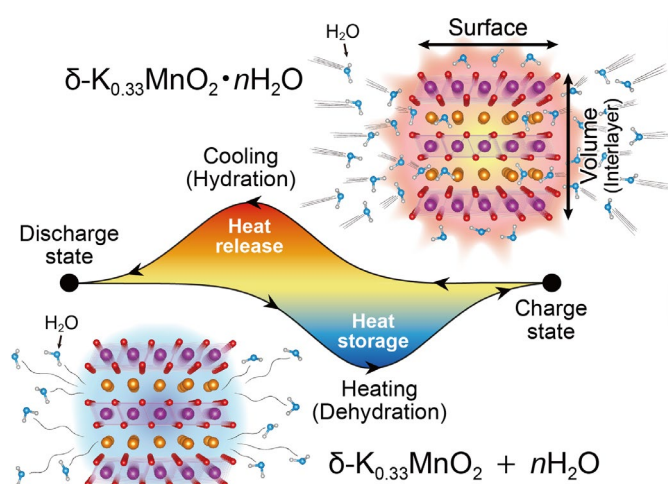


Figure 1. Schematic illustration of heat storage/release operation of the layered manganese dioxide utilizing endo/exothermic reactions by desorption/absorption of the environmental moisture.

References

- [1] A. C. Gaillot, et al., *Chem. Mater.* 2003, 15, 24, 4666–4678.
- [2] T. Hatakeyama, N. L. Okamoto, S. Otake, H. Sato, H. Li, and T. Ichitsubo, *Nat Commun* **13**, 1452 (2022).

A new AB₃-based alloy with reversible hydrogen absorption and desorption reactions and less degradation

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T. Honda⁵, H. Sagayama⁵, S. Takagi², T. Kono⁶, H. Yang^{7, 8}, W. Luo⁹, L. Lombardo¹⁰,
A. Züttel^{7, 8}, S. Orimo^{1, 11}

IMR, Tohoku Univ.¹, QST², Shibaura Inst. of Tech.³, PSI⁴, KEK⁵, Univ. of Tokyo⁶,
EPFL Valais/Wallis⁷, Empa⁸, Shanghai Univ.⁹, Kyoto Univ.¹⁰, AIMR, Tohoku Univ.¹¹

Keywords : Hydrogen storage materials, Crystal structure, Neutron diffraction

Intermetallic compounds AB_x (A: Element in Group 1-5, B: element in Group 6-12 in the periodic table, $0 < x \leq 5$) store hydrogen atoms in interstitial sites in their lattices and release hydrogen gas. Since AB_x exhibits compact hydrogen storage compared to gaseous and liquid hydrogen, they are a promising hydrogen storage material. Although LaNi₅-based alloys have been industrially used for hydrogen storage materials, new materials with reversible hydrogen absorption and desorption reactions at moderate conditions, less degradation and higher hydrogen storage capacity have been demanded.

Recently, we reported (Y, Mg)(Co, Ni)₂, which was synthesized from YCo₂ and MgNi₂, with reversible hydrogen absorption and desorption reactions at 303 K.^{1,2} In the results, their equilibrium hydrogen pressures and hydrogen storage capacities were depended on amounts of Mg and Co. On the other hand, using YCo₂ and MgCo₂ as starting materials, (Y, Mg)Co₃ were formed instead of (Y, Mg)Co₂. Interestingly, (Y, Mg)Co₃ exhibited reversible hydrogen absorption and desorption reactions at 303 K. The crystal structure and chemical composition of (Y, Mg)₃ was determined by synchrotron radiation X-ray diffraction and became to be Y_{0.68}Mg_{0.32}Co_{3.00}. In addition, hydrogen absorption and desorption reactions were investigated up to 100 cycles. The cycling results exhibited less degradation, which meant maintaining of hydrogen storage capacities, equilibrium hydrogen absorption and desorption pressures (Figure 1), crystallinities, and so on.

To understand the reactions viewed from atomic arrangements, we observed crystal structures by neutron diffraction under D₂ pressure.

Based on the Rietveld refinements on the neutron diffraction data, the experimentally observed neutron diffraction patterns before and after deuterium absorption reactions were reasonably reproduced by rhombohedral crystal structure models ($a = 4.99719(67)$ Å and $c = 24.16062(533)$ Å before D₂ absorption reaction, and $a = 5.27370(64)$ Å and $c = 25.68827(553)$ Å after D₂ absorption reaction).

In the E-IMR International Workshop 2024, we will introduce hydrogen storage materials and present details of syntheses, hydrogen storage properties, and crystal structures of Y_{0.68}Mg_{0.32}Co_{3.00}.

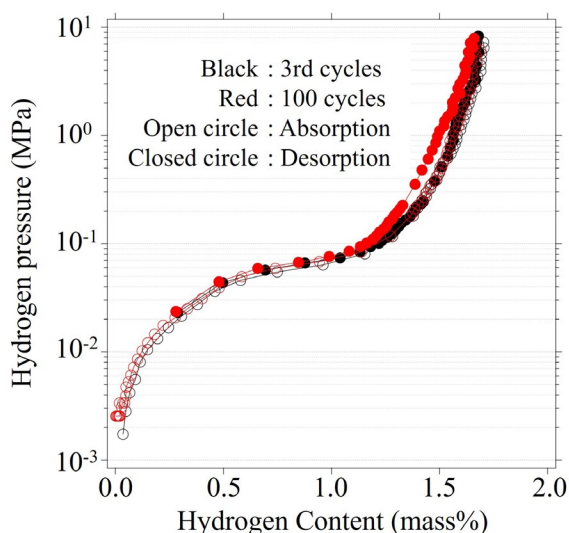


Fig. 1 Hydrogen absorption and desorption reactions of Y_{0.68}Mg_{0.32}Co_{3.00} at 303 K. Black and red indicate on the 3rd and 100th cycles, respectively. Open and closed circles indicate absorption and desorption, respectively.

References:

- 1) T. Sato et al., J. Phys. Chem. C 126, 16943-16951 (2022).
- 2) T. Sato et al., ACS Omega 5, 31192-31198 (2020).

Interface Design for Room-Temperature Rechargeable Magnesium Batteries with Transition Metal Oxide Cathodes

Hongyi Li, Xiatong Ye, Yue Qi, Norihiko L. Okamoto and Tetsu Ichitsubo
Institute for Materials Research, Tohoku University

Keywords : solvation environment, electrode-electrolyte interface, surface modification

It is essential to develop rechargeable batteries that offer high safety, long cycle life, and low production costs towards the construction of sustainable energy systems. Among the candidate technologies, rechargeable magnesium batteries (RMBs) have emerged as a promising alternative due to their lower resource limitations compared to commercial lithium-based batteries. However, progress in the development of RMBs has stagnated since the initial report of a prototype system that combined a Chevrel phase cathode (Mo_6S_8) with a Cl-contained electrolyte.[1] To promote the practical application of RMBs, researchers have aimed at improving oxide cathodes with higher potential and capacity, alongside developing non-corrosive, Cl-free electrolytes capable of reversible magnesium deposition and dissolution and good chemical stability.

These efforts have significantly advanced the field in recent years. Specifically, transition metal oxides, such as hollandite-type MnO_2 , have demonstrated the ability to support genuine Mg^{2+} intercalation through a metastable phase transformation pathway.[2] Additionally, electrolytes that dominated by solvent-separated ion pairs (SSIPs), such as $\text{Mg}[\text{B}(\text{hfp})_4]_2$ in G3 (triglyme), can effectively prevent the passivation of Mg metal anodes and offer a wide potential window.[3] However, in construction of full cells with these oxide cathodes and SSIP-dominated electrolytes, complex side reactions usually occur due to the absence of stable electrode-electrolyte interface, which leads to rapid structural degradation of the oxide cathodes and the progressive consumption of the electrolyte during cycling.[4]

To pave the way for a new era of RMBs, in this presentation, we highlight our efforts to clarify the relationship between the solvation environment of electrolytes and the interfacial reaction behavior on both oxide cathodes and Mg metal anodes. Based on these findings, we further propose several effective strategies to stabilize the oxide cathode interface to suppress unwanted side reactions in full cells with SSIP-dominated electrolytes.

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Recent Advances of Silicon Crystal for Solar Cells

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Keywords : silicon, solar cell, crystal growth

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Last two decades, photovoltaic industry has increased rapidly all over the world. In 2023, 390 GW solar cells were installed, and increased about 70% in comparison with the installation of solar cells in 2022. The total accumulated installation is about 1500 GW. Clearly, the photovoltaic has been an important renewable energy source in the world.

Silicon crystal, specially Czochralski (Cz) silicon, is the mainstream material for solar cells, and currently occupies ~ 98% market share in photovoltaic industry. In this talk, recent advances of silicon crystal for solar cells, including the high purity polycrystalline silicon used as the raw material and Cz silicon, is reviewed.

Trichlorosilane (TCS) process and Fluidized bed silane (FBS) process are two main processes to fabricate high purity polycrystalline silicon. In recent years, the mount of raw silicon materials increases step by step and reaches to 16% market share. In the talk, the progress of technical parameters including production rate, production cost, energy consumption, silicon consumption and et al are analyzed.

The growth technology of silicon crystal also includes two methods, (Cz) silicon and multicrystalline (mc) silicon. In current, Cz Si becomes the main material due to its high quality of crystal which is suitable for the fabrication of higher efficiency solar cells, such as PERC, TopCon and HJT cells. In the talk, the RCz growth technology is introduced. The growth parameters, including dopant, diameter of crystal, inner diameter of furnace, crucible size, production yield, pulling rate, power consumption and so on, are discussed. Furthermore, the property of oxygen impurity, as the main impurity in Cz silicon, and its effects on solar cells is also presented.

Probing the Multipolar Structure of Berry Curvature in Magnetization Space by the In-plane Anomalous Hall Effect

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Keywords : Berry Curvature, anomalous Hall effect

Berry curvature is a fundamental concept underlying numerous phenomena in condensed matter physics. While prior researches have primarily concentrated on the structure and distribution of Berry curvature in real space and reciprocal space, its geometric properties in other parameter spaces remain unexplored. In this work, we reveal the multipolar structure of Berry curvature in magnetization space through Hall measurements and demonstrate its universal presence in various ferromagnetic materials. Our experiments show that Berry curvature multipoles can induce an anomalous Hall effect (AHE) under in-plane magnetization, a configuration distinct from the conventional out-of-plane scenario. Through the measurements of the in-plane AHE in Fe, Ni, and Cr_{1.2}Te₂, we quantitatively resolve the AHE contributions beyond the magnetization dipole term of Berry curvature, which exhibit distinct magnetization angle dependencies consistent with our theoretical predictions. This study provides direct experimental evidence of the multipolar structure of Berry curvature in magnetization space, fundamentally expanding the origins of the AHE and other Berry curvature-driven effects in magnetic systems.

Reference:

Wenzhi Peng et al., arXiv:2402.15741

Formation Rate as a Key Factor in Enhancing the Stability of Anode-Less Lithium Metal Batteries

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Keywords : Li-Ion Batteries, Anode-less Batteries, Formation protocol

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Lithium-metal (Li-metal) anodes have been studied since the 1970s due to their high specific capacity, low redox potential, and low density, making them an ideal alternative to traditional graphite anodes. However, Li-metal's processing complexities, including the need for controlled oxygen and moisture free environments, complicate manufacturing and increase costs. To address these challenges, anode-free lithium-metal batteries (AFBs) have recently been proposed. In AFBs, a copper foil serves as the anode current collector, allowing Li to plate and strip during cycling. Despite theoretical benefits in battery performance and simplicity of manufacture, AFBs experience rapid capacity loss due to lithium depletion during cycling, as they lack excess Li reserves as is the case with Li metal foils.

Research has proposed various solutions to improve AFB stability, such as enhanced current collector designs, advanced electrolytes, and optimized cycling protocols, which all improve the battery performance. In this work, we look at a synergetic alternative approach, where we investigate how different current densities (CD) during initial formation cycles affect AFB cycling stability. Varying CD levels in formation cycles influence the Li structure and solid-electrolyte interphase (SEI) composition on the anode, affecting Li-metal stripping during discharge. Optimal formation CD varies by electrolyte composition, suggesting that customized protocols are essential for AFBs.

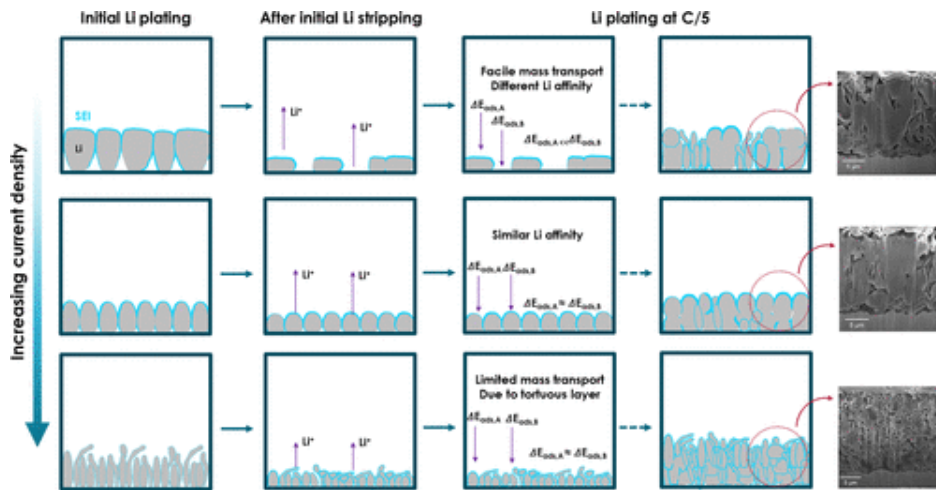


Figure1: Schematic of how different formation current densities affect the morphology of plated Li and influences the long term stability of AFBs.

Depending on the initial charging CD, Li-metal with different morphologies and SEIs with different chemical compositions were formed, which affect the Li plating and stripping during cycling (see figure 1). Unlike classic anodes, which are best formed very slowly, we found for three different classes of electrolytes that the most stable cycling behavior was observed for cells formed at the highest CD before Li dendrites were developed. This CD is a unique property of the specific electrolyte used, and the rationale developed herein offers a powerful tool to identify and optimize the formation conditions.