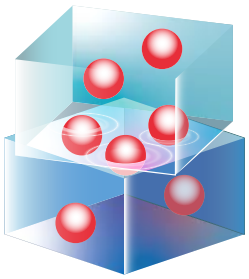


Interface IONICS

Science on Interfacial Ion Dynamics for Solid State Ionics Devices

Newsletter Vol.5

March 2022

Interface Ionics toward Sustainable Society

2019 – 2023 Japan Society for the Promotion of Science
Grant-in-Aid for Scientific Research on Innovative Areas

Preface

The postponed Olympics and Paralympic Games Tokyo 2020 were held in the summer of 2021, and a variety of electric vehicles with modern forms supported Tokyo 2020. In September, an electric car that led the marathon course was powered by an all-solid-state battery, and its driving movie was released. At the same time, the electrode–solid electrolyte interface issues affecting the lifespan of all-solid-state batteries (SSBs) were highlighted. The COP26 meeting held in November outlined a target that all new vehicle sales by 2040 should be "Zero Emission" like electric vehicle that emit no CO_2 during the driving. We hope that our achievements of Interface IONICS will contribute to the further improvement of SSBs and then sustainable society. While the vaccination rate is increasing, the global end of COVID-19 may take more time because of the emergence of new mutant strains. We would like to continue our domestic and international collaborative research activities via online and limited face-to-face meetings.

Yasutoshi Iriyama, Principal Investigator
Nagoya University

Contents

Member Introductions

Researchers

Gp-A02

Hirofumi Tsukasaki

Osaka Prefecture Univ. Specially-appointed Associate Professor (Mori Gr.)
/ Transmission electron microscopy

I obtained my PhD in 2016 from Waseda University, where I analyzed the domain structure of ferroelectrics using transmission electron microscopy (TEM). Thereafter, I moved to materials science research at Osaka Prefecture University as a postdoctoral fellow under Professor Shigeo Mori. Since April 2021, I have been involved in the Interface IONICS project as a specially appointed associate professor. My current research focuses on glass and glass ceramics, whose physical properties are affected by their crystallite size, crystallinity, and crystal/amorphous interface structure. To understand their ionic conduction mechanism, I am currently analyzing the microstructure of glasses and glass ceramics by TEM. Figure 1 shows a high-resolution TEM image of Li_3PS_4 glass, where Li_3PS_4 nanocrystallites are dispersed in an amorphous matrix. Figure 2 shows dark-field images capturing the crystallization process of $Li_{10}GeP_2S_{12}$ glass. Nanocrystallites precipitate upon heat-treatment of the glass, as denoted by the bright contrast. I would like to contribute to the development of materials for all-solid-state batteries by utilizing various TEM observation techniques.

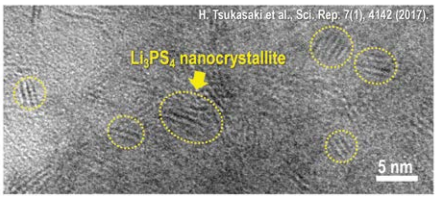


Figure 1. High-resolution TEM image of Li_3PS_4 glass.

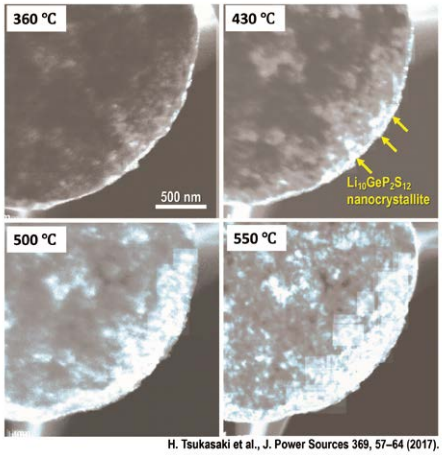


Figure 2. Dark-field images of the $Li_{10}GeP_2S_{12}$ glass heated in a TEM.

Gp-A04

Wataru Namiki

NIMS Postdoctoral Researcher (Tsuchiya Gr.)
/ Solid state ionics

I received my PhD from Tokyo University of Science in 2021. My research focuses on nanoionic devices with magnetic properties, for memory storage and artificial intelligence. In my PhD course, I fabricated an all-solid-state redox device with a solid-state Li-ion conductor (Fig. 1); this device could manipulate the magnetic anisotropy *in situ*. I also established a quantitative method to analyze the direction of spontaneous magnetization in a stacked device structure. The developed technique represented a breakthrough new manipulation method that enables the rotation of magnetization vectors (56°) at room temperature. In addition, substantial manipulation of the magnetic anisotropy could also be achieved (lowered as much as 40%) (Fig. 2). Such technology is applicable to new-generation devices with spin dynamics, e.g., spin–torque oscillators and spin-wave waveguides. At present, I am actively involved in the study of artificial intelligence with nanoionic devices.

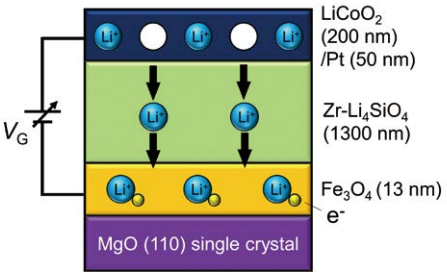


Figure 1. Schematic of an all-solid-state redox device.

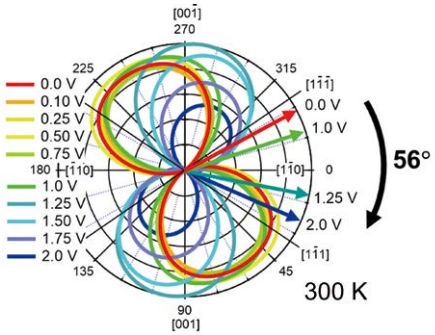


Figure 2. Distributions of magnetic anisotropy variations at various gate voltages.

Research Assistants

Gp-A01

Satoshi Yamamoto

Nagoya Univ. M2 (Iriyama Gr.)
/ Electrochemistry, Solid state ionics

My research subject is the elucidation of Li^+ insertion/extraction mechanisms in the graphene/LiPON (lithium phosphorus oxynitride glass) system. The Li^+ desolvation reaction is the rate-limiting process for the Li^+ insertion reaction into graphite in an organic liquid electrolyte, and this reaction is absent in a solid electrolyte such as LiPON.

Epitaxial graphene with controlled layer numbers can be synthesized by thermal decomposition of single-crystalline SiC. Hence, using SiC-derived graphene with an amorphous LiPON electrolyte enables the study of a model interface of graphite (graphene)/solid-state electrolyte.

I often visit Prof. Norimatsu's group (A01) at Nagoya University to prepare graphene samples and also collaborate with Prof. Kumatani's group (A02) at Tohoku University on scanning electrochemical microscopy experiments. Visiting other labs is very exciting for me, and I am grateful to have had the opportunity to participate in this project. There are still numerous aspects of my research that I feel I do not fully understand, but I intend to do my best while enjoying research.

Figure. Instrument for preparing epitaxial graphene samples via thermal decomposition of SiC.

Gp-A02

Masaki Abe

Tohoku Univ. M2 (Takahashi Gr.)
/ X-ray microscopy

Since I was assigned to the Takahashi group in 2020, I have been working on developing an X-ray ptychographic measurement system for use in the "tender" X-ray region (2–5 keV). X-ray ptychography using coherent X-rays is a lensless microscopy technique that provides real-space sample images with a resolution of several tens of nanometers or better. We can also obtain chemical-state images of a sample by analyzing the spatially resolved absorption spectra obtained using ptychographic measurements at continuous energies near the absorption edge of the target elements. We are the first group to establish a ptychographic measurement system in the tender X-ray region and have successfully obtained spatially resolved absorption spectra (~24 × 24 nm^2) of sulfur-containing polymer particles at the S *K*-edge (~2.47 keV) (right figure). One of the promising applications of this method is cathode-active materials of lithium–sulfur batteries, and we aim to elucidate the reaction and degradation mechanisms of these materials during the charge–discharge process by conducting operando measurements.

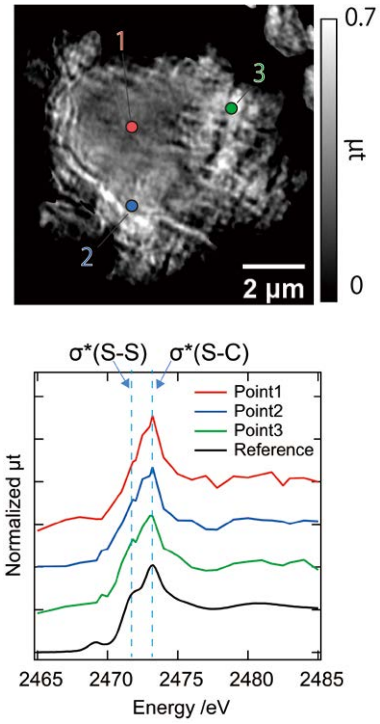


Figure. Reconstructed image of a sulfur-containing polymer particle (top) and the spatially resolved absorption spectrum (~24 × 24 nm^2) obtained from the image (bottom).

Research Achievements

2021.7– 2021.12

Gp-A01 Model Interface

Gp-A01 has provided model electrode materials such as epitaxial thin-film electrodes and single-crystalline solid electrolytes to its members, and collaborative research with Gp-A02 and Gp-A03, in addition to that within Gp-A01, has progressed continually. A low-resistive graphene–solid electrolyte interface was realized by eliminating the desolvation process commonly observed in organic liquid electrolyte systems. In addition, a standard solid-state battery fabricated using NASICON-structured LATP combined with $Fe_2(MoO_4)_3$ electrodes that can be treated even in air was proposed. The results are highlighted as follows.

Highlight 1 A01-A02 joint paper

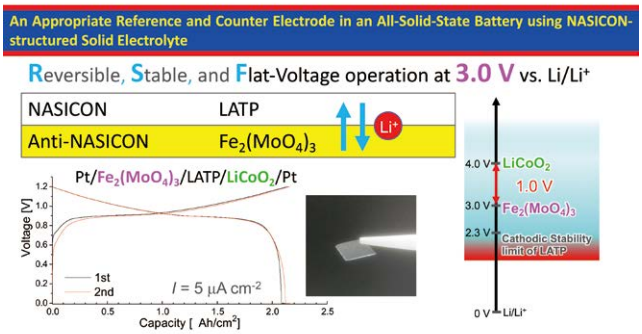
An appropriate reference and counter electrode in an all-solid-state battery using NASICON-structured solid electrolyte

Y. Kee, Y. Suzuki, N. Ishigaki, M. Motoyama, Y. Kimura, K. Amezawa, Y. Iriyama.

Electrochem commun vol. 130, 107108 (2021)
https://doi.org/10.1016/j.elecom.2021.107108

Abstract

Anti-NASICON-structured $Fe_2(MoO_4)_3$ (FMO) thin films are formed on NASICON-structured LATP solid-state electrolyte by pulsed laser deposition. The FMO thin films operate at 3.0 V flat voltage vs. Li/Li$^+$ within the potential window of LATP. The FMO thin films on LATP operates as with that in conventional organic liquid electrolyte. Combining crystalline electrode-solid electrolytes with a similar framework structure at relatively low temperatures will play an important role in realizing reversible electrode reactions. An all-solid-state battery, FMO/LATP/$LiCoO_2$, is developed to apply the FMO as a reference and counter electrode, and the SSB operates at 1.0 V without visible capacity fading. [Reproduced with permission of Elsevier]



Highlight 2 A01 Research Gp Public Offering joint paper

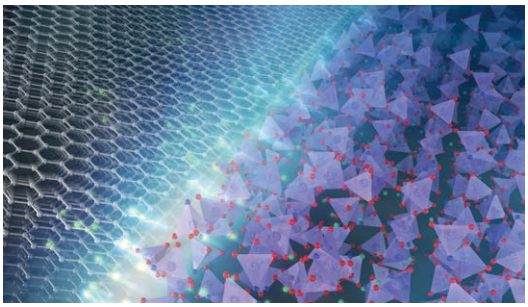
Charge/discharge reactions via LiPON/multilayer-graphene interfaces without Li$^+$ desolvation/solvation processes

M. Motoyama, K. Miyoshi, S. Yamamoto, R. Sakakibara, Y. Yamamoto, T. Yamamoto, W. Norimatsu, Y. Iriyama.

ACS Appl. Energy Mater. vol. 4, 10442 (2021)
https://doi.org/10.1021/acsaem.1c00628

Abstract

Li$^+$ desolvation process has been regarded as the rate-limiting process in Li$^+$ insertion reaction with graphite anode in lithium-ion batteries. In contrast, Li$^+$ desolvation process is absent in solid-state batteries. We fabricated thin-film all-solid-state cells by depositing lithium phosphorus oxynitride glass (LiPON) electrolyte onto a multilayer-graphene (MGr) film by RF magnetron sputtering and measured the charge/discharge performance of the cells. The charge transfer resistance at the LiPON/MGr interface was significantly small, although the LiPON/MGr interface was supposed to have inorganic solid electrolyte interphase resulting from the LiPON reduction decomposition. Consequently, the dominant factor for the overall overpotential was the ohmic loss for LiPON, and hence the capacity retention was still maintained at 60% even at nearly 900C when the LiPON film thickness was 4 μm. [Reproduced with permission of the American Chemical Society.]



Gp-A02 Advanced Analysis

This group aims to understand unique ion transport/storage phenomena at solid-state interfaces through comprehensive analyses. We have been establishing/improving various novel and advanced analytical techniques and systematically applying them to typical model solid-state interfaces, such as a well-defined film electrode on a solid electrolyte and glass-ceramic electrolytes, which were supplied by Gp-A01 and Gp-A04, respectively. Based on the obtained results, together with assistance from theoretical calculations and simulations conducted by Gp-A03, we will establish scientific principles that enable the design of high-performance solid-state interfaces.

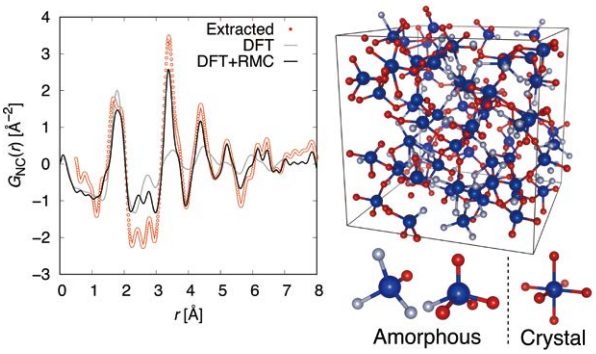
Highlight 3

Structural characterization of the delithiated noncrystalline phase in a Li-rich Li_2VO_2F cathode material

S. Hiroi, K. Ohara, O. Sakata.
Chem. Mater. vol. 33, pp. 5943–5950 (2021)
https://doi.org/10.1021/acs.chemmater.1c01466

Abstract

As a cathode material for lithium-ion batteries, the disordered rock-salt-type Li_2VO_2F has a high theoretical capacity of 462 mA h/g; however, this capacity fades rapidly upon cycling. The atomic pair distribution function obtained from the X-ray total scattering measurements indicates that the disordered rock-salt crystal partially transforms to an amorphous phase on delithiation. Using the extracted structural information of the amorphous phase, a three-dimensional atomic configuration was modeled by a combination of the density functional theory and reverse Monte Carlo method. The structural model constructed the tetrahedral or pyramidal structure by V and anions.



These polyhedral structures are likely to involve the anion transfer between the crystalline and amorphous phases. It induces the concentration fluctuation of anions, O and F, in the crystalline phase and might be a factor for capacity fading of the Li_2VO_2F cathode material. [Reproduced with permission of the American Chemical Society.]

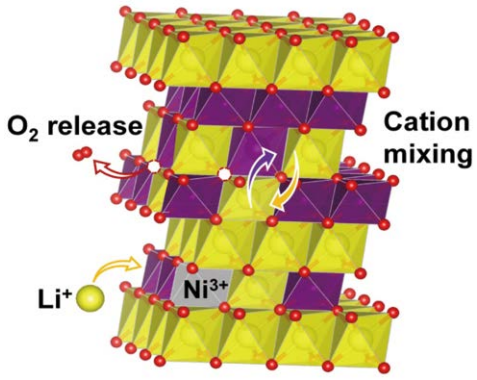
Highlight 4

Lattice oxygen instability in oxide-based intercalation cathodes: A case study of layered $LiNi_{1/3}Co_{1/3}Mn_{1/3}O_2$

X. Hou, K. Ohta, Y. Kimura, Y. Tamenori, K. Tsuruta, K. Amezawa, T. Nakamura.
Adv. Energy Mater. vol. 11, pp. 2101005 (2021)
https://doi.org/10.1002/aenm.202101005

Abstract

Lattice oxygen stability in layered rock-salt $LiNi_{1/3}Co_{1/3}Mn_{1/3}O_{2-\delta}$ is investigated with a focus on oxygen release behavior and relevant changes in crystal and electronic structures. Release of lattice oxygen facilitates cation mixing, transition metal slab expansion, and Li slab contraction, thus deteriorating the layered structure. As is revealed by X-ray absorption spectroscopy, in the beginning stage of oxygen release, the charge balance is compensated by selective reduction of Ni^{3+}. This suggests that high valent Ni generated by delithiation or negative defect species, that is, lithium at the transition metal site, aggravates oxygen release severely. These findings



provide a new research direction and guidelines for the stabilization of lattice oxygen in oxide-based intercalation cathodes. [Reproduced with permission of the Wiley-VCH GmbH.]

Gp-A03 Computational & Data Science

To construct a new theoretical framework for Interface IONICS, Gp-A03 has introduced two strategies: a computational approach and a data science approach. With the development of several novel techniques and deep collaboration with the other experimental groups (Gp-A01, -A02, and -A04), we have achieved a new understanding of interfacial phenomena. Recently, two molecular dynamics studies based on machine-learning potential provided novel insights into the mixing and migration of atoms and ions, leading to a deeper understanding of ionics.

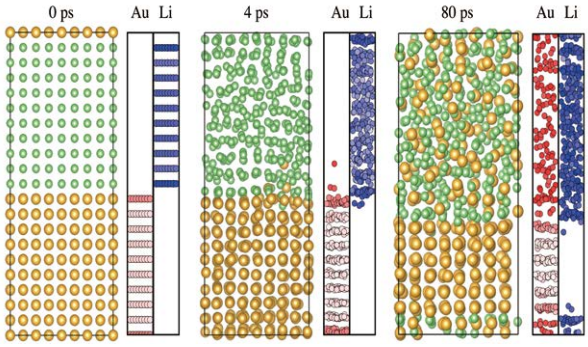
Highlight 5

Phase stability of Au-Li binary systems studied using neural network potential

K. Shimizu, E.F. Arguelles, W. Li, Y. Ando, E. Minamitani, S. Watanabe.
Phys. Rev. B vol. 103, pp. 094112 (2021)
https://doi.org/10.1103/PhysRevB.103.094112

Abstract

The miscibility of Au and Li exhibits a potential application as an adhesion layer and electrode material in secondary batteries. To explore alloying properties, we constructed a neural network potential (NNP) of Au-Li binary systems based on density functional theory (DFT) calculations. Using the constructed NNP, we investigated the mixing energy of $Au_{1-x}Li_x$ with fine composition grids, showing excellent agreement with DFT verifications. We found the existence of various compositions with structures on and slightly above the convex hull. Moreover, we found other stable phases.



Finally, we examined the alloying process starting from the phase separated structure to the complete mixing phase. We found that when multiple adjacent Au atoms dissolved into Li, the alloying of the entire Au/Li interface started from the dissolved region. [Reproduced based on Creative Commons license (CC BY 4.0).]

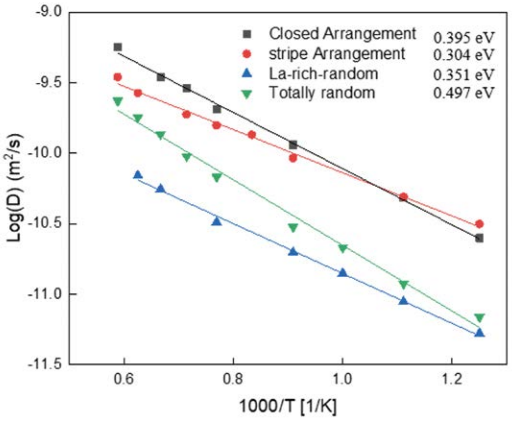
Highlight 6

Exploring the diffusion mechanism of Li ions in different modulated arrangements of $La_{(1-x)/3}Li_xNbO_3$ with fitted force fields obtained via a metaheuristic algorithm

Z. Yang, R. E. Ward, N. Tanibata, H. Takeda, M. Nakayama, R. Kobyashi.
Solid State Ion vol. 366-367, pp. 115662 (2021)
https://doi.org/10.1016/j.ssi.2021.115662

Abstract

Li ion conductivity of A-sites deficient perovskite-type $Li_xLa_{(1-x)/3}NbO_3$ (LLNO) has been investigated by materials simulation. Our previous reports revealed that two types of modulated structures, namely closed and striped structures, derived from cation/vacancy arrangements coexist in the La-rich layer, which affects Li-ion migration. In this study, DFT-derived force-field molecular dynamics (FFMD) simulations were performed to investigate the effect of a modulated structure on the migration behavior of Li ions in LLNO compounds. The results indicate that the type of modulated arrangements of La/Vac has a significant influence on the migration of Li ions. Moreover, the estimated diffusion coefficients of the modulated structures are higher by a factor of 10 than those of La/Vac disordered models at 800 K. The migration energy in



the ab plane appeared to be much lower than along the c-axis, controlling the modulated arrangement of LLNO is beneficial to eliminate La-ion blockage during long-distance migration. Accordingly, the present study reveals that the controlling cation/Vac arrangement at perovskite A-sites is crucial for achieving high Li-ion conductivity. [Reproduced based on Creative Commons license (CC BY 4.0).]

Gp-A04 Design of Functional Interface

Gp-A04 designs innovative solid-state ionics materials (SSIMs) through interface engineering. With an increase in the concentration of grain boundaries, charge carriers are efficiently accumulated in SSIMs, resulting in new structures and functionalities. Such functionalities have been applied to new solid-state ionics devices. Collaborative studies with members of Gp-A02 and Gp-A03 have further accelerated the development of new solid-state devices.

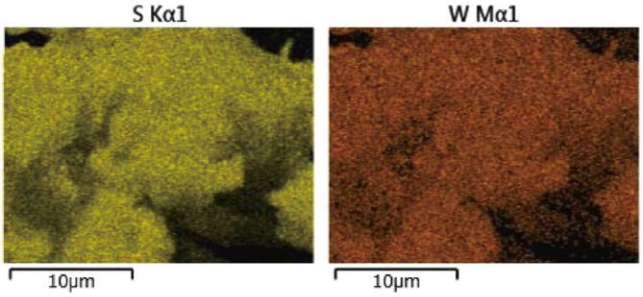
Highlight 7

Mechanochemical synthesis and characterization of $Na_{3-x}P_{1-x}W_xS_4$ solid electrolytes

F. Tsujia, A. Nasua, A. Sakuda, M. Tatsumisago, A. Hayashi.
J. Power Sources vol. 506, 230100 (2021)
https://doi.org/10.1016/j.jpowsour.2021.230100

Abstract

All-solid-state sodium batteries are attracting attention as next-generation batteries, owing to their improved safety and abundance of sodium resources. To realize all-solid-state sodium batteries, solid electrolytes with high sodium-ion conductivities are required. In this study, Na_3PS_4 electrolytes with partial substitution of P^{5+} with W^{6+} were investigated. The $Na_{3-x}P_{1-x}W_xS_4$ sulfide-based solid electrolytes were prepared via a mechanochemical process and consecutive heat treatment. The $Na_{2.85}P_{0.85}W_{0.15}S_4$ electrolyte with Na vacancies exhibited an ionic conductivity of 8.8×10^{-3} S cm^{-1} at 25 °C, which was higher than that of Na_3PS_4 solid elect rolyte. The all-solid-state batteries (Na-Sn/$Na_{2.85}P_{0.85}W_{0.15}S_4$/$TiS_2$) exhibited a reversible capacity of 140 mA h g^{-1} at a current density of 0.038 mA cm^{-2} and retained the capacity of 115 mAh g^{-1} for 40 cycles at 0.130 mA cm^{-2} at 25 °C. The $Na_{3-x}P_{1-x}W_xS_4$ samples prepared via mechanochemistry are homogeneous electrolytes free of crystalline WS_2 impurities and are effective for application to all-solid-state sodium batteries. [Reproduced with permission of Elsevier.]



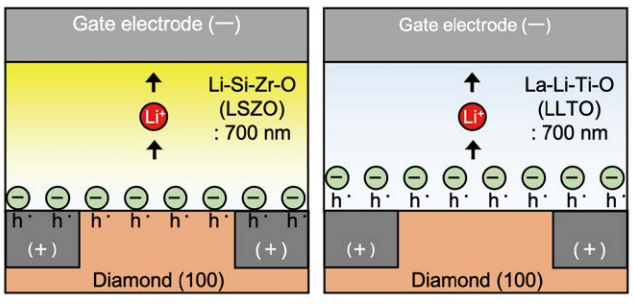
Highlight 8

The electric double layer effect and its strong suppression at Li^+ solid electrolyte/hydrogenated diamond interfaces

T. Tsuchiya, M. Takayanagi, K. Mitsuishi, M. Imura, S. Ueda, Y. Koide, T. Higuchi, K. Terabe.
Commun. Chem. vol. 4, 117 (2021)
https://doi.org/10.1038/s42004-021-00554-7

Abstract

The electric double layer (EDL) effect at solid electrolyte/electrode interfaces has been a key topic in many energy and nanoelectronics applications (e.g., all-solid-state Li^+ batteries and memristors). However, its characterization remains difficult in comparison with liquid electrolytes. Herein, we use a novel method to show that the EDL effect, and its suppression at solid electrolyte/electronic material interfaces, can be characterized on the basis of the electric conduction characteristics of hydrogenated diamond(H-diamond)-based EDL transistors (EDLTs). Whereas H-diamond-based EDLT with a Li-Si-Zr-O Li^+ solid electrolyte showed EDL-induced hole density modulation over a range of up to three orders of magnitude, EDLT with a Li-La-Ti-O (LLTO) Li^+ solid electrolyte showed negligible enhancement, which indicates strong suppression of the EDL effect. Such suppression is attributed to charge neutralization in the LLTO, which is due to variation in the valence state of the Ti ions present. The method described is useful for quantitatively evaluating the EDL effect in various solid electrolytes. [Reproduced with permission of Springer Nature.]



Activity Reports

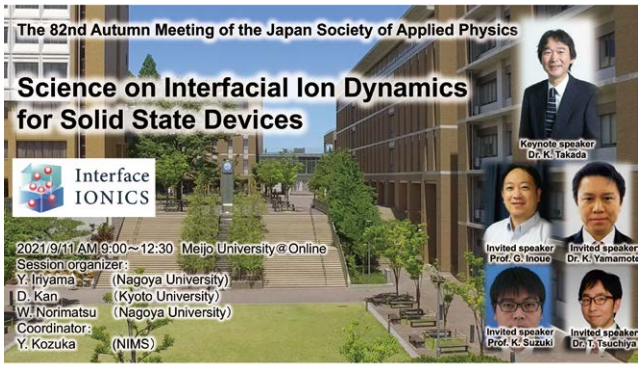
Conferences Partially Supported by the Interface IONICS Project

Co-organized Symposium "Science on Interfacial Ion Dynamics for Solid State Devices" of the 82nd Autumn Meeting of the Japan Society of Applied Physics (Online)

Sep. 11, 2021

Prof. Yasutoshi Iriyama, Nagoya Univ.
Prof. Daisuke Kan, Kyoto Univ.
Prof. Wataru Norimatsu, Nagoya Univ.

One keynote lecture from Dr. Takada (NIMS); four invited lectures from Prof. Suzuki (Tokyo Institute of Technology), Dr. Tsuchiya (NIMS), Dr. Yamamoto (JFCC), and Prof. Inoue (Kyushu University); and six general lectures were presented. The number of participants was approximately 80. The symposium provided a good opportunity to introduce the activities of Interface IONICS to researchers closely associated with the Japan Society of Applied Physics.



Symposiums and Seminars

The 3rd Public Symposium on Interface IONICS (Online)

Sep. 16, 2021

Prof. Naoaki Yabuuchi, Yokohama National Univ.

The 3rd Public Symposium on Interface IONICS was held online on Sep. 16, 2021. More than 300 people registered for the symposium, which provided an opportunity for scientists, engineers, and students to discuss the diverse aspects of interfacial phenomena related to solid-state chemistry, science, and technology. The conference featured three invited talks from the academic and industrial communities. Four representatives from each group in the Interface IONICS project also delivered talks on recent research advances in the project. In addition, a poster session was held from all members of Interface IONICS using Zoom breakout rooms. These presentations triggered detailed and exciting discussions throughout the symposium.

Our first invited speaker, Dr. Mikinari Shimada, who is the director of LIBTEC, delivered a presentation related to the development of solid-state batteries in LIBTEC. Our second speaker, Prof. Kiyoshi Kanamura, who is a distinguished professor studying the technology of lithium-ion batteries, presented a history of the research progress on batteries, especially those with a metallic Li electrode. Finally, our third invited speaker, Dr. Masayuki Nagamine, who is a chief scientist at Murata Manufacturing Co., Ltd. delivered a talk on the history and development of Li-ion batteries in his company and future prospects for the development of solid-state Li-ion batteries.

International Training Program Reports

Visiting the Liquid Structure Research Group in the Wigner Research Centre for Physics, Budapest, Hungary

Oct. 17–Dec. 9, 2021

Dr. Hiroki Yamada, Japan Synchrotron Radiation Research Inst.

I visited the Liquid Structure Research Group in the Wigner Research Centre for Physics in Budapest, Hungary. The purpose of this visit was to reveal the structural differences between Li_3PS_4 electrolytes prepared by a typical mechanical milling method (denoted as "Glass") and by mechanical milling under different conditions (denoted as "MM"). These two materials have the same composition and density, but MM exhibits greater Li-ion conductivity than Glass; thus, understanding their structural differences is important. For this reason, I worked with Dr. Laszlo Puztai and Dr. Laszlo Temleitner, who are leading developers of the Reverse Monte Carlo (RMC) software and specialists in analyzing amorphous/liquid materials.

During my visit, I was interested in combining machine-learning potential (MLP) with RMC simulation and focused on developing this new method. In a previous study, the structure of Li_3PS_4 electrolytes was investigated by using the density functional theory (DFT) method. However, because of the associated calculation costs, this method is difficult to apply to larger models (e.g., those with more than 1000 atoms in total) for comparison with experimental data. However, classical RMC sometimes produces a large structure that compares favorably with experimental results but has a thermodynamically unfavorable local structure. This thermodynamically unfavorable local structure hinders deep understanding of certain aspects of materials, such as their physical properties. Therefore, combining RMC with MLP, whose calculation cost is much lower than that of DFT but provides comparable results, is considered a promising approach to overcoming these limitations.

Our procedure for using RMC-MLP in this manner is described as follows. First, classical RMC was conducted to fit both X-ray and neutron scattering patterns. After a constant number of movements, the energy difference between the models before and after RMC was calculated using MLP and the program decided whether these movements generated by RMC were acceptable. From a continuous loop of RMC and energy evaluations, structure models satisfying both the experimental results and the thermodynamic requirements were obtained at the end of the simulation. The latest results will be presented at the 3rd Meeting for Young Scientists in the Interface IONICS Project.

Using this new RMC-MLP approach, structure models of MM and Glass were obtained. From these sophisticated models, a slight difference in bond lengths was observed, consistent with the results related to Li-ion conductivity. In the next step, this approach will be used to analyze the interface between amorphous electrolytes, which can be characterized using X-ray/neutron/electron diffraction measurements at the region of interest. The experimental data from these analytic methods might be noisy because of the smaller beam and higher background. However, by tuning the potential and experimental weight in the RMC-MLP to minimize the effects from experimental errors, we expect to extract the essential structural features of the interface.

I am grateful for this opportunity to participate in the international training program of the Interface IONICS project and to gain valuable experience in collaborating with prominent researchers abroad.

Photos of the meeting to share the latest results. In addition to the group members, Prof. Eckhard Spohr (University of Duisburg-Essen) and Prof. Philippe Bopp (Université Bordeaux) kindly attended the meeting and provided helpful comments.

Domestic Training Program Reports

Visiting the Kan group at Kyoto University

Jul. 7–9, 2021

Ms. Nanaka Shimada, Yokohama National Univ.

I visited Prof. Kan's group at Kyoto University with Prof. Yabuuchi, who is my supervisor at Yokohama National University, to learn high-pressure synthesis methods for metal oxides. I am currently studying high-capacity positive electrode materials, and the larger reversible capacity for these electrode materials originates from an anionic redox reaction. This conclusion (i.e., charge compensation by anionic species), was made on the basis of experimental observations using X-ray absorption spectroscopy at the oxygen K-edge region. Nevertheless, the lack of a reference material for anionic redox, i.e., stable materials in the ambient condition with holes (or radicals on oxygen), hinders clear understanding of the electronic structures for oxygen in high-capacity electrode materials. Therefore, a reference material is necessary. High-pressure synthesis enables us to synthesize such a unique material, e.g., $SrFeO_3$. We expect that the high-pressure method can be used to synthesize reference materials for spectroscopic studies of oxygen. We are grateful to the Interface IONICS project for providing excellent collaboration opportunities.

Domestic Training Program Reports

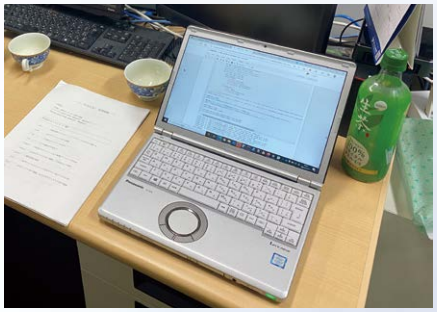
Visiting the Nakayama's laboratory in Nagoya Institute of Technology

Nov. 11–12, 2021

Assist. Prof. Kosuke Kawai, Waseda Univ.

I visited Prof. Nakayama's laboratory at Nagoya Institute of Technology to learn machine learning techniques. Machine learning is an information processing technology based on statistical mathematics and has become a promising analytical tool in the materials science field. Applying machine learning to experimental data enables experimental scientists to develop battery materials and attain new findings in battery research.

On the first day, Prof. Nakayama gave an overview of materials' descriptors for machine learning (e.g., composition, structure, and physical properties) and Bayesian optimization. After his lecture, students in the laboratory taught me how to use Python scripts, which they had developed, through hands-on training. On the second day, I built a programing environment on my laptop by installing software and revising the scripts for our datasets. We hope that the machine learning techniques will be useful for developing battery materials in our laboratory. I am grateful to the Interface IONICS project for providing such beneficial collaboration opportunities.



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