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  G: Advances in Smart Energy Storage for a Sustainable Energy Future – Electrochemistry, Mechanics and Applications
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Friday - 8 July, 2016 | Symposium G

Oral Presentations

Session G: Sodium Batteries II; Advanced Materials & Technology: Solid Electrolytes and Solid State Batteries
Friday, July 08, 2016 | 11:00 - 13:00 | 311
Chairs: Daniel RETTENWANDER, Stefan ADAMS

G-1
30 min

ICEM16-A-1201 Invited

Sodium Intercalation Chemistry in Graphite

Kisuk KANG[1#+]
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The insertion of guest species in graphite is the key feature utilized in applications ranging from energy storage and liquid purification to the synthesis of graphene. Recently, it was discovered that solvated-Naion intercalation can occur in graphite even though the insertion of Na ions alone is thermodynamically impossible; this phenomenon enables graphite to function as a promising anode for Na-ion batteries. In an effort to understand this unusual behavior, we investigate the solvated-Na-ion intercalation mechanism using in operando X-ray diffraction analysis, electrochemical titration, real-time optical observation, and density functional theory (DFT) calculations. The ultrafast intercalation is demonstrated in real time using millimeter-sized highly ordered pyrolytic graphite, in which instantaneous insertion of solvated-Na-ions occurs (in less than 2 s). The formation of various stagings with solvated-Na-ions in graphite is observed and precisely quantified for the first time. The atomistic configuration of the solvated-Na-ions in graphite is proposed based on the experimental results and DFT calculations. The correlation between the properties of various solvents and the Na ion co-intercalation further suggests a strategy to tune the electrochemical performance of graphite electrodes in Na rechargeable batteries.

G-2
30 min

ICEM16-A-0129 Invited

Atomic-Level Insights Into Solid-State Lithium Ion Battery Materials

Craig A. J. FISHER[1#+], Takafumi OGAWA[1], Akihide KUWABARA[1], Shunsuke KOBAYASHI[1], Yumi H. IKUHARA[1], Hiroki MORIWAKE[1], Yuichi IKUHARA[1]
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Solid-state lithium ion batteries (SSLIBs) promise to provide a safer, higher density form of energy storage than conventional liquid-electrolyte batteries. Because SSLIBs are often fabricated in thin film form, two-dimensional defects such as surfaces, grain boundaries, stacking faults, and heterointerfaces between the different components can significantly affect charge/mass transfer kinetics (and hence battery cell performance, cyclability and lifetime), and thus need to be controlled or minimized. This requires a good understanding of the nature of such defects at the atomic level. A combination of state-of-the-art scanning transmission electron microscopy (STEM) and theoretical modeling is one powerful means of probing these important features at the atomic level.

In this paper we present a number of examples of the use of computer simulation to examine the structures and properties of various interfaces and defects in SSLIB materials that have been observed by STEM. Examples will include stacking faults in layered oxide cathodes $LiMO_2$ (M = Cr, Fe, Co, and Ni) and surfaces of cathode materials $LiFePO_4$. The paper aims to show how improvements in computing power are allowing more sophisticated theoretical models to be treated, and how the insights gained are contributing to our understanding of fundamental materials phenomena.

G-3
30 min

ICEM16-A-0246 Invited

On Structure-Property Relationships in Li-Oxide Garnets: New Insights by Studying a Large Li6La3ZrTaO12 Single Crystal Made by Czochralski Method

Daniel RETTENWANDER[1#+], Stefan BERENDTS[2], Reinhard UECKER[3], Günther REDHAMMER[4], Martin WILKENING[5], Jürgen FLEIG[6], Georg AMTHAUER[4]
[1]Massachusetts Institute of Technology, United States, [2]Technical University Berlin, Austria, [3]Leibniz Institute for Crystal Growth (IKZ), Germany, [4]Universitaet Salzburg, Austria, [5]Graz University of Technology, Austria, [6]Vienna University of Technology, Austria
[#]Corresponding author: drett@mit.edu [+]Presenter

Li-ion batteries (LiB) using a solid-state electrolyte are in the spotlight of battery research due to its significant improved safety compared to current commercial LiB equipped with flammable liquid electrolytes. Among all solid electrolytes, $Li_7La_3Zr_2O_{12}$ (LLZO) garnets and its variants are the most promising candidates; they benefit from a high Li-ion conductivity and high chemical stability. Moreover, the wide electrical potential window enables the realization of Li-metal based battery concepts such as Li-air, Li-flow or Li-S.

Since the initial study of Murugan *et al.* in 2007[1] an enormous amount of papers has been published in order to understand the underlying structure-property relationships for this class of material.[2] Considering the global importance of energy research and the need for new energy storage systems such knowledge is crucial to improve LLZO-based electrolytes for their applications by crystal chemical engineering.

The accuracy or meaningfulness of most of the published studies is limited by using inhomogeneous polycrystalline samples. Unfortunately, for LLZO, as for many other oxides, no large single crystals are available. In the present study, however, we have successfully grown a large $Li_7La_3ZrTaO_{12}$ single crystal by the Czochralski method. The availability of large single crystals enables the application of a broad spectrum of methods (*e.g.*, single crystal X-ray/neutron diffraction, NMR, Raman, and impedance spectroscopy) on identical parts of the same single crystal without any, *e.g.*, inhomogeneities and variations in the composition, structure or morphology. In this talk, the state of research on such large LLZO-single crystals will be presented.

1. Murugan, R.; Thangadurai, V. Weppner, W. *Angew. Chem. Int. Ed.* **2007**, 46, 7778.

2. Thangadurai, V.; Narayanan, S.; Pinzaru, D. *Chem. Soc. Rev.* **2014**, 43, 4714.

G-4
15 min

ICEM16-A-0491 Contributed

Low Temperature Sintering of NASICON Solid Electrolyte with Na3BO3 Additive

Kousuke NOI[1+], Kenji SUZUKI[1], Akitoshi HAYASHI[1#], Masahiro TATSUMISAGO[1]
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[#]Corresponding author: hayashi@chem.osakafu-u.ac.jp [+]Presenter

$Na_3Zr_2Si_2PO_{12}$ (NASICON) is a promising candidate as a solid electrolyte for all-solid-state sodium batteries with high safety and low cost because of its high Na^+ ion conductivity, chemical stability, and lack of rare elements. The dense NASICON ceramics that show the high room temperature conductivities of about 10^{-3} S cm^{-1} are usually prepared by sintering at over 1200^oC. However, the sintering at such high temperatures promotes the volatilization of sodium contents. Protection such as covering a green compact in its mother powder of the same composition is essential to avoid the decomposition of NASICON during sintering. Moreover, undesirable side reactions with electrode materials at the high temperatures are concerned when batteries are fabricated through a co-sintering process in order to form close solid-solid interfaces. Hence it is necessary to decrease the sintering temperature of the NASICON ceramics.

	In the present research, highly conducting NASICON solid electrolytes were prepared by the liquid phase sintering at lower temperatures. The low melting glass of Na_3BO_3 (680°C of melting point) was used as a sintering additive. The NASICON based ceramics were prepared by sintering at 900°C without mother powder. The obtained ceramic with 5 wt% of Na_3BO_3 showed the ambient temperature conductivity of 1.0×10^{-3} S cm^{-1}, which was comparable to that of the pure NASICON ceramic sintered at 1220°C. The high relative density of 95% was achieved for the sintered body. SEM observation demonstrated the highly dense microstructure of the ceramic. The XRD pattern for the sintered body showed that the dominant phase was $Na_3Zr_2Si_2PO_{12}$ and any crystalline boron compounds were not detected. Consequently, these results suggest that Na_3BO_3 acts as a liquid sintering additive without a harmful reaction to NASICON and that sodium borates, which remain as an amorphous phase, do not adversely affect the conductivity of the sintered body.
G-5 *15 min*	ICEM16-A-0933 Contributed **Structural Stability of Li+/H+ Ionic-Exchanged Garnet-Related Li7La3Zr2O12 Solid Electrolyte** Zhen Feng YOW[1+], Wenyi GU[1], Stefan ADAMS[1#] [1]*National University of Singapore, Singapore* [#]*Corresponding author: mseasn@nus.edu.sg* [+]*Presenter* Among the garnet-related fast ion conducting solids, aliovalently doped $Li_7La_3Zr_2O_{12}$ (LLZ) solid electrolytes have received much attention due to their particularly high chemical and thermal stability with a wide electrochemical window versus lithium metal. LLZ was previously claimed to be chemically stable in exposure to ambient air, but Li^+/H^+ exchange in LLZ under air humidity and water has been successfully demonstrated lately. Stability of LLZ in contact with water thus poses a major concern especially in handling and storing of this solid electrolyte. In this work, Ta-doped LLZ, $Li_{7-x}La_3Zr_{2-x}Ta_xO_{12}$ (LLZTa) was prepared by solid-state method. Lattice parameters of Ta-doped LLZ were found to increase after water treatment in accordance to literature data and our molecular dynamics (MD) simulations of LLZ. The extent and kinetics of such Li^+/H^+ exchange can be controlled by the pH of the immersion solution, as demonstrated by immersion in LiOH solution. MD simulations clarify the proton distribution and suggest that for compositions $Li_3H_4La_3Zr_2O_{12}$ corresponding to the equilibrated powder samples after immersion in water the material becomes essentially a moderate proton conductor with higher activation energy and significantly reduced room temperature Li^+ ion conductivity compared to H^+-free cubic LLZ. For the minor levels of proton exchange in alkaline solutions (e.g. $Li_{6.5}H_{0.5}La_3Zr_2O_{12}$) the hardly affected lithium ion mobility however dominates over the proton mobility. Therefore, despite the ion exchange, structural stability with limited Li^+/H^+ exchange suggests LLZTa solid electrolyte to be suitable as anode-protecting membrane in Li-air battery with sufficiently alkaline catholytes.
G-6 *15 min*	ICEM16-A-0681 Contributed **Synthesis, Characterization and Conductivity Investigation of Ce1-x-yDyx-yCayO1.90/ (Li0.52Na0.48)2CO3 (CDC/INCO) for Their Use as a Solid Electrolyte in Lt-SOFCs** Khagesh TANWAR[1+], Om Parkash CHADDHA[2#], Nandini JAISWAL[2], Devendra KUMAR[2] [1]*ceramic engineering, Indian Institute of Technology, BHU, India*, [2]*Indian Institute of Technology, BHU, India* [#]*Corresponding author: oprakash.cer@itbhu.ac.in* [+]*Presenter* $Ce_{1-x-y}Dy_{x-y}Ca_yO_{1.90}$ (CDC) nano-crystalline powder has been synthesized by citrate-nitrate auto-combustion route. The nanopowder has been characterized using XRD and DTA. Solid oxide fuel cell nanocomposite electrolyte with high ionic conductivity at low temperature has been prepared by mixing CDC and eutectic mixture of lithium carbonate and sodium carbonate in various ratios to optimize the maximum conductivity. The mixture has been heated to 650 °C and cooled down to room temperature to introduce amorphous nature of carbonates. The powders have been pressed into pellets and sintered at 700 °C. The density of composites have been calculated and found to be more than 85%. Complex plane impedance analysis has been carried out to investigate ionic conduction behavior of electrolyte in the temperature range of RT to 600°C. The presence of amorphous nature of carbonates in electrolyte has been confirmed by SEM analysis. The total conductivity of composite electrolyte found to be enhanced of two orders with compare to the pure CDC electrolyte.
G-7 *15 min*	ICEM16-A-0717 Contributed **Piezoelectricity and Electrostriction in Gd-Doped CeO2 Bulk Ceramics Studied by Laser Interferometry** Andrei KHOLKIN[1,2#+], Andrey USHAKOV[2], Denis ALIKIN[2], Ivan BATURIN[2] [1]*University of Aveiro, Portugal*, [2]*Ural Federal University, Russian Federation* [#]*Corresponding author: kholkin@ua.pt* [+]*Presenter* Recently Korobko et al [1] have shown that thin films of ionic conductors Ce0.8Gd0.2O1.9 demonstrate giant electrostriction (and notable piezoelectricity in the biased state) with the electrostriction coefficient in the range 2-10 kPa/(kV/cm2). The ability to generate exceptional strain (> 7 MPa) and absence of lead (together with very stable structure without ferroelectric domains and phase transition) opened a new perspective for the new generation of electromechanical sensors and actuators. Another advantage is its ability to work at high temperatures and possible multifunctionality due to notable ionic conductivity. Here, we demonstrate that Gd-doped CeO2 ceramics (Gd content 20 mol%) can also exhibit a piezoelectric effect without any bias. The measurements were done with the Michelson-Morley interferometer adapted for the measurements of small strains. Special measures were taken to avoid the effect of the sample bending that could lead to the overestimation of the piezoelectric and electrostriction coefficients. The resulting electrostriction coefficient is about 10-19 m2/V2 at 13 kHz but increased to higher values with decreasing frequency. We show that the electric field induced strain depends on whether Pt or Pd/Au electodes are used and strongly varies with frequency and temperature. We show that weak piezoelectric effect is also present due to the internal bias field induced by Pt. The data are complemented by the detailed dielectric relaxation measurements that hint to the increased grain boundary conductivity. The mechanisms of the electric field induced strain in doped ceria ceramics are discussed. 1. R. Korobko et al, Giant Electrostriction in Gd-doped Ceria, Adv. Mat. 24, 5857 (2012). **Acknowledgement:** The equipment of the Ural Center for Shared Use “Modern Nanotechnology” Ural Federal University has been used. The research was made possible with the financial support of RFBR (grant 15-52-06006 MSTI_a).
G-8 *15 min*	ICEM16-A-0752 Contributed **Ionic Conductivity Behaviour of Ceria Reinforced Yttria Stabilized Zirconia (8YSZ) Nanocomposite Electrolyte for Solid Oxide Fuel Cell Application** Alka GUPTA[1#+], Kantesh BALANI[1] [1]*Indian Institute of Technology, India* [#]*Corresponding author: gupta.alkag@gmail.com* [+]*Presenter* Solid oxide fuel cells (SOFCs) based on 8 mol.% Y_2O_3 – ZrO_2 (8YSZ) electrolyte requires high working temperatures (800-1000°C) to render a reasonable power density. Most of the research and development work on SOFCs worldwide has been devoted on lowering its high operational temperature to intermediate temperature range (400-600°C). In the present work, the novel CeO_2-8YSZ nano-composites were synthesized and tested with the aim to develop higher ionic conductive electrolyte materials for SOFCs. Spark plasma sintering (SPS) method was utilized to synthesize nano-composites of 8YSZ with different CeO_2 contents (0, 5, and 10 wt. %). The SPS was performed on the powder mixtures of 8YSZ and CeO_2 under 30 MPa at 1200°C and with the soaking time of 5 min. Densities of all the sintered samples were estimated to be 96% of theoretical density or above. The XRD profiles collected at room temperature suggest dissolution of CeO_2 in 8YSZ matrix, whereas TEM investigation shows isolated CeO_2 rich regions indicating the formation of composite. The ionic conductivity measurement was performed using AC impedance spectroscopy in air from 300°C to 450°C. The effect of CeO_2 addition on the structure and ionic conductivity of 8YSZ will be discussed.