【Grant-in-Aid for Scientific Research (S)】

Science and Engineering (Chemistry)

Title of Project : Creation of superionic conductors

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Research Project Number : 17H06145 Researcher Number : 90135426
Research Area : Solid State Ionics, Solid State Chemistry
Keyword : Superionic conductors, Electrochemical devices, Neutron, Synchrotron X-ray

【Purpose and Background of the Research】

Superionic conductors are the materials showing fast ionic diffusion in the solids. These materials are expected to be used as solid electrolytes in the electrochemical devices and enable the development of novel energy devices such as lithium / sodium batteries with extremely high energy density and power characteristics (Fig. 1).
These materials also provide the oxygen / proton systems with high efficiency power system. On the other hand, novel conducting species such as hydride ion expands novel research fields and energy devices.
In the present study, the key materials which show superionic conductivity will be searched and developed for the energy devices in the future. Especially, the current research focuses on the lithium or hydride ion conductors.
1. Material system to exploit: (i) Bulk material search with wide composition range and (ii) Interfacial design of nano-region of the electrochemical system, which shows superionic conduction.
2. Purpose: Development of the methods for new materials search: (i) Conventional synthesis technique by element substitutions, (ii) Systematic synthesis based on phase diagram, and (iii) Computational chemistry.

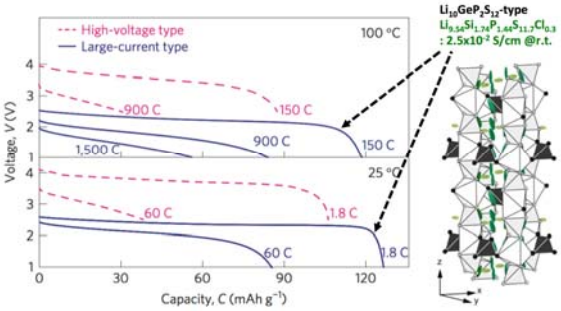

Figure 1 Performances of all solid-state battery using Li superionic conductor, $Li_{9.51}Si_{1.74}P_{1.44}S_{11.7}Cl_{0.3}$.

【Research Methods】

Bulk superionic conductors: Conventional sintering technique and high-pressure synthesis for creating phase diagrams and new materials.
Development of nano interface: Creating a hetero-interface for fast ionic diffusion by single crystal film synthesis under vacuum.
Construction of systematic synthesis method: Introducing computational chemistry method.
Characterization, device construction, and establishment of material search direction: physical property evaluation, evaluation of device characteristics.

【Expected Research Achievements and Scientific Significance】

New materials: Material development based on our new synthesis strategy could provide new energy storage and conversion devices which strongly impact on our society.
Material search method: While the conventional synthesis methods were efficient for the materials search, new methodology is necessary for the developments of materials for the next generation. By combining the conventional technique and new computational chemistry, new methodology for the materials search will be looked for. New superionic conductors will be developed.
Ionic conduction at nano interface: Systematic investigation of the nano region for the ideal hetero-interface is important for designing electrochemical interface in the devices.
Development of ion conduction species: Hydride ion conductor is a new superionic conducting system and may lead to new science in solid-state chemistry and energy chemistry fields.

【Publications Relevant to the Project】

・*Nat Mater*, **10**, 682-686 (2011).
・*Nature Energy*, **1**, 16030 (2016).
・*Science*, **351**, 1314-1317 (2016).

【Term of Project】 FY2017-2020
【Budget Allocation】 129,500 Thousand Yen

【Homepage Address and Other Contact Information】

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