

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

Broad Section D



Title of Project : Construction of new mechanism for dual-ion storage batteries concerted by lithium and multivalent ions

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Keyword : Polyvalent-ion conductivity, Concerted interaction, Dendrite free, Metal anode battery

【Purpose and Background of the Research】

Construction of energy storage technology is indispensable in the modern society. Although the mechanism of a storage battery using a monovalent carrier ion such as a lithium ion battery is well known or understood, the basic science of storage batteries system using multivalent ions such as magnesium as a carrier is almost unknown. We have been making efforts to develop positive electrode materials for magnesium storage batteries that utilize divalent carriers earlier and succeeded in proposing several potential candidates as positive electrode materials for magnesium storage batteries. We have also pioneered to propose the concept of dual-carrier rechargeable batteries that simultaneously utilize monovalent ions and divalent ions so far. Therefore, in this research, we aim to establish the material science for storage batteries that utilize multivalent ions as carriers and to construct the theory/concept of cooperative collaborations, i.e., concerted interaction, played between Li and multivalent careers.

【Research Methods】

The fundamental problems to be solved in this research are as follows.

[1] Coherent strain-field effect due to phase transition: While a phase transition occurs along with the insertion and extraction of carrier ions, the coherent strain field yielded by lattice mismatch greatly affects electrode characteristics. Evaluation of the strain field is carried out by scanning / transmission electron microscope, soft X-ray spectroscopy, synchrotron radiation or X-ray diffraction analysis, and the strain energy is evaluated by the first principles calculation, micromechanics calculation.

[2] Elucidation of concerted effects between dual ions: We have found that the activation energy of diffusion is markedly reduced under the dual-career situation, as shown in Fig. 1, by using first principles calculations. So, we try to clarify such “concerted interaction” between monovalent and multivalent ions. As a final goal, we try to find a mechanism by which multivalent ions can move even at room temperature.

[3] Proposal of dendrite suppression mechanism: Prohibiting of dendrite formation during charging is a very critical issue. We have found that dendrite formation tends to be suppressed in the presence of Li/Mg dual-salt electrolyte. Based on the phenomenon, we conversely clarify/deduce the dendrite formation/ inhibition mechanism.

【Expected Research Achievements and Scientific Significance】

Focusing on the fact that two types of carriers of monovalent and multivalent ions can exert a positive concerted effect, we can produce a feature, which cannot be achieved only by a single carrier, and we want to create an innovative mechanism of storage battery carriers.

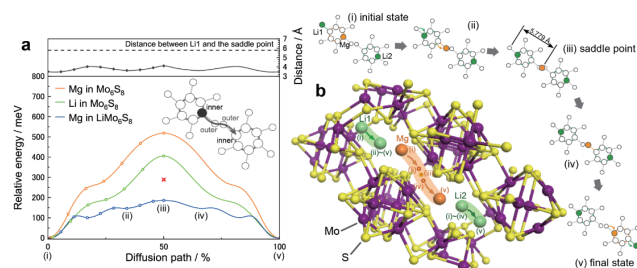


Figure 1 Lowering of diffusion barrier (left) and diffusion path of dual ions (right)

【Publications Relevant to the Project】

- H. Li, N. L. Okamoto, T. Hatakeyama, Y. Kumagai, F. Oba, T. Ichitsubo, *Advanced Energy Materials*, 1801475 (2018).
- H. Li, T. Ichitsubo, S. Yagi, E. Matsubara, *Journal of Materials Chemistry A5*, 3534 (2017).
- T. Ichitsubo, S. Okamoto, T. Kawaguchi, Y. Kumagai, F. Oba, S. Yagi, N. Goto, T. Doi, E. Matsubara, *Journal of Materials Chemistry A3*, 10188 (2015).

【Term of Project】 FY2018-2022

【Budget Allocation】 152,800 Thousand Yen

【Homepage Address and Other Contact Information】

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