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

Fundamental construction of a world woven by dual ions for metal-anode storage batteries

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Project Information	Project Number : 23H05452 Keywords : Multivalent ion conduction, synergistic interactions, dendrite-free, alloy negative electrode battery	Project Period (FY) : 2023-2027

Purpose and Background of the Research

●Outline of the Research

In order to establish a sustainable energy system, battery technologies that combine safety, reliability, high energy density, and low cost are essential. The current lithium-ion batteries have already approached their theoretical limits, and to significantly improve the performance of batteries, the development of new battery systems based on fundamental research is required. The applicant has been establishing mechanisms to enhance ion mobility in the positive electrode through the synergistic effect of dual-ion conduction and successfully suppressing dendrite deposition in the negative electrode during charging. In this research proposal, we aim to further solidify these mechanisms and achieve a metal anode battery with high energy density. By establishing a mechanism to suppress dendrite formation through the dual-ion effect and deriving design principles for the positive electrode that enable simultaneous intercalation and deintercalation of both ions, we will construct a theoretical framework for the world of dual-ion interactions in energy storage devices.

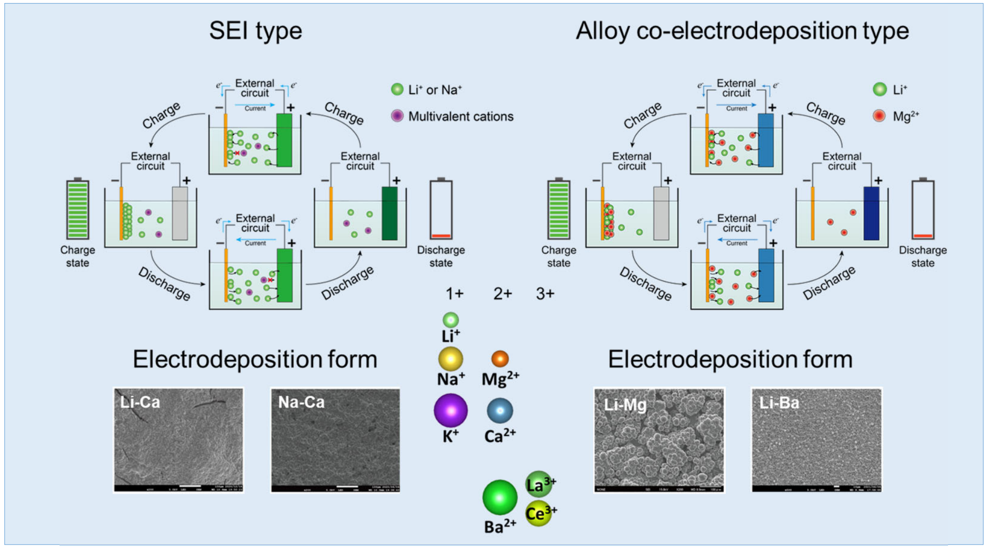

Figure 1. Two types of metal anode batteries aimed in this study. On the left is the SEI (Solid Electrolyte Interphase) type, and on the right is the alloy co-deposition type. In the case of the SEI type, such as Li and Ca, the aim is to contribute to the formation of the SEI layer without involvement in dendrite deposition. In the alloy co-deposition type, such as Li and Mg, alloying occurs during deposition. In both cases, dendrite formation can be expected to be suppressed by the dual-ion effect. By systematic element selection, we will establish mechanisms to suppress dendrite formation. Furthermore, since the design principles for the positive electrode differ between the two types (next page), we will derive the optimal solutions for each type.

●Background and Objectives

The physicochemical mechanisms of batteries that utilize monovalent carriers such as lithium are well understood and have already been established as devices (for example, lithium-ion battery: LIB). On the other hand, the fundamental science of battery systems that use multivalent ions or a combination of multivalent ions is still in its early stages. We have been conducting materials science research on innovative dual-ion batteries that utilize multivalent ions and have obtained support for our findings, demonstrating the synergistic effect in ion mobility in the positive electrode (where the movement of multivalent ions becomes faster following the movement of monovalent ions) and the suppression of dendrite formation in the negative electrode. The reason for applying for this research project as the Grant-in-Aid for Scientific Research (S) is to aim for further development and expansion, and to systematically explore the world of dual-ion interactions in order to achieve metal anode (metal/alloy negative electrode) batteries with high energy density.

Expected Research Achievements

To establish a theoretical framework for dendrite suppression and achieve metal anode (metal/alloy negative electrode) batteries with high energy density (target: 500-600 Wh/kg), we will systematically explore the world of dual-ion interactions. The dual-ion effect on dendrite suppression can be broadly categorized into two types: SEI type and alloy co-deposition type. The following tasks are defined for this research:

Task 1: Establishing dendrite suppression mechanisms of Li or Na metal anodes through the dual-ion (SEI) effect.

Task 2: Establishing dendrite suppression mechanisms through dual-ion alloy co-deposition (or alloy negative electrodes).

Task 3: Establishing design guidelines for positive electrode materials that enable simultaneous intercalation of dual ions at room temperature.

By addressing these tasks, we aim to construct the fundamental scientific principles of the next-generation batteries.

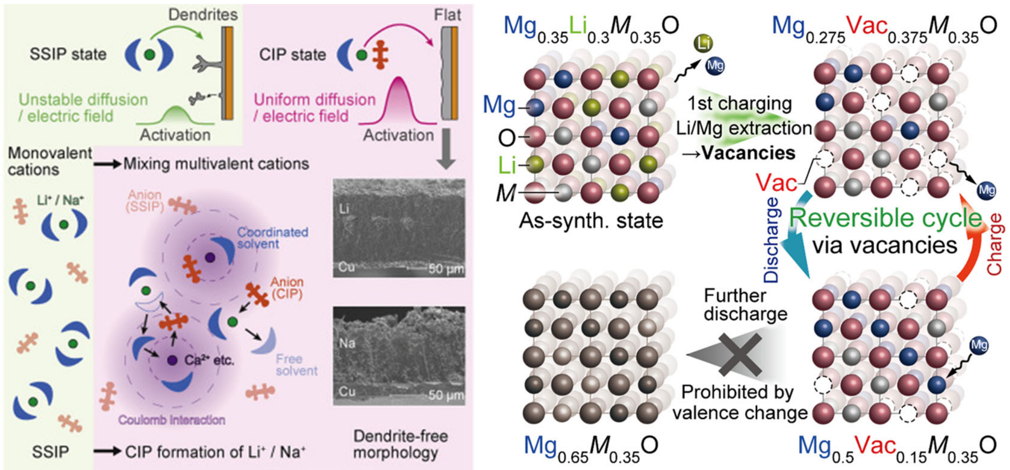

Figure 2. Left: Constructing mechanisms to suppress dendrite formation by modifying the solvation structure through the dual-ion effect. Right: Establishing design guidelines for positive electrode active materials that allow dual-ion insertion (e.g., through making them high entropy state, etc.).

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