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

Title of Project : Materials Science on Hydrides with High-Density Hydrogen – Overcoming the Hydride-Gap by Controlling the Bonding State of Hydrogen in Hydrides

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Research Area : Materials Engineering, Materials Chemistry
Keyword : Energy Materials, Inorganic Materials Designing and Synthesis Processing, Atomic and Electronic Structure Characterization

【Purpose and Background of the Research】

Materials science on hydrides with high-density hydrogen will be advanced; by synthesizing new hydrides composed mainly of *3d*-Transition-Metals (TMs) for which hydrogen-densification is difficult (so called, the Hydride-Gap), by analyzing and building-up databases on them, and by enhancing their energy-related functions.

Specifically, extensive studies are to be carried out for various perovskite and complex hydrides that have been never synthesized with traditional techniques; by combining fusion researches such as predicting the properties through Hydrogen Diagram (Fig. 1) and first-principles calculations focusing on the flexibility in the bonding state of hydrogen in hydrides, by high-pressure syntheses using hydrogen fluid, and by *in-/ex-situ* analyses using quantum beams. Optimizations of their compositions as high-density hydrogen storage materials and fast-ionic conducting materials are also planned, along with measurements of hydrogen- and lithium-dynamics.

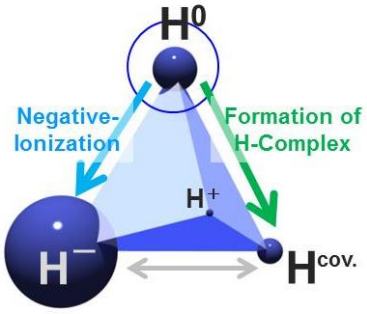

Figure 1 Concept of Hydrogen Diagram

【Research Methods】

1. Controlling the Bonding State of Hydrogen in Hydrides:
With the goal of synthesizing perovskite hydrides through the negative-ionization of hydrogen, and also of synthesizing complex hydrides through the formation of hydrogen-complexes, starting materials and promising hydrides will be appropriately selected by the theoretical and experimental analyses on the bonding state of hydrogen upon hydrogenation.

2. Overcoming the Hydride-Gap:
Donor-addition and high-pressure techniques will be introduced and improved to synthesize the promising hydrides with high-density hydrogen, composed mainly of *3d*-TMs like iron and nickel.

3. Enhancing the Energy-Related Functions:
The databases will be built-up on the starting materials and the synthesis conditions, combined with the atomic and electronic analyses. A materials-designing strategy will then be established for the development of high-density hydrogen storage materials and fast-ionic conducting materials.

【Expected Research Achievements and Scientific Significance】

The present project focusing on the flexibility in the bonding state of hydrogen in hydrides will massively boost the academic and social values of hydrides composed mainly of *3d*-TMs that are vital in terms of Element Strategy. The project will not only lead to revitalization of energy-related industries and strengthening of international competitiveness, but will also lead to the elucidation of unsolved academic issues such as novel superconductivity and quantum phenomena related to hydrogen/hydrides.

【Publications Relevant to the Project】

- M. Matsuo et al., "Experimental studies of complex hydride YMn_2H_6 on formation kinetics and X-ray absorption fine structure analyses", Appl. Phys. Lett., 100 (2012) 044101.
- S. Takagi et al., "Theoretical investigation of Fe substitution for Mn in complex hydride YMn_2H_6", Appl. Phys. Lett., 100 (2012) 021908.

【Term of Project】 FY2013-2017

【Budget Allocation】 158, 300 Thousand Yen

【Homepage Address and Other Contact Information】

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