Search for Novel Metal Hydrides utilizing High Pressure Technique
- Structural Studies Using Synchrotron Radiation X-rays and Neutrons -

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Materials research for various applications to hydrogen usage is progress to realize the hydrogen society. To make stable use of hydrogen, the fundamental knowledges such as interaction between hydrogen atoms and their surrounding atoms in the material are also important. However, it is not yet sufficient to apply them to material developments. High pressure technique is one of the effective parameters for obtaining knowledge about interaction between neighboring atoms. By changing the interatomic distance directly by compression, new structures and/or changes of physical properties can be induced. In addition, the chemical potential of hydrogen molecule rapidly increases above 1 GPa, and then it is expected that hydrogenation reaction of some metals or alloys which never realize at ambient condition would be occurred. To search novel metal hydrides synthesized under high pressure and to determine crystal structure including the position of interstitial hydrogen atoms, we have performed structural studies using synchrotron radiation x-rays and neutrons under high pressure. Obtained structural information would provide the fundamental knowledge such as the interaction between interstitial hydrogen atoms and their surrounding atoms.

In studies of metal hydrides, we observe a new phenomenon, pressure-induced phase separation, on LaH_2 by x-ray diffraction under high pressure in SPring-8 [1]. Results combining the high-pressure neutron diffraction performed at J-PARC and the mentioned x-ray diffraction are indicated that a monohydride (rock salt structure), which has not been existed in La-H system, is formed (Fig. 1) [2]. In addition, we succeed in in-situ observation of the hydrogenation process of iron by neutron diffraction under high pressure and high temperature, and elucidated the hydrogen occupation state in an fcc-iron hydride [3].

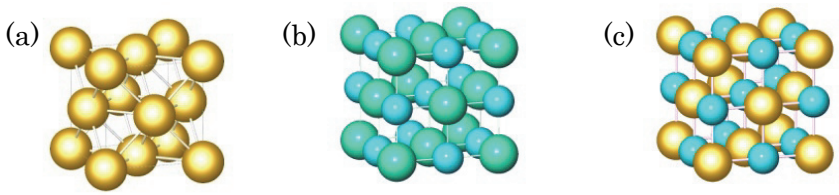

Fig. 1: Atomic arrangements of lanthanum monohydride obtained from (a) x-ray diffraction, (b) neutron diffraction. (c) Crystal structure of lanthanum monohydride elucidated by both x-ray and neutron diffraction results.

Bibliography

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[2] A. Machida *et al.*; Phys. Rev. Lett., **108**, 205501 (2012).
[3] A. Machida *et al.*; Nat. Commun., **5**, 5063 (2014).

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