5–5 Development of an Aluminum-Based Hydrogen Storage Alloy

— To Realize Light-Weight Hydrogen Storage Alloys —

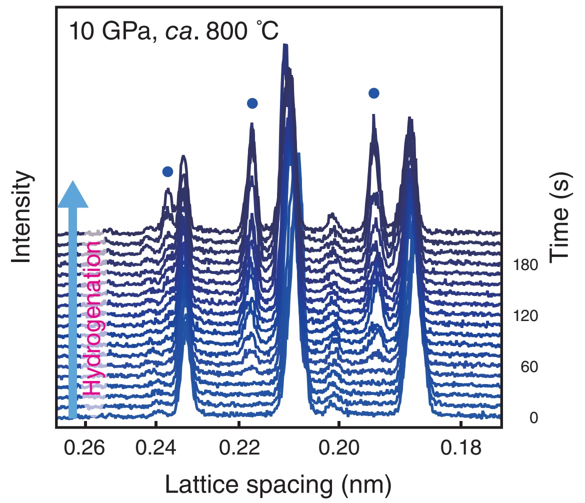

Fig.5-17 *In situ* synchrotron radiation X-ray diffraction profiles of hydrogenated Al_2Cu
Closed circles (●) indicate the Bragg peaks from Al_2CuH. The hydrogenation reaction began 60 s after incubation of the sample at *ca*. 800 °C.

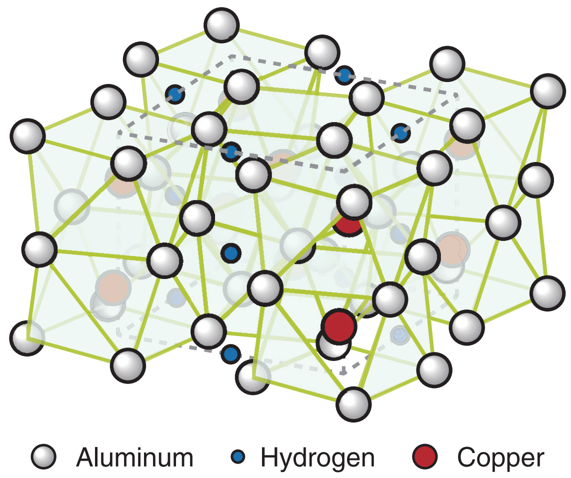

Fig.5-18 Crystal structure of Al_2CuH
The interstitial nature of the synthesized aluminum-based hydride, Al_2CuH, was confirmed both experimentally and by theoretical calculations.

Developing safe and efficient hydrogen storage is among the primary technological challenges to realizing a hydrogen-based economy. Lightweight hydrogen storage materials are required for automotive applications. Aluminum is a suitable material because it is lightweight, harmless, and abundant in nature. However, although complex aluminum hydrides have been extensively investigated, they have not been considered for hydrogen storage applications. Apart from complex aluminum hydrides, few aluminum-based interstitial hydrides have been synthesized to date, although interstitial hydride —referred to as a "hydrogen-storage alloy"—exhibits excellent hydrogen reversibility.

We synthesized an aluminum-based interstitial hydride by hydrogenating a powdered aluminum–copper alloy (Al_2Cu) at high pressure and temperature. Under these conditions, hydrogen becomes extremely reactive. High-pressure and high-temperature conditions were generated by a cubic-type multi-anvil apparatus. The hydrogenation conditions were explored by an *in situ* synchrotron radiation X-ray diffraction measurement system installed on the BL14B1 at SPring-8.

Fig.5-17 shows the X-ray diffraction profiles of Al_2Cu hydrogenated at 10 GPa. After 60 s incubation at *ca*. 800 °C, new Bragg peaks (●) began to appear in the profile. The appearance of the peaks indicated that Al_2Cu was hydrogenated to Al_2CuH. The formed hydride was recovered at ambient conditions, and its crystal structure was characterized by a powder X-ray diffractometer. The obtained crystal structure of Al_2CuH (Fig.5-18) is consistent with the formation of an aluminum-based interstitial hydride. This structure is further supported by first-principles calculations.

We conclude that an aluminum-based interstitial hydride, Al_2CuH, was successfully synthesized. The experimental and theoretical results of this study will assist the exploration of other aluminum-based interstitial hydrides, and the development of practical lightweight hydrogen storage materials.

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Reference

Saitoh, H. et al., Synthesis and Formation Process of Al_2CuH_x: A New Class of Interstitial Aluminum-Based Alloy Hydride, APL Materials, vol.1, no.3, 2013, p.032113-1-032113-7.