Structural Study for Lithium Aluminum Amide by the High Intensity Total Diffractometer, NOVA

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Global warming and the resource exhaustion are serious problems to be solved. Nowadays the construction of a clean energy-oriented society based on hydrogen and the electric power has been paid much attention. To achieve the hydrogen energy society, the development of a hydrogen storage material which has high volumetric and gravimetric hydrogen density, high reversibility, and low operating temperature is required. In these days, much interest has been focused on the hydrogen storage materials composed of light elements.

To improve and understand the thermodynamics of the hydrogen storage materials, structural study could be needed. Here, a high-intensity total diffractomerer, NOVA, at J-PARC realized new opportunity to explore structures of these materials. NOVA can observe crystalline as well as amorphous and liquid structure. So it can be clarify the structural changes during the hydriding and dehydriding processes.

Lithium aluminum amide $LiAl(NH_2)_4$ stores hydrogen in the form of amide $[NH_2]^-$ and releases the NH_3 gas with a peak temperature of about 400 K [1-6]. A composite material of $LiAl(NH_2)_4$ and LiH irreversibly releases H_2 gas by 6.1 mass% below 400 K [3,4]. The H_2 desorption mechanism of the composite has been proposed, but it is still controversial because the decomposition pathway of $LiAl(NH_2)_4$ is not well known.

We here examined the detailed structural changes of $LiAl(ND_2)_4$ by using NOVA. Finally, we proposed a thermal decomposition mechanism that $LiAl(ND_2)_4$ became an amorphous phase where the AlN_4 tetrahedral unit was retained as a basic framework and was polymerized with adjacent AlN_4 units on releasing ammonia. In the presentation, the detailed structure of $LiAl(ND_2)_4$ will be described.

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References

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