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利用課題名（日本語）　　：二体分布関数を利用した $CaLi_{2-x}Mg_x$ の水素化物の理解
Program Title (English)　:Insight into hydride phase of $CaLi_{2-x}Mg_x$ from the atomic pair distribution function analysis
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1. 概要（Summary ）

There is no doubt that materials which are able to absorb and desorb a large amount of hydrogen (more than 5 mass%) at ambient conditions will play a key role in the realization of a hydrogen society. At present, metal hydrides are the only materials capable of reversibly absorbing a large amount of hydrogen at ambient conditions [1]. Conventional metal hydrides are, however, composed of heavy transition and rare-earth metals resulting in low hydrogen capacity in weight (less than 3 mass%). Therefore, it is necessary to develop light weighted metal hydrides using elements lighter than transition metals. This limits our choice to only few metals like Li, Mg, Al and Ca but their hydrides, like LiH, MgH_2 and CaH_2, require high temperatures to desorb hydrogen. Therefore, it is important to thoroughly understand hydrogen absorption and desorption properties of lightweight materials to develop new lightweight metal hydrides.

2. 実験(目的,方法)（Experimental）

To understand hydrogenation properteis of lightweight materials, we prepared CaLiMg and 400 nm Mg-thin film with a Pd cap (50 nm or 10 nm) deposited on a kapton substrate. CaLiMg powder sample was loaded in a kapton capillary and sealed with epoxy using a glovebox. Thin film samples were cut into small pieces and loaded in cells developed for an in-situ hydrogenation study. Synchrotron X-ray total scattering experiment was carried out at BL22XU [2] at SPring-8 using RA-PDF setup [3]. The X-ray energy was 70.2054 keV. Total scattering data were collected at room temperature and converted into the atomic pair distribution function (PDF) [4].

3. 結果と考察(Results and Discussion)

The X-ray PDF of CaLiMg is well explained by a C14 Laves phase structural model. For Mg-thin film sample with a 50 nm Pd cap, peaks from Pd are too large and it is difficult to see Mg peaks from PDF. For the sample with a 10 nm Pd cap, Pd peaks are still larger than Mg peaks but we can clearly differentiate Mg peaks from Pd peaks in PDF. Both Mg and Pd were fully hydrogenated using in-situ hydrogen gas loading setup. Further analysis is currently underway.

4. その他・特記事項（Others）

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