
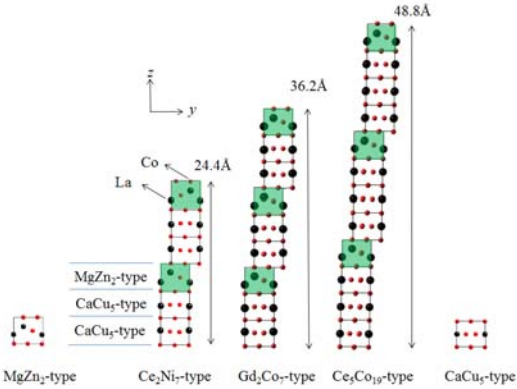


(※本報告書は英語で記述してください。ただし、産業利用課題として採択されている方は日本語で記述していただいても結構です。)

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|  MLF Experimental Report | 提出日 Date of Report 2018/1/17 |
| 課題番号 Project No. 2017B0038 実験課題名 Title of experiment The phase transformation from crystallite to amorphous phase of $\text{La}_2\text{Co}_7\text{D}_x$ during deuterium absorption-desorption process by in-situ neutron diffraction 実験責任者名 Name of principal investigator Kenji Iwase 所属 Affiliation Ibaraki University | 装置責任者 Name of responsible person Prof. T.Ohtomo 装置名 Name of Instrument/(BL No.) BL21 実施日 Date of Experiment 2017/12/11-13 |

試料、実験方法、利用の結果得られた主なデータ、考察、結論等を、記述して下さい。(適宜、図表添付のこと)
Please report your samples, experimental method and results, discussion and conclusions. Please add figures and tables for better explanation.

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| 1. 試料 Name of sample(s) and chemical formula, or compositions including physical form. |
| La_2Co_7 , $\text{La}_2\text{Co}_7\text{D}_{1.9}$, $\text{La}_2\text{Co}_7\text{D}_{7.8}$, $\text{La}_2\text{Co}_7\text{D}_{3.8}$, $\text{La}_2\text{Co}_7\text{D}_{6.6}$, $\text{La}_2\text{Co}_7\text{D}_{7.8}$ |

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| 2. 実験方法及び結果 (実験がうまくいかなかった場合、その理由を記述してください。) Experimental method and results. If you failed to conduct experiment as planned, please describe reasons. |
| <p>The alloy sample and deuteride samples were taken at room temperature. Fig. 1 shows La-Co binary alloy with super lattice structures. Fig. 2 shows the $S(q)$ profiles (BS bank) of the measured samples. The $S(q)$ decreased with increasing deuterium content as shown in Fig. 1. The profile of La_2Co_7 corresponded to Ce_2Ni_7-type structure and the Bragg peaks were sharp. Ce_2Ni_7-type structure is shown in Fig. 1. MgZn_2- and CaCu_5-type structures stacked along the c-axis in ratios of 1:2. $\text{La}_2\text{Co}_7\text{D}_{1.9}$ and $\text{La}_2\text{Co}_7\text{D}_{3.8}$ contained the solid solution phase and the deuteride phase. $\text{La}_2\text{Co}_7\text{D}_{6.6}$ and $\text{La}_2\text{Co}_7\text{D}_{7.8}$ showed single phase profile. The peak broadening increased with increasing deuterium content. The $S(q)$ of $\text{La}_2\text{Co}_7\text{D}_{7.8}$ showed particularly heavy broadening, however, the Bragg peaks were clearly observed in the profile</p> <div style="text-align: right;">  </div> <p>Fig. 1 La-Co binary alloy with super lattice structure</p> |

2. 実験方法及び結果(つづき) Experimental method and results (continued)

as shown in Fig. 3.

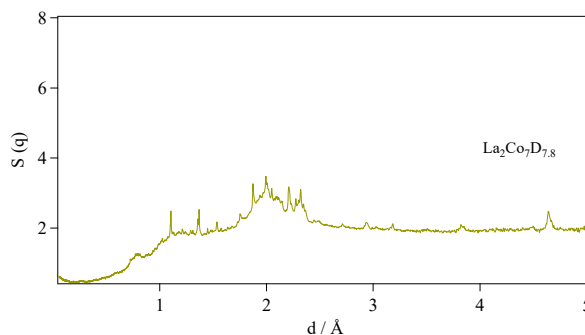
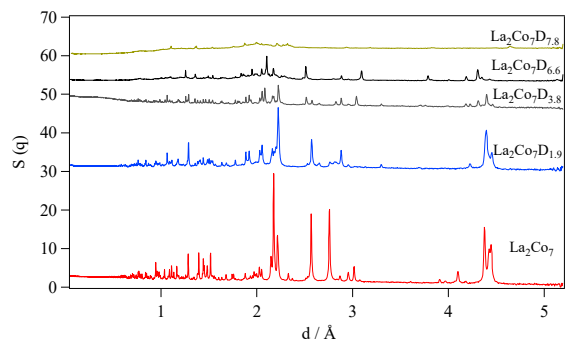


Fig. 2 $S(q)$ profiles (BS bank) of $\text{La}_2\text{Co}_7\text{D}_x$ ($X = 0 \sim 7.8$)

Fig. 3 $S(q)$ profile (BS bank) of $\text{La}_2\text{Co}_7\text{D}_{7.8}$

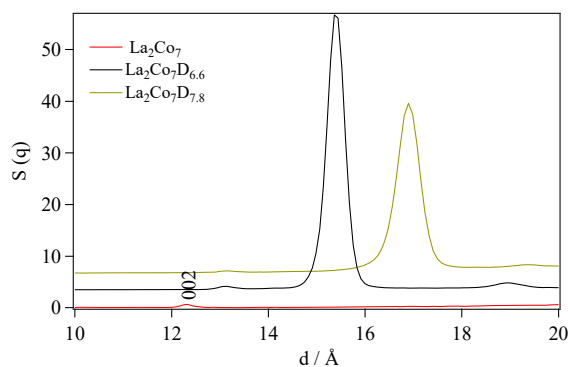


Fig. 4 $S(q)$ profile (20 degrees bank) of $\text{La}_2\text{Co}_7\text{D}_7$, $\text{La}_2\text{Co}_7\text{D}_{6.6}$ and $\text{La}_2\text{Co}_7\text{D}_{7.8}$.

Considering the change of $S(q)$ and peak profile, the symmetry of deuteride phases is lower than that of the original alloy (Ce_2Ni_7 -type, hexagonal, No. 194).

Fig. 4 shows the $S(q)$ profile of La_2Co_7 , $\text{La}_2\text{Co}_7\text{D}_{6.6}$ and $\text{La}_2\text{Co}_7\text{D}_{7.8}$ by 20 degrees bank. The superlattice peak 002 of La_2Co_7 with Ce_2Ni_7 -type structure was observed in the profile. The $S(q)$ of peaks of $\text{La}_2\text{Co}_7\text{D}_{6.6}$ and $\text{La}_2\text{Co}_7\text{D}_{7.8}$ was appreciably larger than that of La_2Co_7 , which indicates that the superlattice structures retain in $\text{La}_2\text{Co}_7\text{D}_{6.6}$ and $\text{La}_2\text{Co}_7\text{D}_{7.8}$.

The structure model of deuteride phases are considering by combined XRD and $S(q)$ profiles. Orthorhombic model is attempting to $\text{La}_2\text{Co}_7\text{D}_{6.6}$. Deuterium occupation sites exist in 6 sites in MgZn_2 -type cell and 8 sites in CaCu_5 -type cell. It is necessary to check D-D, La-D and Co-D bonds length. Westlake's criterion for H-H distance (2.1 Å) is satisfied or not.