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MLF Experimental Report	提出日 Date of Report 2018/8/30
課題番号 Project No. 2018A0002 実験課題名 Title of experiment Phase transition of Pr2Co7 along P-C isotherm and its deuteration property 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 Dr. M. Yonemura 装置名 Name of Instrument/（BL No.） BL09 実施日 Date of Experiment 2018/5/4-6

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.

1. 試料 Name of sample(s) and chemical formula, or compositions including physical form.

Pr_2Co_7, $Pr_2Co_7D_{2.7}$, $Pr_2Co_7D_{7.2}$

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.

The alloy and deuteride samples were collected at room temperature. Fig. 1 shows the P-C isotherm of Pr_2Co_7 with Ce_2Ni_7-type structure. The maximum hydrogen capacity reached 0.8 H/M (H/M: atomic rations between metal atoms and hydrogen atoms) at the first absorption as shown in Fig. 1. Two plateaus were observed in the absorption-desorption process. The second absorption-desorption process showed the same as the first absorption-desorption process. Fig. 2 shows the neutron diffraction profiles of $Pr_2Co_7D_x$ ($0 < x < 7.2$) during first absorption process (phase I ~ II indicated in Fig. 1). The BS bank data is used for Fig. 2. The phase I, II and III are alloy, half-deuteride and full-deuteride phases. The Bragg peaks increased with increasing deuterium content. The profile of phase III is clearly different from phase I with Ce_2Ni_7-type.

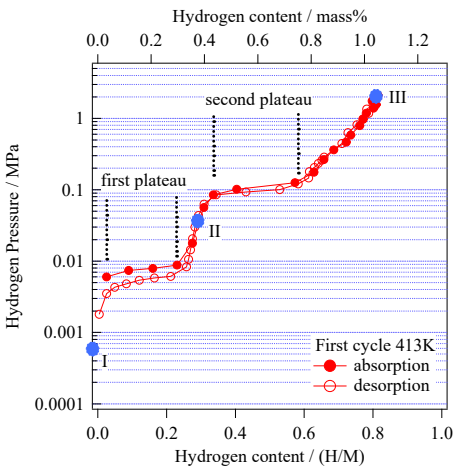

Fig. 1 P-C isotherm of Pr_2Co_7

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

The structure of the phase III (full-deuteride) transformed from $P6_3/mmc$ to lower symmetry, which is correspond to XRD results. The XRD results show the crystal structure of metal sublattice transforms from $P6_3/mmc$ to orthorhombic.

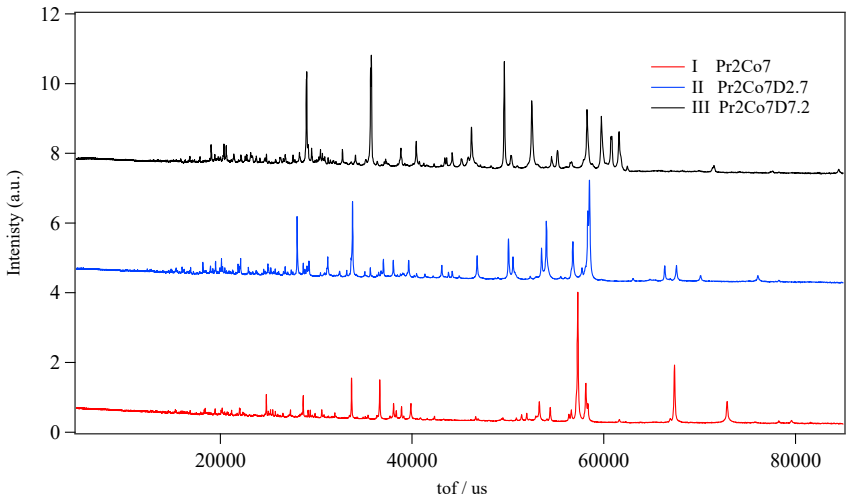

Fig. 2 Neutron diffraction profiles of alloy (I), half-deuteride (II) and full-deuteride (III).

Fig. 3 shows the Rietveld refinement pattern of the phase I (Pr_2Co_7). The structural model Ce_2Ni_7-type was used for refinement. The refined lattice parameters a and c were 5.06244(1) Å and 24.5274(1) Å. The R_{wp}, R_p, R_e and chi-square were 3.84%, 2.55%, 0.7% and 24.6. This result corresponds to that of X-ray diffraction.

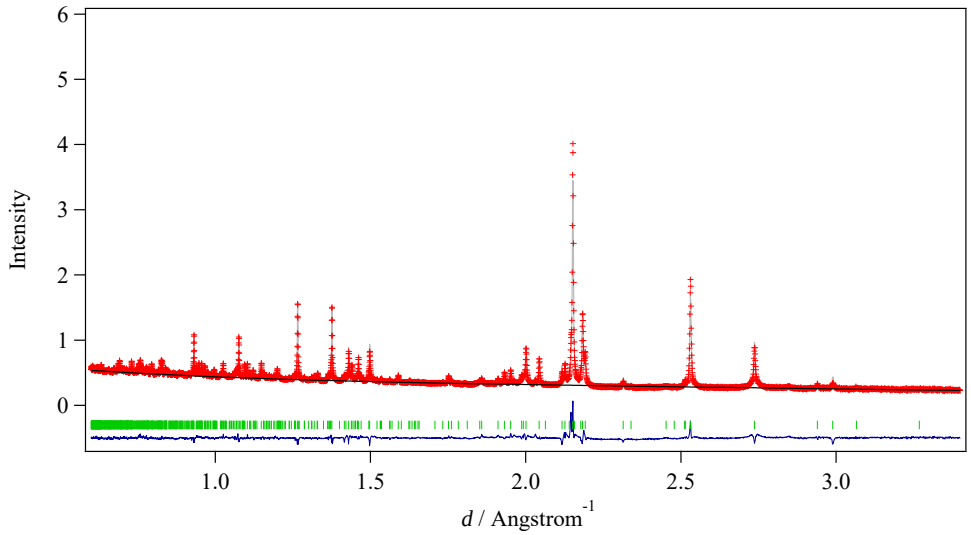

Fig. 3 Rietveld refinement pattern of before deuteration Pr_2Co_7 with Ce_2Ni_7-type structure.

The structure of the deuteride phases, $Pr_2Co_7D_{2.7}$ and $Pr_2Co_7D_{7.2}$, are analyzing using hexagonal symmetry and orthorhombic symmetry. The satisfied fitting is not obtained. It is necessary to attempt the several atomic positions and occupation of deuterium atoms.