MLF Experimental Report	提出日 Date of Report July 4, 2011
課題番号 Project No. 2010B0025 実験課題名 Title of experiment Structural study of $TbPd_{1-x}Ni_xAl$ with isostructural phase transition 実験責任者名 Name of principal investigator Hideaki Kitazawa 所属 Affiliation National Research Institute for Materials Science (NIMS)	装置責任者 Name of responsible person Takashi Kamiyama 装置名 Name of Instrument/（BL No.） BL-08 実施日 Date of Experiment Feb. 4 – Feb. 6, 2011

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.

$TbPd_{1-x}Ni_xAl$ (x = 0, 0.2, 0.4, 0.6, 0.8, 1.0) and $TbNi_{1-x}Cu_xAl$ (x = 0.2, 0.3, 0.4) samples were prepared by arc melting stoichiometric mixtures of the pure elements (Tb:3N; Pd: 3N5; Ni: 4N; Cu:4N; Al:5N) in an argon gas atmosphere. The as-cast buttons were pulverized by an agate mortal. All powder samples were checked by the X-ray diffraction to be single phase of the hexagonal ZrNiAl-type structure (P6-2m). The powder sample of 8.1 g to 9.9 g was filled in a vanadium cylinder with 10 mm in outer diameter and 25 mm to 33 mm in length.

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.

2-1. Experimental methods

We have performed the powder neutron diffraction measurements using a high-resolution neutron diffractometer, BL-08 (SuperHRPD) installed at the megawatt-class pulsed spallation neutron sources, J-SNS, at the Japanese particle accelerator research complex (J-PARC). The exposure time for data collection in 0.2 MW operation was approximately 5 hours for each sample contained in a cylindrical vanadium cell 10 mm in outer diameter. Rietveld refinements were carried out using the program Z-Rietveld ver. 0.9.36 for time-of-flight neutron powder diffraction analyses.

All the diffraction peaks could be indexed by the the hexagonal ZrNiAl-type structure (P6-2m). When we tried to fit all powder patterns by Z-Rietveld, we could find the tentative structure parameters at room temperature as shown in the Table 1 and 2. The nominal concentration was fixed in the process of Riedveld analysis for simplicity. However, we could not achieve further reduction of

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

Table 1 Tentative structure parameters of $TbPd_{1-x}Ni_xAl$ at room temperature with a single phase fitting.

x	a (Å)	c (Å)	c/a	R_{wp} (%)
0	7.19178(2)	3.99425(2)	0.55539	6.3
0.2	7.11500(0)	4.01527(1)	0.56434	8.0
0.4	7.04986(1)	4.02518(1)	0.57095	6.6
0.6	7.01000(0)	4.00235(1)	0.57095	8.8
0.8	7.017592(6)	3.931178(6)	0.56019	7.1
1	7.00613(1)	3.87749(1)	0.55344	6.6

Table 2 Tentative structure parameters of $TbNi_{1-x}Cu_xAl$ at room temperature with a single phase fitting.

x	a (Å)	c (Å)	c/a	R_{wp} (%)
0	7.00613(1)	3.87749(1)	0.55344	6.6
0.2	7.022901 (3)	3.898384 (4)	0.56434	5.8
0.3	6.978217 (7)	3.967262 (9)	0.56852	10.8
0.4	7.01000(0)	4.00235(1)	0.57095	6.3

the R-factor. One reason is that the alloying transition element of Ni or Cu for Pd or Ni, respectively, induces the isostructural phase transition (IPT). When we apply the empirical rule that the IPT appears in the forbidden range of c/a from 0.56 to 0.57, IPT should occur at around x = 0.2 and 0.8 in $TbPd_{1-x}Ni_xAl$ and x = 0.2 - 0.3 in $TbNi_{1-x}Cu_xAl$, respectively. The double peaks of (210) peak in Fig.1 indicate that the 2 phases with low and high c/a ratio clearly coexist in $TbPd_{1-x}Ni_xAl$. The two phases coexist at around x = 0.3 in $TbNi_{1-x}Cu_xAl$ as shown in Fig.2. We could detect the coexistence of both phases owing to the high resolution neutron diffractometer, BL-08 (SuperHRPD). We need further investigation with different concentration of Ni and Cu to describe the whole phase diagram.

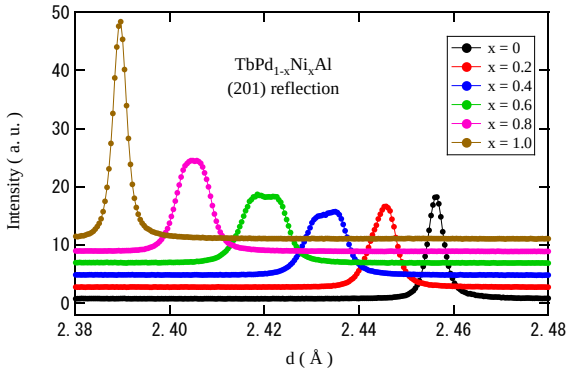

Fig. 1 Ni concentration dependence of a (201) Bragg peak position in $TbPd_{1-x}Ni_xAl$.

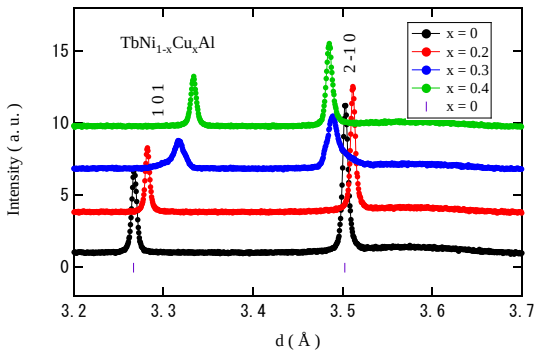

Fig. 2 Ni concentration dependence of (1 0 1) and (2-1 0) Bragg peak position in $TbNi_{1-x}Cu_xAl$.