Powder diffraction data of the $PrAlFeNi_3$ quaternary compound

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(Received 12 June 2014; accepted 31 August 2014)

A new quaternary compound $PrAlFeNi_3$ was synthesized and studied by means of X-ray powder diffraction technique. The powder pattern of $PrAlFeNi_3$ was indexed and refined, giving a hexagonal structure, space group *P*6/mmm (No. 191) with the $CaCu_5$ structure type, $a = 5.1132(2)$ Å, $c = 4.0737(1)$ Å, $V = 92.19$ Å^3, $Z = 1$, $\rho_x = 7.20$ g cm^{-3}, $F_{30} = 173.61$ (0.0054, 32) and RIR = 0.77. © *2014 International Centre for Diffraction Data.* [doi:10.1017/S0885715614000839]

Key words: $PrAlFeNi_3$, powder X-ray diffraction data

I. INTRODUCTION

Many AB_5 intermetallic compounds, a metal hydride with hexagonal $CaCu_5$ type structure, can react reversibly with hydrogen at moderate pressure and temperature and exhibit excellent hydrogen storage properties. These compounds are extensively investigated and pseudobinary compounds obtained by partial replacement of the constituents in $LaNi_5$ have also been examined in order to improve hydriding properties for specific applications. It has been found that these substitutions induce a large change in both the stability and the capacity of the related hydrides (Percheron-Guegan *et al.*, 1985). So far, powder diffraction data of the quaternary compound $PrAlFeNi_3$ have not included in the PDF (ICDD, 2011). Therefore, in this paper, we present high-quality experimental powder XRD data for $PrAlFeNi_3$.

II. EXPERIMENTAL

A. Synthesis

The sample of $PrAlFeNi_3$ with a total mass of 2 g was prepared by arc melting using a non-consumable tungsten electrode and a water-cooled copper tray under argon atmosphere. Praseodymium (purity of 99.9%), aluminum (purity of 99.8%), iron (purity of 99.9%), and germanium (purity of 99.9%) were used as the starting materials. Titanium was used as an oxygen getter during the melting process. The sample was remelted three times in order to ensure the complete fusion and

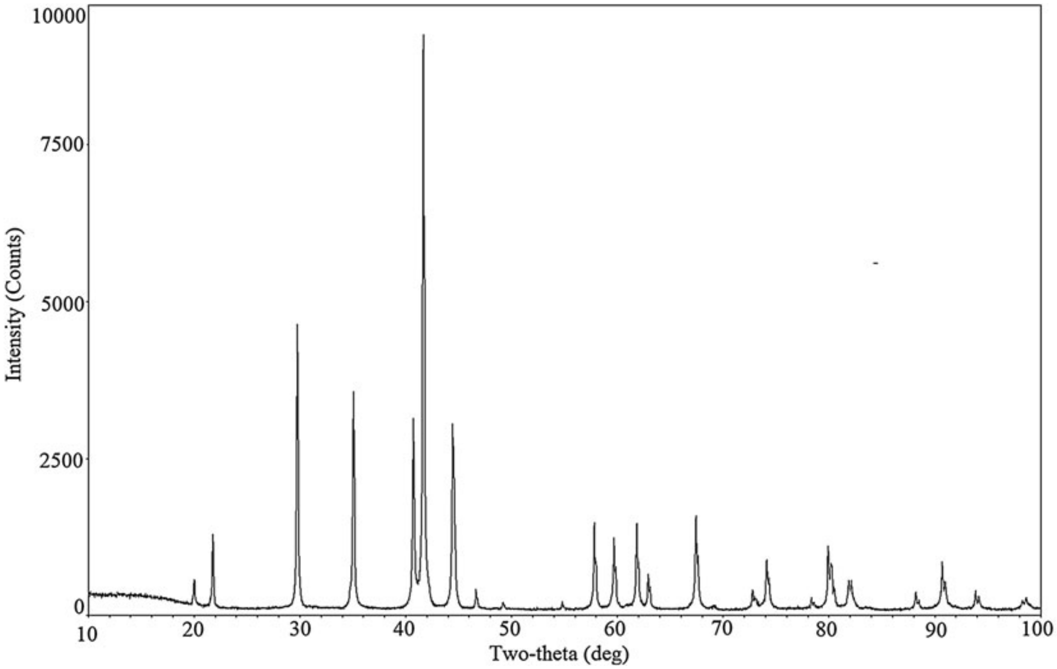

Figure 1. X-ray powder diffraction pattern for $PrAlFeNi_3$.

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TABLE I. Powder diffraction data of a new quaternary compound $PrAlFeNi_3$ ($CuK\alpha_1$, with $\lambda = 1.5406$ Å).

No.	h	k	l	$2\theta_{obs}$	$2\theta_{cal}$	$\Delta 2\theta^a$	I/I_o	d_{obs}	d_{cal}
1	1	0	0	20.039	20.040	0.001	4.4	4.4273	4.4270
2	0	0	1	21.800	21.799	−0.001	12.7	4.0735	4.0737
3	1	0	1	29.779	29.779	0	49.5	2.9977	2.9977
4	1	1	0	35.079	35.079	0	37.6	2.5560	2.5560
5	2	0	0	40.721	40.729	0.007	32.3	2.2139	2.2135
6	1	1	1	41.681	41.682	0.001	100	2.1651	2.1651
7	0	0	2	44.459	44.441	−0.018	32	2.0361	2.0368
8	2	0	1	46.662	46.662	0	3.1	1.9449	1.9449
9	1	0	2	49.198	49.200	0.002	1.1	1.8505	1.8504
10	2	1	0	54.832	54.819	−0.014	1.3	1.6729	1.6733
11	1	1	2	57.841	57.837	−0.003	14.8	1.5928	1.5929
12	2	1	1	59.699	59.691	−0.008	12.1	1.5476	1.5478
13	2	0	2	61.843	61.850	0.008	14.2	1.4990	1.4988
14	3	0	0	62.939	62.931	−0.009	5.6	1.4755	1.4757
15	3	0	1	67.442	67.446	0.004	16	1.3875	1.3875
16	0	0	3	69.128	69.119	−0.01	0.7	1.3577	1.3579
17	1	0	3	72.788	72.789	0.001	2.9	1.2982	1.2982
18	2	1	2	73.135	73.134	−0.001	1.2	1.2929	1.2929
19	2	2	0	74.139	74.132	−0.007	8.1	1.2779	1.2780
20	2	2	1	78.361	78.351	−0.01	1.8	1.2193	1.2194
21	1	1	3	79.939	79.933	−0.006	10.6	1.1991	1.1992
22	3	0	2	80.260	80.268	0.008	7.2	1.1951	1.1950
23	3	1	1	81.880	81.873	−0.007	4.7	1.1755	1.1756
24	2	0	3	83.439	83.440	0.001	0.4	1.1575	1.1575
25	4	0	0	88.201	88.210	0.009	2.9	1.1069	1.1068
26	2	2	2	90.710	90.722	0.012	7.9	1.0827	1.0825
27	2	1	3	93.863	93.865	0.002	3.1	1.0544	1.0544
28	3	1	2	94.191	94.195	0.004	2.2	1.0516	1.0516
29	0	0	4	98.287	98.286	−0.001	1.4	1.0184	1.0184
30	3	2	0	98.658	98.651	−0.007	1.9	1.0156	1.0156

[a] $\Delta 2\theta = 2\theta_{cal} - 2\theta_{obs}$.

homogeneity. Weight losses were less than 1 wt%. After melting, the sample was enclosed in an evacuated quartz tube and annealed at 1073 K for 720 h, then cooled down at a rate of 10 K h^{-1} to room temperature. The sample was ground in an agate mortars and pestled to particle sizes of no larger than 45 μm.

B. Data collection

Powder X-ray diffraction (XRD) patterns of $PrAlFeNi_3$ compound were collected at room temperature using a Rigaku Smart Lab 2006 powder diffractometer equipped with a $CuK\alpha$ radiation and a diffracted-beam graphite monochromator. The diffractometer was operated at 40 kV and 180 mA, the 2θ scan range was from 10 to 100° with a step size of 0.02° and a count time of 3 s per step. Two sets of XRD data were collected, one with SRM 640 Si added as an internal standard to correct for possible systematical errors in the observed peak positions and the other without SRM 640 Si. The XRD pattern recorded from the specimen added with Si internal standard was used for indexing and for determining space group and unit-cell information, while the XRD pattern without Si internal standard was used for determining diffraction intensities. The $2\theta_{obs}$ values of the peaks were determined by the Savitzky–Golay second derivative using JADE 6.0 (Materials Data Inc., 2002) XRD Pattern Processing software of Materials Data, Inc. after smoothing the patterns, fitting and removing the background, and stripping the $CuK\alpha_2$ peaks. Values of unit-cell parameters were then obtained by the least-squares method using JADE 6.0.

III. RESULTS

The experimental XRD pattern of compound $PrAlFeNi_3$ is shown in Figure 1. All lines were successfully indexed using the Jade6.0 program in hexagonal structure. By comparing powder XRD data of $PrAlFeNi_3$ with those of $LaMn_{1.13}Ni_{3.87}$ (PDF2, 00-033-0707#), it was found that $PrAlFeNi_3$ and $LaMn_{1.13}Ni_{3.87}$ (Achard *et al.*, 1979) have the same structure type $P6/mmm$ (No. 191). Using the corrected diffraction data of $PrAlFeNi_3$, the accurate lattice parameters were obtained: $a = 5.1132(2)$ Å, $c = 4.0737(1)$ Å, $V = 92.19$ $Å^3$, $Z = 1$, and $\rho_x = 7.20$ g cm^{-3}. The figure of merit for indexing F_N (Smith and Snyder, 1979) is 173.61 (0.0054, 32) and the value of RIR (RIR = 0.77) was obtained from the value of the ratio of the strongest line in the pattern to the strongest line of corundum in a 50–50 wt percent mixture of the two compounds. The observed and the calculated X-ray powder diffraction data (Prince, 2004) for $PrAlFeNi_3$ are listed in Table I.

ACKNOWLEDGEMENT

This work was supported by the Scientific Foundation of Guangxi High Education (2013ZD070).

SUPPLEMENTARY DATA

The supplementary material for this article can be found at http://www.journals.cambridge.org/PDJ

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