Powder diffraction data of the $AlCeCo_2Ni_2$ quaternary compound

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A new quaternary compound $AlCeCo_2Ni_2$ was synthesized and studied by means of X-ray powder diffraction technique. The powder pattern of $AlCeCo_2Ni_2$ was indexed and refined, giving a hexagonal structure, space group P_6/mmm (No. 191) with the $CaCu_5$ structure type. $a = 4.9242(2)$ Å, $c = 4.0524(1)$ Å, $V = 85.1$ Å^3, $Z = 1$, $\rho_x = 7.85$ g cm^{-3}, $F_{30} = 130.2(0.010, 30)$, and RIR = 0.71(2). © *2016 International Centre for Diffraction Data.* [doi:10.1017/S0885715616000300]

Key words: $AlCeCo_2Ni_2$, quaternary compound, $CaCu_5$ structure type, powder X-ray diffraction data

I. INTRODUCTION

The development and application of high and new technology is often inseparable from discovery of new materials, and most of the new materials research and development starts with synthesis and characterization. Polynary compounds compared with binary compounds have additional constituent elements and potentially a diversity of structure. These compounds may exhibit excellent properties for developing new function materials. As far as we know, previous studies of the RE–Al–Cu–Ni quaternary system have reported several quaternary compounds: $AlCeCu_2Ni_2$ (Sinha and Wallace, 1984), $AlCuLaNi_3$ (Burnasheva *et al.*, 1984), and $AlCu_{0.2}LaNi_{3.8}$ (Li *et al.*, 2009). These compounds have a hexagonal structure, space group P_6/mmm (No. 191) with the $CaCu_5$ (Haucke, 1940) structure type. So far, we have not found any powder diffraction patterns of quaternary compounds of RE–Al–Co–Ni quaternary system included in the Inorganic Crystal Structure Database (ICSD Database, 2015.01). Therefore, in this paper, we present high-quality experimental powder X-ray diffraction (XRD) data for $AlCeCo_2Ni_2$.

II. EXPERIMENTAL

A. Synthesis

Polycrystalline specimen of $AlCeCo_2Ni_2$ was prepared by arc melting using a non-consumable tungsten electrode and a water-cooled copper tray under argon atmosphere. Aluminum (purity of 99.9%), cobalt (purity of 99.9%), cerium (purity of 99.99%), and nickel (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 several times in order to ensure complete fusion and homogeneity. Weight losses were <1 wt%. After melting, the sample was enclosed in an evacuated quartz tube and annealed at 1053 K for 720 h, then cooled down at a rate of 12 K h^{-1} to room temperature. Before X-ray measurements, the sample was ground in an agate mortar and pestle to particle sizes of no larger than 30 μm.

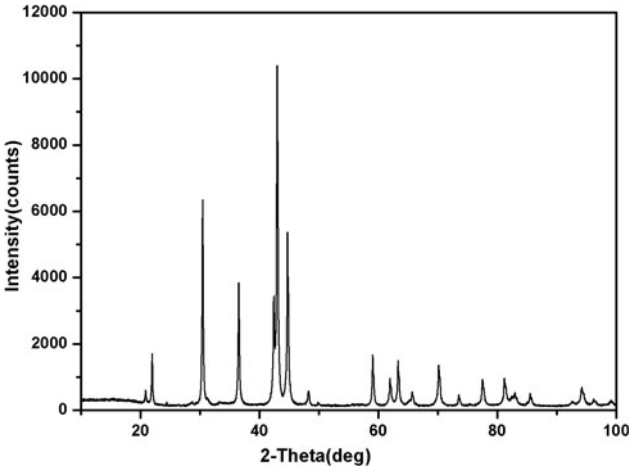


Figure 1. The powder XRD pattern of $AlCeCo_2Ni_2$.

B. Data collection

The powder XRD patterns of $AlCeCo_2Ni_2$ compound were collected at room temperature on a Rigaku Smart Lab 2006 powder diffractometer using Cu$K\alpha$ radiation and a diffracted-beam graphite monochromator. The diffractometer was operated at 40 kV and 150 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. The X-ray goniometer optics were 300 mm goniometer radius, receiving slit of 0.3 mm, ½ deg. incident and diffracted beam anti scatter slits, incident and diffracted beam solar slits, and a scintillation counter detector, the stabilities of both the X-ray source and the specimen were checked by recording again the diffraction lines at low angles. Two sets of XRD data were collected: one with SRM 640a Si added as an internal standard to correct for possible systematical errors in the observed peak positions and the other pure sample do not add anything. All the XRD data samples used a flattened surface when data were collected. In order to reduce the preferred orientation for the intensity data, the samples were ground to particle sizes of no larger than 30 μm, and do not exert external force as far as possible. 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

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TABLE I. Powder diffraction data for $AlCeCo_2Ni_2$ ($CuK\alpha_1$, with $\lambda = 1.540\,60$ Å).

No.	$2\theta_{obs}$	h	k	l	$2\theta_{cal}$	$\Delta 2\theta$[a]	I_{obs}	d_{obs}	d_{cal}
1	20.801	1	0	0	20.813	0.012	37	4.2669	4.2645
2	21.900	0	0	1	21.915	0.015	150	4.0551	4.0524
3	30.398	1	0	1	30.403	0.005	614	2.9380	2.9376
4	36.459	1	1	0	36.463	0.003	365	2.4623	2.4621
5	42.359	2	0	0	42.354	−0.005	323	2.1320	2.1322
6	42.940	1	1	1	42.947	0.007	1000	2.1045	2.1042
7	44.680	0	0	2	44.688	0.008	505	2.0265	2.0262
8	48.181	2	0	1	48.185	0.004	30	1.8871	1.8870
9	49.781	1	0	2	49.782	0.001	10	1.8301	1.8301
10	57.080	2	1	0	57.096	0.016	05	1.6122	1.6118
11	58.982	1	1	2	58.989	0.008	152	1.5647	1.5645
12	61.900	2	1	1	61.902	0.002	76	1.4978	1.4977
13	63.260	2	0	2	63.260	0.000	122	1.4688	1.4688
14	65.641	3	0	0	65.623	−0.018	37	1.4212	1.4215
15	69.543	0	0	3	69.534	−0.008	14	1.3507	1.3508
16	70.099	3	0	1	70.094	−0.005	119	1.3413	1.3414
17	73.478	1	0	3	73.477	0.000	33	1.2877	1.2877
18	75.292	2	1	2	75.274	−0.018	7	1.2611	1.2614
19	77.460	2	2	0	77.468	0.008	77	1.2312	1.2311
20	81.139	1	1	3	81.148	0.008	71	1.1844	1.1843
21	81.271	3	1	0	81.273	0.002	50	1.1828	1.1828
22	81.683	2	2	1	81.679	−0.003	7	1.1779	1.1779
23	82.902	3	0	2	82.895	−0.007	28	1.1636	1.1637
24	84.901	2	0	3	84.915	0.014	7	1.1412	1.1411
25	85.440	3	1	1	85.442	0.002	35	1.1354	1.1354
26	92.539	4	0	0	92.524	−0.015	10	1.0660	1.0661
27	94.115	2	2	2	94.133	0.018	46	1.0522	1.0521
28	96.159	2	1	3	96.149	−0.010	17	1.0352	1.0353
29	96.680	4	0	1	96.678	−0.002	6	1.0310	1.0310
30	97.900	3	1	2	97.893	−0.007	2	1.0214	1.0215
31	99.001	0	0	4	98.986	−0.015	9	1.0130	1.0131

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

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 $AlCeCo_2Ni_2$ is shown in Figure 1. All lines were successfully indexed using the Jade6.0 program in the hexagonal system. By comparing powder XRD data with those of $AlCeCu_2Ni_2$ (Sinha and Wallace, 1984) and $AlCuLaNi_3$ (Burnasheva *et al.*, 1984), it was found that $AlCeCo_2Ni_2$, $AlCeCu_2Ni_2$, and $AlCuLaNi_3$ have the same structure type P_6/mmm (No.191). Using the corrected diffraction data of $AlCeCo_2Ni_2$, the accurate unit-cell parameters were obtained with $a = 4.9242(2)$ Å, $c = 4.0524(1)$ Å, $V = 85.1$ Å^3, $Z = 1$, and $\rho_x = 7.85$ g cm^{-3}, which is very close to the experimental density (about 7.55 g cm^{-3}). The figure of merit for indexing F_N (Smith and Snyder, 1979) is $F_{30} = 130.2$ (0.010, 30) and the value of RIR (RIR = 0.71) 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.% mixture of the two compounds. The observed and the calculated X-ray powder diffraction data for $AlCeCo_2Ni_2$ are listed in Table I.

SUPPLEMENTARY MATERIAL

The supplementary material for this article can be found at http://dx.doi.org/10.1017/S0885715616000300.

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Burnasheva, V. V., Petrova, K. A., Semenenko, K. N., Zhang, J., and Bobev, S. (**1984**). "The reaction of hydrogen with the compounds $LaNi_{5-x}$ (T1, T2)$_x$ where T1, T2 = Al, Cr, Fe, Cu," Zh. Neorg. Khim. **29**, 869–874.

Haucke, W. (**1940**). "Kristallstruktur von $CaZn_5$ und $CaCu_5$," Z. Anorg. Allg. Chem. **244**, 17–22.

Inorganic Crystal Structure Database (**2015**). *Fachinformationszentrum Karlsruhe, Germany, and the U.S. Department of Commerce on the behalf of the United States* (Inorganic Crystal Structure Database, Germany).

JADE Version 6.0 (**2002**). *XRD Pattern Processing* (Materials Data Inc., Livermore, CA).

Li, S. L., Wang, P., Chen, W., Luo, G., Chen, D. M., and Yang, K. (**2009**). "Hydrogen storage properties of $LaNi_{3.8}$ $AlM_{0.2}$ (M = Ni, Cu, Fe, Al, Cr, Mn) alloys," J. Alloy Compd. **485**, 867–871.

Sinha, V. K. and Wallace, W. E. (**1984**). "Effect of neodymium, copper and aluminium on the hydriding characteristics of $CeNi_5$," J. Less Common Met. **96**, 283–290.

Smith, G. S. and Snyder, R. L. (**1979**). "FN: a criterion for rating powder diffracton patterns and evaluating the reliability of powder pattern indexing," J. Appl. Crystallogr. **12**, 60.

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