

# NEW DIFFRACTION DATA

## The X-ray powder diffraction data for CeCo<sub>3</sub>Ni<sub>2</sub>

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The CeCo<sub>3</sub>Ni<sub>2</sub> compound was synthesized by arc melting under argon atmosphere. High-quality powder X-ray diffraction (XRD) data of CeCo<sub>3</sub>Ni<sub>2</sub> have been collected using a Rigaku SmartLab X-ray powder diffractometer. The refinement of the XRD pattern for the CeCo<sub>3</sub>Ni<sub>2</sub> compound shows that the CeCo<sub>3</sub>Ni<sub>2</sub> is a hexagonal structure, space group *P6/mmm* (No.191) with  $a = b = 4.9081(2)$  Å,  $c = 4.0034(2)$  Å,  $V = 83.52$  Å<sup>3</sup>,  $Z = 1$ , and  $\rho_x = 8.6347$  g cm<sup>-3</sup>. The Smith–Snyder FOM  $F_{30} = 112.7$  (0.0089, 30) and the intensity ratio RIR = 0.48. © 2014 International Centre for Diffraction Data. [doi:10.1017/S0885715614000463]

Key words: CeCo<sub>3</sub>Ni<sub>2</sub>, X-ray powder diffraction

### I. INTRODUCTION

The AB<sub>5</sub>-type hydrogen storage alloy is widely used in nickel-metal hydride batteries as anode material because of its good comprehensive performance, such as easy activation, dynamic performance, moderate capacity, relatively low price, etc. Researchers have done a lot of work with experimental and theoretical studies since LaNi<sub>5</sub> hydrogen storage alloy was found in the 1960s of the past century, resulting in the development of a large number of AB<sub>5</sub>-type hydrogen storage alloys using the method of element substitution. At present, the structure of AB<sub>5</sub> alloy materials has been investigated, and several AB<sub>5</sub>-type alloys have been confirmed, such as LaNi<sub>4.5</sub>Si<sub>0.5</sub>, LaMn<sub>3</sub>Ni<sub>2</sub>, LaMnNi<sub>4</sub>, LaNi<sub>4.25</sub>Al<sub>0.75</sub>, LaNi<sub>4.75</sub>Sn<sub>0.25</sub>, FeLaNi<sub>4</sub>, Cu<sub>3</sub>LaNi<sub>2</sub>, Ga<sub>1.2</sub>LaNi<sub>3.8</sub>, La<sub>0.5</sub>Ni<sub>5</sub>Y<sub>0.5</sub>, Ce<sub>0.5</sub>La<sub>0.5</sub>Ni<sub>5</sub>, Co<sub>2.5</sub>LaNi<sub>2.5</sub>, Cr<sub>0.5</sub>Cu<sub>1.5</sub>LaNi<sub>3</sub>, CuFeLaNi<sub>3</sub>, Al<sub>0.3</sub>Co<sub>0.75</sub>LaMn<sub>0.4</sub>Ni<sub>3.55</sub>, and others. The X-ray diffraction (XRD) patterns of a new phase in the Ce–Co–Ni ternary system have not been extensively studied, and there are very few reports about the structure of a CeCoNi phase from inorganic crystal structure database (Da *et al.*, 1983) and ICDD's PDF4+ database (Klyamkin *et al.*, 2005).

So far, the experimental X-ray powder diffraction data of the CeCo<sub>3</sub>Ni<sub>2</sub> phase have not been included in the ICDD's Master Database. We report here the high-quality powder XRD data for the compound CeCo<sub>3</sub>Ni<sub>2</sub>.

### II. EXPERIMENTAL

#### A. Synthesis

The sample of CeCo<sub>3</sub>Ni<sub>2</sub> was generated from the melt of stoichiometric amounts of elemental constituents (99.9 wt% Ce, 99.99 wt% Co, and 99.99 wt% Ni by China New Metal Materials Technology Co. Ltd.) under high-purity argon atmosphere in a vacuum arc furnace, which has a tungsten

electrode and a water-cooled copper tray. During the melting process, titanium was used as an oxygen capture agent. In order to ensure fused together and uniform composition, multiple melting processes (three times in this experiment) have been executed. Weight losses of the sample were <1 wt% with a total mass of 2 g. After melting, the sample was enclosed in an evacuated quartz tube and annealed at 1173 K for 480 h, and then cooled down to room temperature at a rate of 18 K h<sup>-1</sup>. Finally, the sample was ground to powder with a particle size smaller than 20 µm, in an agate mortar.

#### B. Data collection

The X-ray powder diffraction data for CeCo<sub>3</sub>Ni<sub>2</sub> compound were collected at room temperature using a Rigaku SmartLab X-ray powder diffractometer, using CuKα radiation and a diffraction beam graphite monochromator. The diffractometer was operated at 40 kV and 150 mA, the scan range of 2θ was from 10° to 100° with a step size of 0.02° and a count-time of 10 s step<sup>-1</sup>.

X-ray powder diffraction data for the mixture of CeCo<sub>3</sub>Ni<sub>2</sub> and an internal standard material (SRM Si) were

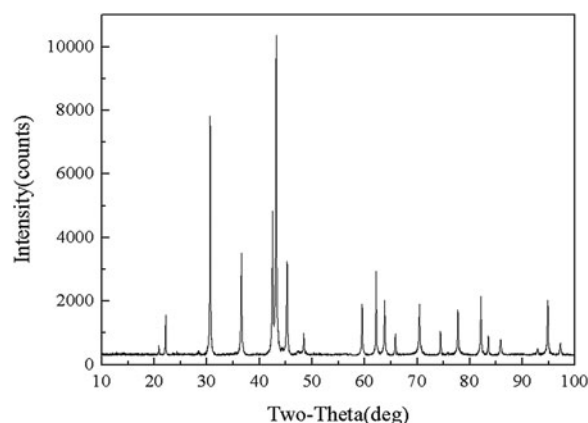


Figure 1. The X-ray powder diffraction pattern of CeCo<sub>3</sub>Ni<sub>2</sub>.

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TABLE I. X-ray powder diffraction data for CeCo<sub>3</sub>Ni<sub>2</sub> (CuK  $\alpha_1$ , with  $\lambda = 1.5406 \text{ \AA}$ ).

No.	<i>h</i>	<i>k</i>	<i>l</i>	$2\theta_{\text{obs}}$	$2\theta_{\text{cal}}$	$\Delta 2\theta^a$	<i>l</i> / <i>I</i> <sub>0</sub>	<i>d</i> <sub>obs</sub>	<i>d</i> <sub>cal</sub>	$\Delta d^b$
1	1	0	0	20.864	20.882	-0.018	2.9	4.2541	4.2505	0.0036
2	0	0	1	22.180	22.187	-0.007	12.7	4.0045	4.0034	0.0011
3	1	0	1	30.645	30.652	-0.007	75.4	2.9149	2.9143	0.0006
4	1	1	0	36.573	36.587	-0.014	32.4	2.4549	2.454	0.0009
5	2	0	0	42.499	42.500	-0.001	46	2.1253	2.1253	0
6	1	1	1	43.201	43.205	-0.004	100	2.0924	2.0922	0.0002
7	0	0	2	45.260	45.265	-0.005	29	2.0019	2.0017	0.0002
8	2	0	1	48.460	48.453	0.007	6.8	1.8769	1.8771	-0.0002
9	1	0	2	50.340	50.346	-0.006	0.6	1.8111	1.8109	0.0002
10	2	1	0	57.319	57.301	0.018	0.5	1.6061	1.6065	-0.0004
11	1	1	2	59.559	59.550	0.009	16.4	1.5509	1.5511	-0.0002
12	2	1	1	62.221	62.213	0.008	27	1.4908	1.491	-0.0002
13	2	0	2	63.839	63.825	0.014	17.6	1.4568	1.4571	-0.0003
14	3	0	0	65.879	65.866	0.013	6.9	1.4166	1.4168	-0.0002
15	3	0	1	70.428	70.438	-0.010	13.1	1.3358	1.3357	0.0001
16	0	0	3	70.510	70.511	-0.001	8	1.3345	1.3345	0
17	1	0	3	74.459	74.458	0.001	7.5	1.2732	1.2732	0
18	2	1	2	75.880	75.873	0.007	0.9	1.2528	1.2529	-0.0001
19	2	2	0	77.760	77.771	-0.011	13.7	1.2272	1.227	0.0002
20	3	1	0	81.580	81.597	-0.017	0.1	1.1791	1.1789	0.0002
21	2	2	1	82.065	82.081	-0.016	6	1.1733	1.1732	0.0001
22	1	1	3	82.140	82.150	-0.010	18.2	1.1725	1.1723	0.0002
23	3	0	2	83.539	83.529	0.010	5.9	1.1563	1.1565	-0.0002
24	3	1	1	85.857	85.865	-0.008	4.8	1.131	1.1309	0.0001
25	2	0	3	85.918	85.934	-0.016	5	1.1303	1.1301	0.0002
26	4	0	0	92.920	92.918	0.002	1.7	1.0626	1.0626	0
27	2	2	2	94.855	94.838	0.017	17.6	1.046	1.0461	-0.0001
28	4	0	1	97.183	97.178	0.005	1.9	1.027	1.0271	-0.0001
29	2	1	3	97.250	97.247	0.003	3.7	1.0265	1.0265	0
30	3	1	2	98.625	98.628	-0.003	0.2	1.0158	1.0158	0

<sup>a</sup> $\Delta 2\theta = 2\theta_{\text{obs}} - 2\theta_{\text{cal}}$

<sup>b</sup> $\Delta d = d_{\text{obs}} - d_{\text{cal}}$

collected. The obtained values of the Bragg angle,  $2\theta$ , were calibrated for instrumental errors using a parabolic fit with reference material SRM Si. Once the  $2\theta$  values were corrected, precise lattice parameters were obtained by a least-squares refinement (Zeng *et al.*, 2007). The observed intensity (peak heights) of each diffraction peak was determined from the XRD data of a pure CeCo<sub>3</sub>Ni<sub>2</sub> sample. The RIR value was calculated from the XRD data that were collected from a mixture of 50 wt% CeCo<sub>3</sub>Ni<sub>2</sub> and 50 wt% corundum.

### III. RESULTS

The experimental XRD pattern for the pure CeCo<sub>3</sub>Ni<sub>2</sub> compound is shown in Figure 1. All peaks were successfully indexed by Jade 6.0 (2002, Materials Data Inc.) software with a hexagonal structure. It was found that CeCo<sub>3</sub>Ni<sub>2</sub> and LaNi<sub>5</sub> (Kisi *et al.*, 1992) have the same structure type (*P6/mmm*, No.191) by comparing the X-ray powder diffraction pattern of CeCo<sub>3</sub>Ni<sub>2</sub> with that of LaNi<sub>5</sub>. The accurate lattice parameters were obtained with  $a = b = 4.9081(2) \text{ \AA}$ ,  $c = 4.0034(2) \text{ \AA}$ ,  $V = 83.52 \text{ \AA}^3$ ,  $Z = 1$ , and the density is  $8.6347 \text{ g cm}^{-3}$  by indexing and refining for the corrected X-ray powder diffraction data of CeCo<sub>3</sub>Ni<sub>2</sub>. The figure of merit for indexing  $F_N$  (Smith and Snyder, 1979) is  $F_{30} = 112.7(0.0089, 30)$  and the intensity ratio RIR value is 0.48. The observed and the

calculated X-ray powder diffraction data for CeCo<sub>3</sub>Ni<sub>2</sub> are listed in Table I.

### ACKNOWLEDGMENTS

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