The X-ray Powder Diffraction Pattern of Co_4NiNd Ternary Compound

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Abstructs. The new ternary compound Co_4NiNd had been prepared by melting with stoichiometric elemental constituents, and the crystal structure had been studied by the means of X-ray powder diffraction technique. The results show that the new compound of Co_4NiNd is the hexagonal structure, space group ***p6/mmm(No.191)***, with the lattice parameters a = b = 5.0082(2) Å, c=3.9852(2) Å, V = 86.57 $Å^3$, Z = 1 and the density is 8.4145 g/cm^3, and the Smith-Snyder figure-of-merit F_{30} is 157.6(0.0071, 30). The intensity ratio RIR of Co_4NiNd compound is 0.53.

Introduction

The alloys AB_5(A=Rare earth elements or their mixtures, B=Ni, Al, Mn, Cr, Fe, Co, Cu, Ag, Pd, Si, Ti, Zr, V, et al.) have been researched extensively because of their good comprehensive performance in the hydrogen storage. A lot of new ternary compounds had been reported in the process of studies on experimental and theoretical with the method of element substitution from inorganic crystal structure database (***ICSD Database***, 2014.02), such as $FeNdNi_4$, $CoLaNi_4$, $Co_{2.5}LaNi_{2.5}$, $Co_{0.3}LaNi_{4.7}$, Co_2Ni_3Tb, $Co_{2.5}Ni_{2.5}Y$, Co_3Ni_2Y, Co_2Ni_3Sm, $Co_{3.5}Ni_{1.5}Pr$, Co_3HoNi_2, Co_3Ni_2Th, etc.. But there are only one compound of $Co_{2.5}NdNi_{2.5}$(***Y.C. Chuang, et al,*** 1982.02) with Co-Ni-Nd system have been reported and a large number of new compound in the Co-Ni-Nd ternary system need to be developed, AB_5 structure especially. In this work, we present the high-quality powder X-ray diffraction data and structure information for the ternary compound Co_4NiNd.

Experimental Details

The sample of Co_4NiNd compound had been synthesized by melting with the stoichiometric elemental constituents(53.74 wt % Co, 13.38 wt.% Ni and 32.88 wt % Nd) in the arc furnace under high purity argon atmosphere, and the constituents of raw materials coming from China new metal materials technology Co., Ltd. with 99.99 wt % Co, 99.99 wt % Ni and 99.9 wt % Nd. In the process of melting, the sample was turned upside down and melted at least three times in order to fuse together for the constituents and distribute uniformly for the elemental component. The sample is available when the weight loss is less than 1% after melting. The sample of Co_4NiNd compound was sealed in an evacuated quartz galss tube, and was annealed at the temperature of 1123 K for one month, then cooled down to room temperature at the rate of 12 K/h. The X-ray powder diffraction data of the sample were collected at room temperature by the Rigaku Smart Lab powder diffractometer equipped with a Cu target and a graphite monochromator. The scan range of Bragg angle (two theta) was from 10.00^o to 100.00^o with the step size of 0.02^o and the scan speed of 10 s per step. The internal standard

method has been used for correcting the Bragg angle, and the X-ray powder diffraction data for the mixture of Co_4NiNd and the internal standard material silicon were collected. The whole pattern was calibrated with the calibration curve of standard silicon, and the lattice constants were refined by Jade 6.5 software(*Materials Data Inc.*, 2002). The observed intensity of diffraction peaks were determined by the X-ray diffraction pattern of Co_4NiNd compound. The RIR value was calculated by the ratio of the highest diffraction peak intensity between Co_4NiNd and corundum, and so the X-ray powder diffraction data of the mixture of 50 wt % Co_4NiNd and 50 wt % corundum were collected.

Conclusions

The X-ray powder diffraction pattern of Co_4NiNd was showed in figure 1, and the X-ray powder diffraction pattern of Co_4NiNd was successfully indexed by the MDI Jade 6.5 program with the hexagonal structure. It was found that the compound of Co_4NiNd and Co_4NiHo have the same structure type (space group P6/mmm, $CaCu_5$-type structure) by comparing crystallographic characteristics of the Co_4NiNd compound with those of Co_4NiHo presented in the inorganic crystal structure database. The lattice parameters have been determined with a = b = 5.0082(2) Å, c = 3.9852(2) Å, V = 86.57 $Å^3$, Z = 1 and the density is 8.4145 g/cm^3 after cell refinement with spcac group P6/mmm(No. 191). The Smith-Snyder figure-of-merit(*G.S. Smith and R.L. Snyder*, 1979) is F_{30} = 157.6(0.0071, 30). The X-ray powder diffraction data for Co_4NiNd were showed in table 1. The intensity ratio RIR value is 0.53 that was calculated from the ratio of the strongest peak intensity between Co_4NiNd and corundum in the X-ray powder diffraction pattern for the mixture of Co_4NiNd and corundum.

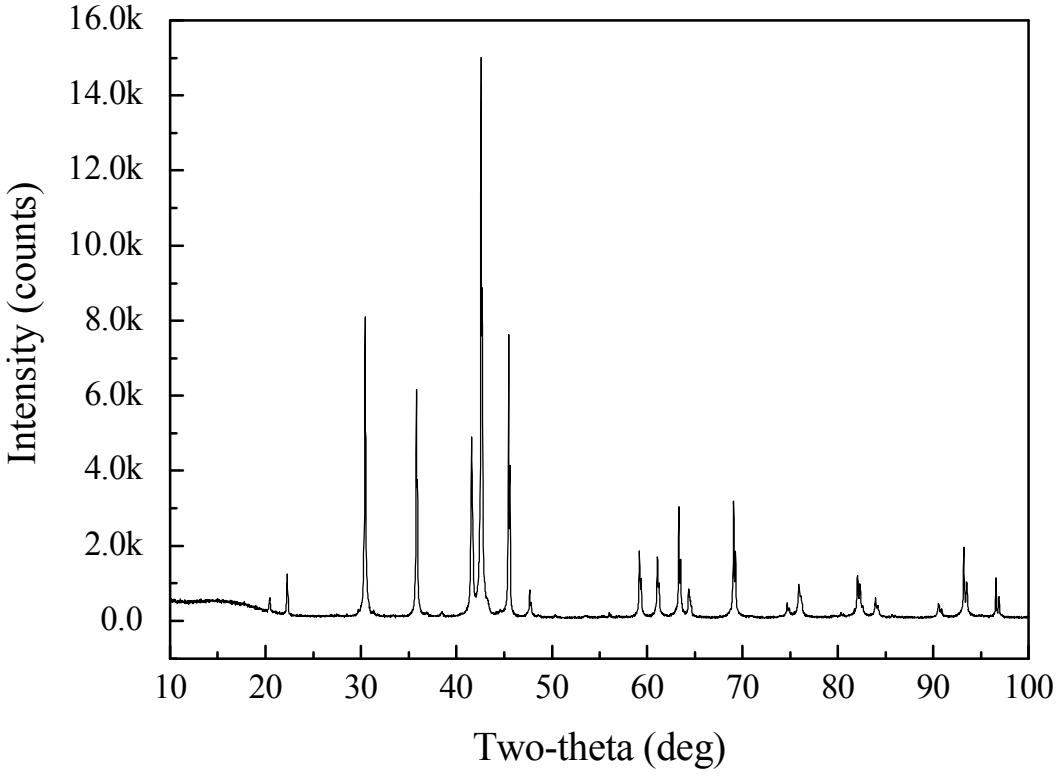

Fig.1 The X-ray powder diffraction pattern of Co_4NiNd

Table 1 X-ray powder diffraction data for Co_4NiNd (Cu $K\alpha_1$, with λ = 1.5406 Å)

No.	*h*	*k*	*l*	$2\theta_{cal}$	$2\theta_{obs}$	$\Delta 2\theta$ [a]	I/I_0	d_{cal}	d_{obs}	Δd [b]
1	1	0	0	20.460	20.452	0.008	1.7	4.3372	4.3388	-0.0016
2	0	0	1	22.289	22.282	0.007	6.5	3.9852	3.9865	-0.0013
3	1	0	1	30.435	30.430	0.005	50.6	2.9345	2.9351	-0.0006
4	1	1	0	35.830	35.824	0.006	39.2	2.5041	2.5045	-0.0004
5	2	0	0	41.611	41.601	0.010	31.6	2.1686	2.1691	-0.0005
6	1	1	1	42.605	42.600	0.005	100	2.1203	2.1205	-0.0002
7	0	0	2	45.482	45.478	0.004	52.8	1.9926	1.9928	-0.0002
8	2	0	1	47.704	47.701	0.003	4.7	1.9048	1.9050	-0.0002
9	1	0	2	50.354	50.347	0.007	0.5	1.8107	1.8109	-0.0002
10	2	1	0	56.053	56.060	-0.007	0.8	1.6393	1.6391	0.0002
11	1	1	2	59.211	59.202	0.009	12.1	1.5592	1.5594	-0.0002
12	2	1	1	61.072	61.079	-0.007	10.8	1.5161	1.5159	0.0002
13	2	0	2	63.333	63.325	0.008	20.3	1.4673	1.4674	-0.0001
14	3	0	0	64.389	64.380	0.009	4.9	1.4457	1.4459	-0.0002
15	3	0	1	69.050	69.040	0.010	21.7	1.3591	1.3592	-0.0001
16	0	0	3	70.881	70.883	-0.002	0.3	1.3284	1.3284	0
17	1	0	3	74.665	74.670	-0.005	2.3	1.2702	1.2701	0.0001
18	2	1	2	74.956	74.955	0.001	0.5	1.2660	1.2660	0
19	2	2	0	75.935	75.935	0	5.6	1.2520	1.2520	0
20	3	1	0	79.634	79.641	-0.007	0.2	1.2029	1.2028	0.0001
21	2	2	1	80.311	80.301	0.010	0.8	1.1945	1.1946	-0.0001
22	1	1	3	82.051	82.060	-0.009	7.6	1.1735	1.1734	0.0001
23	3	0	2	82.334	82.340	-0.006	2.9	1.1702	1.1701	0.0001
24	3	1	1	83.960	83.968	-0.008	3.5	1.1516	1.1515	0.0001
25	2	0	3	85.687	85.696	-0.009	0.5	1.1328	1.1327	0.0001
26	4	0	0	90.533	90.537	-0.004	2.4	1.0843	1.0843	0
27	2	2	2	93.202	93.202	0	13.2	1.0601	1.0601	0
28	4	0	1	94.820	94.825	-0.005	0.3	1.0463	1.0462	0.0001
29	2	1	3	96.548	96.541	0.007	7.6	1.0321	1.0321	0
30	3	1	2	96.830	96.839	-0.009	1	1.0298	1.0298	0

[a] $\Delta 2\theta = 2\theta_{cal} - 2\theta_{obs}$, [b] $\Delta d = d_{cal} - d_{obs}$

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