The X-ray Powder Diffraction Data for Al_8GdNi_4 Compound

De-Gui LI[1, a], Liu-Qing LIANG[1, b], Chang-Sheng QIN[1, c], Bing HE[1, d], Ming QIN[1,e], Shu-Hui LIU[1, f], Pei-Lin QING[1, g], Zhi-Jun XIAO[1, h], Ling-Min ZENG[2, i]

[1]College of Materials Science and Engineering, Baise University, Baise, Guangxi 533000, China

[2]School of Materials Science and Engineering, Guangxi University, Nanning, Guangxi 530004, China

[a]lidegui354@163.com, [b]114560196@qq.com, [c]87629749@qq.com, [d]bsxyhb@21cn.com, [e]qm6327@sohu.com, [f]wert887@126.com, [g]plqing110@163.com, [h]272464254@qq.com, [i]lmzeng@gxu.edu.cn

Keywords: Al_8GdNi_4, X-ray Powder Diffraction.

Abstract. The new ternary compound Al_8GdNi_4 had been synthesized by melting in arc furnace and annealing in vacuum. The crystal structure of Al_8GdNi_4 was analyzed by X-ray powder diffraction technique. The whole pattern of Al_8GdNi_4 had been indexed, and the lattice constants had been refined with tetragonal structure type of space group *I4/mmm* (No.139). The lattice parameters are presented, $a = b = 8.7661(1)$ Å, $c = 5.0498(1)$ Å, $Vol = 388.06$ Å^3, $Z = 2$, $Density = 5.2022$ g/cm^3, $F_{30} = 278.5$ (0.0051, 30) and $RIR = 1.90$.

Introduction

There are several crystal structures of compounds for Al-Gd-Ni ternary system that have been reported in inorganic crystal structure database[1], such as AlGdNi, $AlGdNi_4$, $AlGd_2Ni_2$, $AlGd_3Ni_8$, $Al_{19}Gd_3Ni_5$, Al_2GdNi, $Al_2Gd_3Ni_6$, $A_{23}Gd_4Ni_6$, Al_4GdNi, Al_9GdNi_3, $Al_9Gd_2Ni_8$, $Al_{1.57}GdNi_{0.43}$, $Al_{12.8}Gd_8Ni_{3.2}$, $Al_{21.65}Gd_{1.35}Ni_4$, etc. So far, the crystal structure of the new compound Al_8GdNi_4 has not been reported. In this work, the experimental X-ray powder diffraction data have been presented, and the crystal structure of Al_8GdNi_4 have been studied by X-ray powder diffraction technique.

Experimental

Sample Preparation

The purity alloy of Al_8GdNi_4 had been synthesized by melting with stoichiometric composition under argon atmosphere in electric arc furnace equipped with a tungsten electrode and a water-cooled copper tray. The high-purity metal of 99.99 wt % aluminum, 99.99 wt % nickel and 99.9 wt % gadolinium is the raw materials that come from China new metal materials technology Co., Ltd. In the melting process, titanium ingot was melted firstly in order to capture the residual oxygen. The alloy was melted at least three times in order to ensure that these metals fused together completely and the composition distributed uniformly, and it is the successful melting process when the weight losses were less than 1 wt%. The alloy ingot was enclosed in an evacuated quartz glass tube and annealed at the temperature of 1173 K for one month, and then cooled down at the rate of 0.2 K/min to room temperature. The powder of Al_8GdNi_4 for testing has been prepared by the alloy ingot ground in a steel mortar.

Data Collection and Analysis

The X-ray powder diffraction data of Al_8GdNi_4 ternary compound were collected at room temperature by using the Rigaku Smart Lab powder diffractometer which equipped with a copper target and a diffracted-beam graphite monochromator. The diffraction instrument was operated at the condition of voltage 40 kV and current 150 mA. The scan range of Bragg angle (two-theta) was

from 10 to 100 °with stepping-scanning-mode that the step size is 0.02 °and the speed is 3s per step. The internal standard method has been adopted for calibrating systematical errors of Bragg angle (2θ) in the observed peak positions, and the XRD data for the mixture of Al_8GdNi_4 and the internal standard material SRM 640 Si were collected. The $2\theta_{obs}$ values of the diffraction peaks were determined by the algorithm based on the Savitzky-Golay 2nd derivatives combined with the counting statistics of intensity data using Jade 6.5 XRD Pattern Processing software (Materials Data Inc., 2002)[2]. The precise values of lattice constants were obtained by the least-squares method using Jade 6.5 after smoothing pattern, stripping Cu $K_{\alpha 2}$ peaks and calibrating two-theta. In order to evaluate the RIR value, the X-ray powder diffraction data of the mixture of 50 wt % Al_8GdNi_4 and 50 wt % corundum were collected.

Results

The experimental X-ray powder diffraction pattern of the Al_8GdNi_4 is shown in figure 1. All diffraction peaks in the pattern were successfully indexed using the Jade 6.5 program with tetragonal structure. The lattice parameters have been refined using the corrected diffraction pattern of Al_8GdNi_4, and the precise lattice parameters were determined with $a = b = 8.7661(1)$ Å, $c = 5.0498(1)$ Å, *Vol* = 388.06 $Å^3$, *Density* = 5.2022, Z = 2. The Smith-Snyder figure-of-merit F*30* (Smith G S and Snyder R L, 1979)[3] is 278.5(0.0051, 30). It was found that Al_8GdNi_4 and Al_8Fe_4Y have the same structure type with space group *I4/mmm* (NO.139) by comparing crystal structure information of Al_8GdNi_4 with those of Al_8Fe_4Y in the report (H. Misiorek, et al, 2004)[4]. The value of *RIR* is 1.90 that was calculated by the ratio of the strongest line between Al_8GdNi_4 and corundum in the XRD pattern for the mixture of Al_8GdNi_4 and corundum. The observed and the calculated X-ray powder diffraction data for Al_8GdNi_4 are listed in table 1.

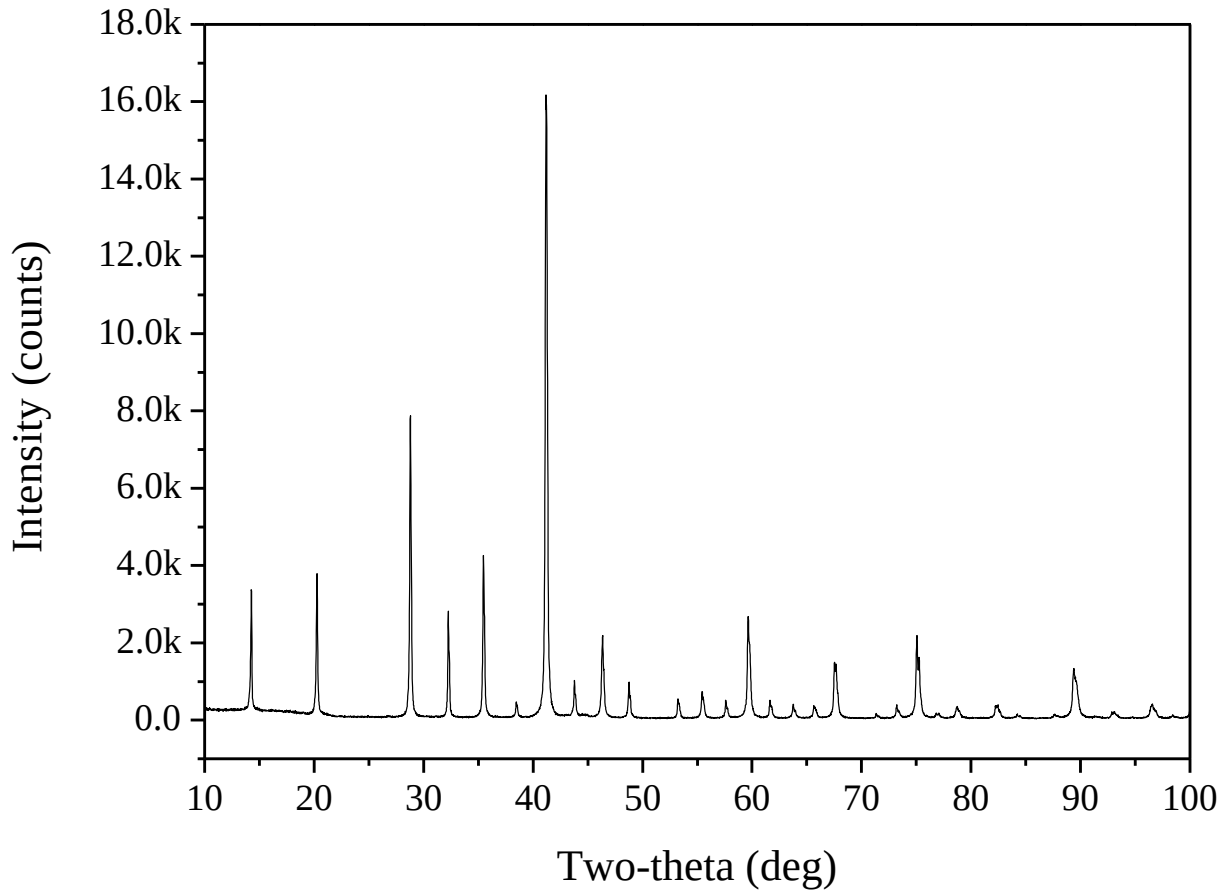

Fig.1 X-ray powder diffraction pattern for Al_8GdNi_4 compound

Tab.1 Powder diffraction data of the new quaternary compound Al_8GdNi_4

(Cu $K\alpha_1$, with λ = 1.5406 Å)

No.	*h*	*k*	*l*	$2\theta_{obs}$	$2\theta_{cal}$	$\Delta 2\theta^b$	I/I_o	d_{obs}	d_{cal}	Δd^b
1	1	1	0	14.277	14.262	0.015	17.2	6.1986	6.2050	-0.0064
2	2	0	0	20.243	20.243	0	18.7	4.3831	4.3832	-0.0001
3	1	0	1	20.278	20.272	0.006	17.3	4.3757	4.3769	-0.0012
4	2	2	0	28.782	28.780	0.002	46.8	3.0993	3.0994	-0.0001
5	2	1	1	28.806	28.811	-0.005	34.4	3.0967	3.0961	0.0006
6	3	1	0	32.266	32.260	0.006	17.4	2.7721	2.7726	-0.0005
7	3	0	1	35.463	35.460	0.003	26.3	2.5292	2.5294	-0.0002
8	0	0	2	35.525	35.527	-0.002	11.9	2.5249	2.5247	0.0002
9	1	1	2	38.466	38.465	0.001	2.4	2.3384	2.3384	0
10	4	0	0	41.156	41.161	-0.005	98.7	2.1915	2.1913	0.0002
11	3	2	1	41.174	41.180	-0.006	100	2.1906	2.1903	0.0003
12	2	0	2	41.228	41.225	0.003	84.6	2.1879	2.1880	-0.0001
13	3	3	0	43.777	43.780	-0.003	5.9	2.0662	2.0661	0.0001
14	4	2	0	46.278	46.280	-0.002	10.5	1.9602	1.9601	0.0001
15	4	1	1	46.295	46.295	1	10.9	1.9595	1.9595	0
16	2	2	2	46.344	46.345	-0.001	12.2	1.9575	1.9575	0
17	3	1	2	48.743	48.742	0.001	6	1.8667	1.8667	0
18	5	1	0	53.237	53.241	-0.004	3.4	1.7192	1.7191	0.0001
19	5	0	1	55.430	55.430	0	4.5	1.6562	1.6562	0
20	4	0	2	55.473	55.470	0.003	3.2	1.6551	1.6552	-0.0001
21	1	0	3	55.546	55.548	-0.002	2.2	1.6531	1.6530	0.0001
22	3	3	2	57.595	57.605	-0.010	3.1	1.5990	1.5988	0.0002
23	4	4	0	59.612	59.607	0.005	11.8	1.5496	1.5498	-0.0002
24	5	2	1	59.626	59.624	0.002	16.5	1.5493	1.5494	-0.0001
25	4	2	2	59.667	59.660	0.007	17.4	1.5483	1.5485	-0.0002
26	2	1	3	59.736	59.734	0.002	8.4	1.5467	1.5468	-0.0001
27	5	3	0	61.643	61.651	-0.008	3.1	1.5034	1.5032	0.0002
28	6	0	0	63.636	63.640	-0.004	0.7	1.4610	1.4609	0.0001
29	3	0	3	63.755	63.759	-0.004	2.3	1.4586	1.4585	0.0001
30	5	1	2	65.647	65.653	-0.006	2.1	1.4211	1.4209	0.0002
31	6	2	0	67.523	67.523	0	8.2	1.3860	1.3860	0
32	6	1	1	67.536	67.541	-0.005	9.7	1.3858	1.3857	0.0001
33	3	2	3	67.639	67.637	0.002	7.7	1.3840	1.3840	0
34	5	4	1	71.317	71.325	-0.008	0.3	1.3213	1.3212	0.0001
35	4	4	2	71.355	71.362	-0.007	0.8	1.3207	1.3206	0.0001

36	4	1	3	71.417	71.414	0.003	0.4	1.3197	1.3198	-0.0001
37	5	3	2	73.212	73.222	-0.010	2.3	1.2917	1.2916	0.0001
38	6	3	1	75.015	75.023	-0.008	12.3	1.2651	1.2650	0.0001
39	6	0	2	75.052	75.059	-0.007	14.4	1.2646	1.2645	0.0001
40	0	0	4	75.199	75.198	0.001	5.5	1.2625	1.2625	0
41	5	5	0	76.827	76.820	0.007	0.8	1.2397	1.2398	-0.0001
42	1	1	4	77.022	77.029	-0.007	0.4	1.2371	1.2370	0.0001
43	6	4	0	78.638	78.638	0	1.5	1.2156	1.2157	-0.0001
44	7	0	1	78.650	78.652	-0.002	1.8	1.2155	1.2155	0
45	6	2	2	78.687	78.693	-0.006	1.9	1.2150	1.2149	0.0001
46	5	0	3	78.747	78.740	0.007	1.9	1.2142	1.2143	-0.0001
47	2	0	4	78.832	78.833	-0.001	0.8	1.2131	1.2131	0
48	7	2	1	82.240	82.242	-0.002	2.2	1.1713	1.1713	0
49	5	2	3	82.336	82.339	-0.003	2.1	1.1702	1.1701	0.0001
50	2	2	4	82.420	82.411	0.009	1.7	1.1692	1.1693	-0.0001
51	7	3	0	84.010	84.003	0.007	0.3	1.1510	1.1511	-0.0001
52	3	1	4	84.201	84.212	-0.011	0.6	1.1489	1.1488	0.0001
53	7	1	2	87.607	87.601	0.006	0.6	1.1128	1.1129	-0.0001
54	8	0	0	89.330	89.323	0.007	7	1.0958	1.0958	0
55	6	5	1	89.342	89.341	0.001	8.3	1.0957	1.0957	0
56	6	4	2	89.377	89.385	-0.008	8.5	1.0953	1.0952	0.0001
57	6	1	3	89.437	89.438	-0.001	6.9	1.0947	1.0947	0
58	4	0	4	89.520	89.518	0.002	5.9	1.0939	1.0940	-0.0001
59	3	3	4	91.290	91.285	0.005	0.3	1.0773	1.0773	0
60	8	2	0	92.870	92.870	0	1.1	1.0631	1.0631	0
61	7	4	1	92.882	92.882	0	0.8	1.0629	1.0629	0
62	5	4	3	92.977	92.977	0	0.8	1.0621	1.0621	0
63	4	2	4	93.061	93.057	0.004	1	1.0614	1.0614	0
64	7	3	2	94.691	94.688	0.003	0.2	1.0474	1.0474	0
65	6	6	0	96.422	96.420	0.002	2	1.0331	1.0331	0
66	6	3	3	96.529	96.520	0.009	2.4	1.0322	1.0323	-0.0001
67	7	5	0	98.206	98.199	0.007	0.2	1.0190	1.0191	-0.0001
68	5	1	4	98.398	98.399	-0.001	0.6	1.0176	1.0176	0

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

Acknowledgments

This work was financially supported by the department of science and technology of Guangxi Zhuang Autonomous Region (project number: 2014AA01018) and department of education of Guangxi Zhuang Autonomous Region (project number: ZD2014134).

References

[1] Inorganic Crystal Structure Database, Fachinformationszentrum Karlsruhe, Germany, and the U.S. Department of Commerce on the behalf of the United States (2014).

[2] Jade version 6.5, XRD pattern processing, Materials Data Inc. (2002).

[3] G.S. Smith and R.L. Snyder: J. Appl. Crystallogr Vol.12 (1979), p. 60.

[4] H. Misiorek, Yu. Stepen' Damm, W. Suski, E. Talik, B.Y. Kotur and V.M. Dmitriev: Journal of Alloys and Compounds, Vol. 363 (2004), p. 78.