Powder diffraction data of the $Al_{0.931}Ni_{1.069}Sc_5$ compound

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A new ternary compound $Al_{0.931}Ni_{1.069}Sc_5$ has been synthesized and studied by means of the X-ray powder diffraction technique. $Al_{0.931}Ni_{1.069}Sc_5$ crystallizes in the hexagonal crystal system with the Al_5Co_2 structure type, space group $P6_3/mmc$, with $a = 8.8287(3)$ Å, $c = 8.6959(4)$ Å, $Z = 4$ and $V = 587.00$ Å^3, $\rho_{calc} = 3.538$ g/cm^3.

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Key words: Al–Ni–Sc compound, $Al_{0.931}Ni_{1.069}Sc_5$, X-ray powder diffraction

I. INTRODUCTION

In the Al–Ni–Sc ternary system, the crystal structure and X-ray powder diffraction (PXRD) data of five ternary compounds, AlNiSc (Teslyuk and Protasov, 1965), $Al_{16}Ni_7Sc_6$ (Markiv and Burnasheva, 1969), $AlNi_2Sc$ (Dwight and Kimball, 1987), Al_2NiSc (Gladyshevskii and Parthe, 1992), and $Al_{0.902}Ni_{1.098}Sc$ (Sahlberg et al., 2012), have been studied and collected in the Inorganic Crystal Structure Database (ICSD) and ICDD's Powder Diffraction File. Recently, our team has studied phase relations of the Al–Ni–Sc ternary system (He et al., 2019) and detected four new phases Ni_2Al_5Sc, Ni_2Al_4Sc, $NiAl_2Sc_3$, and $NiAlSc_5$. The actual composition of the detected phase $NiAlSc_5$ is determined to be $Al_{0.931}Ni_{1.069}Sc_5$ after studied. However, information for the crystal structure of $Al_{0.931}Ni_{1.069}Sc_5$ is not available in the literature. Here, the PXRD data for $Al_{0.931}Ni_{1.069}Sc_5$ is reported.

II. EXPERIMENTAL

A. Sample preparation

The sample of $Al_{0.931}Ni_{1.069}Sc_5$ was prepared by arc melting the stoichiometric amounts of elemental constituents 99.99 Al, 99.99 Ni, and 99.9 Sc (wt%) (supplied by China New Metal Materials Technology Co., Ltd.) under high purity argon atmosphere on a water-cooled copper hearth. To ensure homogeneity of the sample, it was melted four times and weight losses were less than 1 wt%. After melting, the sample was enclosed in an evacuated quartz tube and annealed at 1173 K for 40 days, and then finally cooled down to room temperature at a rate of 10 K/h. The composition (13.40 at.% Al, 15.32 at.% Ni, 71.28 at.% Sc) of the sample was obtained by the electron probe microanalysis (EPMA; JXA-8800R, JEOL, Japan), which is in good agreement with the crystal structure refinement composition of $Al_{0.931}Ni_{1.069}Sc_5$ (13.30 at.% Al, 15.27 at.% Ni, 71.43 at.% Sc). The sample was then grounded to a size smaller than 20 μm for powder diffraction analysis.

B. Data collection

A PXRD pattern (Figure 1) of the new compound $Al_{0.931}Ni_{1.069}Sc_5$ was obtained using a Rigaku D/max 2550 V X-ray diffractometer equipped with Cu$K\alpha$ radiation and a graphite monochromator. The 2θ scan range was from 10.02° to 100.04° with a step size of 0.02° and a count time of 1 s/step. The lattice parameters were calculated with the XRD pattern processing program JADE 6.0 (Materials Data Inc., 2002).

III. RESULTS AND DISCUSSION

The PXRD pattern of $Al_{0.931}Ni_{1.069}Sc_5$ was indexed using the JADE 6.0 program after smoothing the patterns, fitting the background, and stripping the Cu$K\alpha_2$ peaks. All lines were successfully indexed in the hexagonal system with the lattice parameters $a = 8.8287(3)$ Å, $c = 8.6959(4)$ Å, and the Al_5Co_2 (Burkhardt et al., 1998) structure type. Details of the crystal structure for $Al_{0.931}Ni_{1.069}Sc_5$ will be given in our further publication. The observed X-ray powder diffraction data are listed in Table I.

IV. DEPOSITED DATA

The raw data file of $Al_{0.931}Ni_{1.069}Sc_5$ has been deposited with ICDD. You may request this data from ICDD at pdj@icdd.com.

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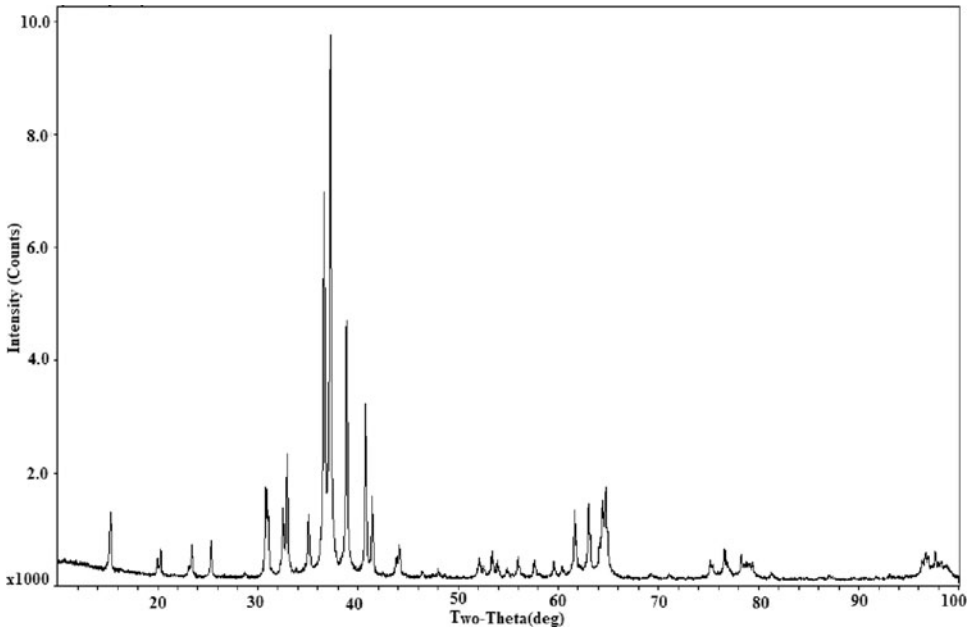

Figure 1. The powder X-ray diffraction pattern of $Al_{0.931}Ni_{1.069}Sc_5$.

TABLE I. Indexed X-ray powder diffraction data for the $Al_{0.931}Ni_{1.069}Sc_5$ compound.

$2\theta_{obs}$ (°)	d_{obs} (Å)	I_{obs}	h	k	l	$2\theta_{cal}$ (°)	d_{cal} (Å)	$\Delta 2\theta$
15.393	5.7514	11	1	0	1	15.418	5.7421	0.025
20.080	4.4184	3	1	1	0	20.098	4.4145	0.018
20.400	4.3498	5	0	0	2	20.408	4.3480	0.008
23.239	3.8244	2	2	0	0	23.248	3.8230	0.009
23.500	3.7825	6	1	0	2	23.518	3.7797	0.018
25.418	3.5012	7	2	0	1	25.429	3.4998	0.011
28.797	3.0977	1	1	1	2	28.796	3.0978	−0.001
30.905	2.8910	17	2	1	0	30.917	2.8899	0.012
31.100	2.8733	13	2	0	2	31.125	2.8711	0.025
32.600	2.7444	13	2	1	1	32.624	2.7425	0.024
33.014	2.7110	23	1	0	3	33.021	2.7105	0.007
35.179	2.5490	10	3	0	0	35.183	2.5487	0.004
36.700	2.4468	72	3	0	1	36.714	2.4458	0.015
37.338	2.4064	100	2	1	2	37.331	2.4068	−0.007
38.941	2.3109	47	2	0	3	38.960	2.3098	0.020
40.840	2.2078	32	2	2	0	40.850	2.2072	0.010
41.499	2.1742	15	0	0	4	41.502	2.1740	0.004
42.586	2.1212	1	3	1	0	42.597	2.1206	0.012
43.918	2.0599	4	3	1	1	43.910	2.0603	−0.008
44.200	2.0474	6	2	1	3	44.218	2.0466	0.019
46.503	1.9512	1	1	1	4	46.525	1.9503	0.022
48.098	1.8902	2	2	0	4	48.107	1.8898	0.009
52.217	1.7503	4	4	0	2	52.232	1.7499	0.015
52.650	1.7370	2	2	1	4	52.638	1.7373	−0.012
53.516	1.7109	5	3	1	3	53.494	1.7115	−0.021
54.020	1.6961	3	1	0	5	54.027	1.6959	0.007
54.991	1.6684	2	4	1	0	54.988	1.6685	−0.003
56.077	1.6387	4	4	1	1	56.079	1.6386	0.002
57.702	1.5963	3	4	0	3	57.723	1.5958	0.022
58.250	1.5826	1	2	0	5	58.230	1.5831	−0.020
59.638	1.5490	3	2	2	4	59.645	1.5489	0.007
60.480	1.5295	2	5	0	0	60.492	1.5292	0.012
61.758	1.5009	12	3	2	3	61.763	1.5007	0.005
63.139	1.4713	13	3	3	0	63.131	1.4715	−0.008
64.200	1.4495	4	0	0	6	64.209	1.4493	0.009
64.522	1.4431	13	5	0	2	64.546	1.4426	0.025
64.845	1.4367	16	3	0	5	64.848	1.4366	0.003
67.100	1.3938	1	3	3	2	67.096	1.3938	−0.004
69.420	1.3527	1	5	0	3	69.432	1.3525	0.011
71.158	1.3239	1	4	1	4	71.175	1.3236	0.017
75.299	1.2610	3	6	0	1	75.310	1.2609	0.011
76.720	1.2412	5	5	1	3	76.730	1.2410	0.010
78.397	1.2188	3	3	3	4	78.411	1.2186	0.014
78.899	1.2123	2	5	2	1	78.890	1.2124	−0.009
79.254	1.2077	2	4	3	2	79.268	1.2076	0.014
79.547	1.2040	3	4	1	5	79.546	1.2040	−0.001
81.398	1.1813	1	2	0	7	81.379	1.1815	−0.019
81.629	1.1785	1	5	2	2	81.627	1.1785	−0.002
87.176	1.1172	1	3	2	6	87.167	1.1173	−0.010
93.182	1.0603	1	6	2	0	93.181	1.0603	−0.001
96.478	1.0326	3	3	3	6	96.486	1.0326	0.007
96.803	1.0300	5	6	2	2	96.792	1.0301	−0.012
97.059	1.0280	2	6	0	5	97.067	1.0279	0.007
97.829	1.0220	3	5	3	3	97.806	1.0221	−0.023
98.398	1.0176	2	2	1	8	98.417	1.0174	0.019
98.907	1.0137	2	3	2	7	98.892	1.0138	−0.015

Continued

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