Powder diffraction data of the Ho_2AlGe_3 ternary compound

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A new ternary compound Ho_2AlGe_3 was synthesized and studied by means of X-ray powder diffraction technique. The powder pattern of Ho_2AlGe_3 was indexed and refined, giving an orthorhombic structure, space group *Pnma* (No. 62) with the Y_2AlGe_3 structure type: $a = 6.743\ 98(8)$ Å, $b = 4.163\ 73(5)$ Å, $c = 17.5834(2)$ Å, $V = 493.74$ Å^3, $Z = 4$, $\rho_x = 7.73$ g cm^{-3}, $F_{30} = 202.7$ (0.004, 37), and RIR = 1.21. © *2013 International Centre for Diffraction Data.*
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Key words: Ho_2AlGe_3, powder X-ray diffraction data, Y_2AlGe_3

I. INTRODUCTION

It is of both academic interest and industrial necessity to study the properties of the Al–Ge–RE ternary compounds. However, up until now, a few researches about these ternary compounds have been reported (Wang *et al.*, 2011). The interesting structural chemistry and the rich magnetic properties make such materials worthy candidates for the investigation of the structural evolution and structure–properties relationships in rare-earth metal compounds (Zhang and Bobev, 2013). The crystal structure of the RE_2AlGe_3 (RE = Y, Dy, Ho, Er, and Tm) compounds was studied for the first time by Johrendt *et al.* (1996). These compounds are orthorhombic, space group *Pnma* (No. 62), with the Y_2AlGe_3 structure type. Later, the crystal structures of Sm_2AlGe_3 and Tb_2AlGe_3 were reported to have the same structure type (Mel'nyk *et al.*, 2005). So far, only two powder diffraction patterns of $HoAl_{2.784}Ge_{0.214}$ (Zhuravleva *et al.*, 2001) and $HoAl_{0.34}Ge_2$ (Zeng *et al.*, 2008) of the Ho–Al–Ge ternary system were included in the PDF (ICDD, 2011). Therefore, in this paper, we present high-quality experimental powder X-ray diffraction (XRD) data for Ho_2AlGe_3.

II. EXPERIMENTAL

A. Synthesis

The sample of Ho_2AlGe_3 with a total mass of 2 g was prepared by arc melting using a non-consumable tungsten electrode and a water-cooled copper tray under argon atmosphere. Holmium (purity of 99.9%), aluminum (purity of 99.9%), and germanium (purity of 99.999%) were used as the starting materials. Titanium was used as an oxygen getter during the melting process. The sample was remelted three times in order to ensure the complete fusion and homogeneity. Weight losses were less than 1 wt%. After melting, the sample was enclosed in an evacuated quartz tube and annealed at 1073 K for 720 h, then cooled down at a rate of 10 K h^{-1} to room temperature. The sample was ground in an agate mortar and pestled to particle sizes no larger than 20 μm.

B. Data collection

XRD patterns of Ho_2AlGe_3 compound were collected at room temperature using 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 180 mA, the 2θ scan range was from 5° to 100° with a step size of 0.02°, and a count time of 6 s per step. Two sets of XRD data were collected, one with SRM 640 Si added as an internal standard to correct for possible systematic errors in the observed peak positions and the other without SRM 640 Si. 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, whereas the XRD 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

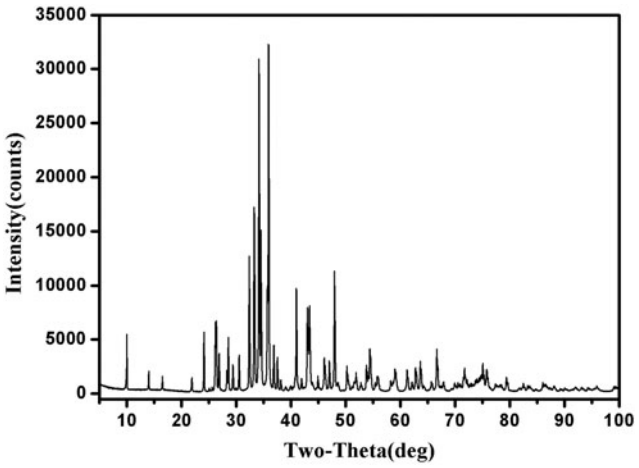

Figure 1. The powder X-ray diffraction pattern of Ho_2AlGe_3.

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smoothing the patterns, fitting and removing the background, and stripping the Cu$K\alpha_2$ 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 Ho_2AlGe_3 is shown in Figure 1. All of the lines were successfully indexed using the Jade6.0 program in an orthorhombic system. By comparing the XRD data of Ho_2AlGe_3 with those of Y_2AlGe_3, it was found that Ho_2AlGe_3 and Y_2AlGe_3 (Johrendt *et al.*, 1996) have the same structure type *Pnma* (No. 62). Using the corrected diffraction data of Ho_2AlGe_3, the accurate unit-cell parameters were obtained with $a =$ 6.743 98(8) Å, $b = 4.163\ 73(5)$ Å, $c = 17.5834(2)$ Å, $V =$ 493.74 Å^3, $Z = 4$, and $\rho_x = 7.73$ g cm^{-3}. The figure of merit for indexing F_N (Smith and Snyder, 1979) is $F_{30} = 202.7$ (0.004, 37) and the value of RIR (RIR = 1.21) 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 XRD data for Ho_2AlGe_3 are listed in Table I.

TABLE I. Powder diffraction data for Ho_2AlGe_3 (Cu$K\alpha_1$, 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	10.058	0	0	2	10.053	0.005	16.3	8.7869	8.7917
2	14.058	1	0	1	14.053	0.005	5.5	6.2945	6.2967
3	16.559	1	0	2	16.553	0.006	4.0	5.3492	5.3510
4	21.920	0	1	1	21.919	0.001	4.1	4.0514	4.0517
5	24.155	1	0	4	24.147	0.008	17.2	3.6814	3.6826
6	25.632	1	1	1	25.628	0.004	1.0	3.4725	3.4731
7	26.238	0	1	3	26.232	0.006	20.2	3.3937	3.3944
8	26.417	2	0	0	26.410	0.007	20.5	3.3711	3.3720
9	26.900	2	0	1	26.900	0.000	10.9	3.3117	3.3116
10	27.112	1	1	2	27.113	−0.001	0.4	3.2863	3.2861
11	28.324	2	0	2	28.324	0.000	5.4	3.1483	3.1484
12	28.600	1	0	5	28.603	−0.003	15.6	3.1185	3.1182
13	29.437	1	1	3	29.435	0.002	7.4	3.0317	3.0320
14	30.559	2	0	3	30.561	−0.002	10.2	2.9229	2.9228
15	32.436	1	1	4	32.430	0.006	38.8	2.7580	2.7585
16	33.318	0	1	5	33.322	−0.004	52.3	2.6870	2.6866
17	34.197	2	1	0	34.189	0.008	95.4	2.6199	2.6204
18	34.579	2	1	1	34.579	0.000	45.2	2.5918	2.5918
19	35.723	2	1	2	35.724	−0.001	29.5	2.5114	2.5113
20	35.957	1	1	5	35.952	0.005	100.0	2.4956	2.4959
21	36.900	2	0	5	36.900	0.000	12.5	2.4339	2.4339
22	37.563	2	1	3	37.567	−0.004	9.4	2.3925	2.3922
23	38.201	1	0	7	38.202	−0.001	3.0	2.3539	2.3539
24	39.883	1	1	6	39.889	−0.006	0.9	2.2585	2.2582
25	40.036	2	1	4	40.024	0.012	1.2	2.2502	2.2509
26	40.417	3	0	1	40.417	0.000	0.3	2.2299	2.2298
27	40.762	2	0	6	40.759	0.003	3.4	2.2118	2.2119
28	41.037	0	0	8	41.031	0.006	29.8	2.1976	2.1979
29	41.976	0	1	7	41.971	0.005	3.0	2.1506	2.1508
30	43.058	3	0	3	43.060	−0.002	15.7	2.0990	2.0989
31	43.432	0	2	0	43.431	0.001	19.8	2.0818	2.0819
32	44.171	1	1	7	44.160	0.011	0.1	2.0487	2.0491
33	44.703	0	2	2	44.696	0.007	0.5	2.0255	2.0258
34	44.962	2	0	7	44.963	−0.001	4.0	2.0144	2.0144
35	45.273	3	0	4	45.270	0.003	0.6	2.0013	2.0015
36	45.869	1	2	1	45.871	−0.002	0.8	1.9767	1.9766
37	46.138	3	1	1	46.140	−0.002	9.2	1.9658	1.9657
38	46.783	1	2	2	46.783	0.000	0.3	1.9402	1.9402
39	47.055	3	1	2	47.049	0.006	8.2	1.9296	1.9299
40	47.998	3	0	5	47.993	0.005	34.8	1.8939	1.8941
41	48.477	1	0	9	48.469	0.008	1.8	1.8763	1.8766
42	48.725	1	1	8	48.714	0.011	1.7	1.8673	1.8677
43	50.280	2	1	7	50.274	0.006	7.2	1.8131	1.8133
44	50.552	3	1	4	50.556	−0.004	2.2	1.8040	1.8039
45	51.177	3	0	6	51.170	0.007	0.6	1.7835	1.7837
46	51.547	2	2	0	51.549	−0.002	1.8	1.7715	1.7714
47	51.634	0	1	9	51.636	−0.002	2.3	1.7687	1.7687
48	51.823	2	2	1	51.829	−0.006	2.6	1.7627	1.7625
49	51.960	0	0	10	51.962	−0.002	5.1	1.7584	1.7583
50	52.665	2	2	2	52.664	0.001	1.0	1.7365	1.7365
51	52.837	1	2	5	52.831	0.006	2.1	1.7313	1.7314

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TABLE I. Continued

No.	$2\theta_{obs}$	h	k	l	$2\theta_{cal}$	$\Delta 2\theta$[a]	I_{obs}	d_{obs}	d_{cal}
52	53.079	3	1	5	53.074	0.005	0.3	1.7239	1.7241
53	53.519	1	1	9	53.518	0.001	0.2	1.7108	1.7108
54	53.840	1	0	10	53.836	0.004	7.0	1.7013	1.7015
55	53.981	0	2	6	53.982	−0.001	5.3	1.6972	1.6972
56	54.032	2	2	3	54.034	−0.002	3.1	1.6958	1.6957
57	54.222	2	0	9	54.215	0.007	4.1	1.6903	1.6905
58	54.441	2	1	8	54.441	0.000	11.7	1.6840	1.6840
59	54.640	4	0	1	54.641	−0.001	3.5	1.6783	1.6783
60	55.457	4	0	2	55.446	0.011	2.1	1.6555	1.6558
61	55.820	1	2	6	55.810	0.010	4.0	1.6456	1.6459
62	55.918	2	2	4	55.914	0.004	4.0	1.6429	1.6430
63	56.049	3	1	6	56.044	0.005	2.6	1.6394	1.6396
64	58.270	2	2	5	58.272	−0.002	3.1	1.5821	1.5821
65	58.700	3	0	8	58.699	0.001	2.5	1.5715	1.5716
66	58.908	2	1	9	58.916	−0.008	3.5	1.5665	1.5663
67	59.062	4	1	0	59.063	−0.001	5.8	1.5628	1.5627
68	59.197	1	2	7	59.200	−0.003	5.4	1.5595	1.5595
69	59.325	4	1	1	59.319	0.006	2.7	1.5565	1.5566
70	61.081	2	2	6	61.075	0.006	1.3	1.5159	1.5160
71	61.278	0	2	8	61.278	0.000	5.6	1.5115	1.5115
72	61.580	3	2	2	61.573	0.007	0.7	1.5048	1.5049
73	62.140	0	1	11	62.151	−0.011	2.0	1.4925	1.4923
74	62.820	3	2	3	62.816	0.004	6.3	1.4780	1.4781
75	62.984	3	0	9	62.981	0.003	5.0	1.4746	1.4746
76	63.680	2	1	10	63.681	−0.001	8.2	1.4601	1.4601
77	63.827	1	1	11	63.829	−0.002	5.8	1.4571	1.4571
78	64.280	2	2	7	64.293	−0.013	1.3	1.4479	1.4477
79	66.702	3	2	5	66.707	−0.005	9.7	1.4011	1.4010
80	67.301	3	1	9	67.304	−0.003	1.1	1.3901	1.3900
81	67.583	3	0	10	67.582	0.001	0.7	1.3850	1.3850
82	67.918	4	1	6	67.919	−0.001	2.7	1.3789	1.3789
83	69.315	3	2	6	69.316	−0.001	0.4	1.3545	1.3545
84	69.897	5	0	1	69.886	0.011	1.6	1.3447	1.3448
85	69.978	0	2	10	69.977	0.001	0.7	1.3433	1.3433
86	70.597	5	0	2	70.587	0.010	1.7	1.3330	1.3332
87	70.984	4	1	7	70.972	0.012	1.2	1.3267	1.3269
88	71.560	1	2	10	71.561	−0.001	2.6	1.3174	1.3174
89	71.768	3	1	10	71.765	0.003	5.4	1.3141	1.3142
90	72.254	4	2	1	72.247	0.007	2.2	1.3065	1.3066
91	72.745	1	3	4	72.755	−0.010	0.6	1.2989	1.2987
92	72.932	4	2	2	72.939	−0.007	0.9	1.2960	1.2959
93	73.359	5	0	4	73.363	−0.004	0.2	1.2895	1.2895
94	73.760	2	3	0	73.764	−0.004	1.1	1.2835	1.2834
95	73.991	2	3	1	73.993	−0.002	1.3	1.2801	1.2800
96	74.068	2	1	12	74.068	0.000	0.2	1.2789	1.2789
97	74.235	4	0	9	74.237	−0.002	0.4	1.2765	1.2764
98	74.426	4	1	8	74.428	−0.002	2.0	1.2736	1.2736
99	74.680	2	3	2	74.678	0.002	1.9	1.2700	1.2700
100	74.800	1	3	5	74.816	−0.016	2.2	1.2682	1.2680
101	75.120	1	1	13	75.119	0.001	6.1	1.2636	1.2636
102	75.834	5	1	3	75.834	0.000	5.9	1.2535	1.2535
103	76.367	1	2	11	76.367	0.000	0.2	1.2460	1.2460
104	76.560	3	1	11	76.567	−0.007	0.2	1.2434	1.2433
105	77.205	1	0	14	77.195	0.010	0.1	1.2346	1.2347
106	77.415	5	1	4	77.417	−0.002	1.4	1.2318	1.2317
107	78.283	4	1	9	78.276	0.007	1.3	1.2203	1.2204
108	78.539	4	0	10	78.538	0.001	0.8	1.2169	1.2170
109	79.433	5	1	5	79.437	−0.004	3.8	1.2055	1.2054
110	79.718	2	1	13	79.715	0.003	0.6	1.2019	1.2019
111	80.192	4	2	6	80.179	0.013	0.1	1.1960	1.1961
112	81.719	3	1	12	81.718	0.001	0.6	1.1774	1.1774
113	82.304	3	3	2	82.311	−0.007	0.8	1.1705	1.1704
114	82.519	4	1	10	82.514	0.005	2.0	1.1680	1.1681
115	83.304	3	0	13	83.308	−0.004	1.4	1.1590	1.1590
116	83.660	1	0	15	83.666	−0.006	1.2	1.1550	1.1549
117	86.035	2	2	12	86.035	0.000	2.3	1.1291	1.1291

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TABLE I. Continued

No.	$2\theta_{obs}$	h	k	l	$2\theta_{cal}$	$\Delta 2\theta^{a}$	I_{obs}	d_{obs}	d_{cal}
118	86.100	0	1	15	86.103	−0.003	1.3	1.1284	1.1284
119	86.641	5	2	2	86.642	−0.001	1.4	1.1227	1.1227
120	87.138	4	1	11	87.153	−0.015	0.1	1.1176	1.1174
121	87.307	1	3	9	87.307	0.000	0.3	1.1159	1.1159
122	88.164	2	0	15	88.163	0.001	1.1	1.1072	1.1072
123	89.263	3	0	14	89.261	0.002	0.7	1.0964	1.0964
124	90.041	6	0	4	90.040	0.001	0.5	1.0890	1.0890
125	90.140	4	2	9	90.123	0.017	0.7	1.0880	1.0882
126	91.916	4	3	0	91.919	−0.003	0.8	1.0716	1.0715
127	92.144	4	3	1	92.140	0.004	0.7	1.0695	1.0696
128	93.181	3	1	14	93.184	−0.003	0.9	1.0603	1.0603
129	94.300	4	2	10	94.305	−0.005	0.8	1.0507	1.0506
130	95.467	0	4	0	95.461	0.006	0.5	1.0409	1.0409
131	95.947	6	1	5	95.951	−0.004	1.3	1.0369	1.0369
132	95.978	2	3	10	95.982	−0.004	0.9	1.0367	1.0367
133	98.965	1	4	3	98.964	0.001	0.8	1.0132	1.0133
134	99.051	3	2	13	99.048	0.003	1.1	1.0126	1.0126
135	99.401	1	2	15	99.408	−0.007	1.2	1.0100	1.0099
136	99.881	4	3	6	99.885	−0.004	0.4	1.0064	1.0064

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

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