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Letter

New ternary aluminides T_5M_2Al having W_5Si_3-type structure

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Abstract

Six new ternary aluminides having W_5Si_3-type structure were found. These are: Zr_5Sn_2Al, Hf_5Sn_2Al, Ti_5Pb_2Al, Zr_5Pb_2Al, Hf_5Pb_2Al and Nb_5Sn_2Al.

Keywords: Ternary aluminides; W_5Si_3-type related crystal structure; Ti_5Sn_2Al; Zr_5Sn_2Al; Hf_5Sn_2Al; Ti_5Pb_2Al; Zr_5Pb_2Al; Hf_5Pb_2Al; Nb_5Sn_2Al

1. Introduction

During the investigation of the phase equilibria in the system Ti–Al–Sn [1] a new ternary compound with the approximate composition Ti_5Sn_2Al [2] was observed. The powder X-ray diffraction pattern was indexed based on a body-centered tetragonal unit cell with $a = 1.0549(2)$ nm and $c = 0.5242(2)$ nm. The intensities of the diffraction peaks can be described satisfactorily by a W_5Si_3-type related crystal structure, space group $I4/mcm$ (Table 1). In this study 20 alloys were prepared by variation of the transition metal T (=Ti, Zr, Hf, V, Nb, Ta, Cr, Mo, W) and the main group element M (=Si, Ge, Sn, Pb) yielding six new W_5Si_3-type ternary compounds: Zr_5Sn_2Al, Hf_5Sn_2Al, Ti_5Pb_2Al, Zr_5Pb_2Al, Hf_5Pb_2Al and Nb_5Sn_2Al.

2. Experimental

Ternary alloys with the composition T:M:Al = 5:2:1 were prepared by compacting ($p \sim 30$ bar) appropriate powder mixtures (1 g) of Ti (purity: m2N), Zr (purity: m3N), Hf (purity: m2N6), Nb (purity: m2N8), Ta (purity: m3N), Cr (purity: m3N5), Mo (purity: 3N), W (purity: 3N), Al (purity: m2N8), Si (purity: m3N+), Sn (purity: m2N5) and Pb (purity: m2N5). V (purity: 99.83%, C: 0.054%, O: 0.014%, Fe: 0.017%, H: 0.0049%, N: 0.0028%), Y (purity: m3N) and Ge (purity: m6N+) were used as lumps. The pellets were placed in alumina crucibles and sealed in quartz tubes. Arc melting had to be avoided for the Pb-containing samples due to high vaporization losses. Except for the alloys in the systems Ti–Si–Al, Ti–Ge–Al and T–Sn–Al the heat treatment involved two steps. First the temperature was raised to the approximate melting temperature of Pb and held there for 1 d. Thereafter all alloys were annealed at 900 °C for 10 d. The analysis of the water-quenched samples was performed by means of XRD (Guinier–Huber cameras, CuKα_1 radiation). The diffraction data were handled and evaluated by using the software package STRUKTUR [3]. It was not attempted to prepare single-phase specimens.

3. Results

The T_5M_2Al alloys prepared were: Ti_5Si_2Al, Ti_5Ge_2Al, Ti_5Pb_2Al, Zr_5Sn_2Al, Zr_5Pb_2Al, Hf_5Sn_2Al, Hf_5Pb_2Al, V_5Sn_2Al, V_5Pb_2Al, Nb_5Sn_2Al, Nb_5Pb_2Al, Ta_5Sn_2Al, Ta_5Pb_2Al, Cr_5Sn_2Al, Cr_5Pb_2Al, Mo_5Sn_2Al, Mo_5Pb_2Al, W_5Sn_2Al, W_5Pb_2Al and Y_5Sn_2Al. The comparison of the XRD pattern intensities observed and calculated showed that in the systems Ti–Pb–Al, Zr–Sn–Al, Zr–Pb–Al, Hf–Sn–Al, Hf–Pb–Al and Nb–Sn–Al ternary compounds exist, which are isomorphous with W_5Si_3 and thus can be described analogously to Ti_5Sn_2Al with space group $I4/mcm$ and 16 T(1) in position 16k, 4 T(2) in position 4b, 8 M in position 8h and 4 Al in position 4a (Table 1). Table 2 shows the lattice parameters of these new compounds and of Ti_5Sn_2Al [2].

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Table 1
X-ray powder diffractogram of Ti_5Sn_2Al [2] in alloy $Ti_{62}Sn_{23}Al_{15}$ ($CuK\alpha_1$ radiation, Ge standard, Guinier camera)

H	K	L	$\sin^2\Theta_{obs}$	$\sin^2\Theta_{calc}$	$Int._{obs}$	$Int._{calc}$	Remarks
1	1	0	0.0107	0.0107	w	8	
2	0	0	0.0213	0.0213	w	6	
2	1	1	0.0483	0.0483	s	66	
0	0	2	0.0862	0.0862	m	28	
3	2	1	0.0909	0.0909	m	28	
3	3	0	0.0959	0.0959	m	30	
4	2	0	0.1066	0.1066	ms	24	coinc. Ti_5Sn_3
2	0	2	0.1078	0.1077	m	27	
			0.1095		vw		TiAl
4	1	1	0.1123	0.1122	vs	100	
			0.1177		w		Ti_5Sn_3
2	2	2	0.1290	0.1290	w	8	
3	1	2	0.1398	0.1397	vw	7	
4	0	2	0.1720	0.1717	w	17	
5	2	1	0.1763	0.1762	w	21	
5	3	0	0.1815	0.1813	vw	5	
3	3	2	0.1827	0.1823	w	18	
6	0	0		0.1919		8	
			0.1925		vw		
4	2	2		0.1930		1	
2	1	3	0.2208	0.2210	vw	9	
7	1	0		0.2666		8	
			0.2670		w		
5	3	2		0.2676		9	
4	1	3	0.2851	0.2849	m	27	
6	2	2	0.2997	0.2996	vw	3	
7	2	1	0.3042	0.3041	vw	3	
7	3	0	0.3089	0.3092	vw	7	
0	0	4	0.3457	0.3456	vw	8	
5	2	3	0.3492	0.3489	vw	9	
7	1	2	0.3527	0.3529	n.d.	11	coinc. Ge
6	4	2	0.3635	0.3634	w	18	
8	1	1	0.3684	0.3683	w	19	
6	6	0	0.3841	0.3840	vw	4	
7	3	2	0.3955	0.3954	vw	15	

Reflections having a calculated intensity <5 are omitted. Crystallographic description: space group: $I4/mcm$; 16 Ti(1) in position 16k; 4 Ti(2) in position 4b; 8 Sn in position 8h; 4 Al in position 4a; $a = 1.0549(2)$ nm, $c = 0.5242(2)$ nm.

Table 2
The lattice parameters of Ti_5Sn_2Al, Ti_5Pb_2Al, Zr_5Sn_2Al, Zr_5Pb_2Al, Hf_5Sn_2Al, Hf_5Pb_2Al and Nb_5Sn_2Al

Compound	a (nm)	c (nm)	V (nm^3)	c/a	Reference
Ti_5Sn_2Al	1.0549(2)	0.5242(2)	0.5833	0.497	[2]
Ti_5Pb_2Al	1.0659(4)	0.5318(2)	0.6042	0.499	This study
Zr_5Sn_2Al	1.1181(2)	0.5538(1)	0.6923	0.495	This study
Zr_5Pb_2Al	1.1209(5)	0.5524(3)	0.6941	0.493	This study
Hf_5Sn_2Al	1.1014(1)	0.5542(1)	0.6724	0.503	This study
Hf_5Pb_2Al	1.1045(2)	0.5543(2)	0.6763	0.502	This study
Nb_5Sn_2Al	1.0629(2)	0.5216(2)	0.5892	0.490	This study

Sn was presented [4], in which a ternary compound of estimated stoichiometry $Y_8Sn_9Al_3$ had been observed. Since the indexing of the diffraction pattern was not yet done, one sample with the estimated composition was prepared assuming a structural relationship to the W_5Si_3-type structures. However, the unknown diffraction pattern did not show any similarity to the structure type presented in this paper.

4. Discussion

As can be expected from the covalent radii of Ti,

Zr, Hf, Sn and Pb the volumes of the unit cell increase in the order $Ti_5M_2Al < Hf_5M_2Al < Zr_5M_2Al$ and are larger for the Pb-containing compounds. In the system Zr–Al there is binary Zr_5Al_3 of W_5Si_3-type structure at temperatures above 950–1000 °C [5]. So it seems that Zr_5Al_3 can be stabilized towards lower temperatures by the addition of Sn and Pb, respectively. In the literature Nb_5Sn_2Ga [6] has been reported to have W_5Si_3-type structure, which might form a continuous series of solid solutions with binary Nb_5Ga_3 (W_5Si_3-type) by substituting large amounts of Ga with Sn. The same is likely to be true for Ta_5Ga_2Sn [7] found to be isomorphous with W_5Si_3. In this case the ratio Ga:Sn is 2:1 and not, as for the others, 1:2. The authors state that successive substitution of Ga by Sn atoms between Ta_5Ga_3 and Ta_5Ga_2Sn is likely to occur.

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