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Phase equilibria in the Dy–Ti–Si system at 1200 K

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Abstract

Phase equilibria in the Dy–Ti–Si system were investigated by X-ray powder diffraction, local X-ray spectral analysis, metallographic analysis and the isothermal cross-section at 1200 K was obtained. The CeFeSi-type (space group *P4/nmm*, No. 129) DyTiSi compound has been confirmed. The new $Sc_2Re_3Si_4$-type (space group $P4_12_12$, No. 92) compound $Dy_2Ti_3Si_4$ [$a=0.6977(1)$ nm, $c=1.2814(2)$ nm] was found. It is obvious that the AlB_2-type (space group *P6/mmm*, No. 191) compound $DyTi_{0.3}Si_{1.7}$ [$a=0.3824(1)$ nm, $c=0.4119(1)$ nm] belongs to an extended region of the AlB_2-type $DySi_{1.56}$-based solid solution.

Keywords: Transition metal compounds; Rare earth compounds; Phase diagram; X-Ray diffraction

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1. Introduction

The interaction between the components in the Dy–Si, Ti–Si and Dy–Ti binary systems have been studied in Refs. [1–4]. However, phase equilibria in the Dy–Si and Dy–Ti systems were not obtained. No binary compounds were detected in the Dy–Ti system. The CeFeSi-type ternary compound DyTiSi was reported earlier [5] (Tables 1 and 2).

2. Experimental

The alloys (Fig. 1) were made in an electric arc furnace under an argon atmosphere using a non-consumable tungsten electrode and a water-cooled copper tray. Silicon, titanium and disprosium (purity of each component ≥99.99%) were used as starting components. Zirconium was used as an O_2 getter during the melting process. The alloys were re-melted three times in order to achieve complete fusion and homogeneous composition. The melted alloys were subjected to an anneal in evacuated quartz ampoules containing titanium chips as an O_2 getter. The ampoules were placed in a resistance furnace. The alloys were annealed at 1200 K for 2 weeks. The samples were quenched from 1200 K in ice-cold water. The phase equilibria in the Dy–Ti–Si system were determined from X-ray phase analysis, local X-ray spectral analysis and metallographic analysis. Powder X-ray data were obtained on a DRON-3.0 diffractometer (Cu Kα radiation, $2\theta=20$–70°, step 0.05°, for 5 s per step).

The powder X-ray diffractograms obtained were identified by means of calculated patterns using the Rietan program [6,7] in the isotropic approximation.

A 'Camebax' microanalyser was employed to perform local X-ray spectral analysis of the samples.

A 'Neophot' microscope was employed for metallographic inspections (×250, ×500).

3. Results and discussion

The results obtained were used in the construction of the isothermal cross-section of the Dy–Ti–Si system at 1200 K, presented in Fig. 2.

The CeFeSi-type DyTiSi compound has been confirmed. The new ternary compounds $Dy_2Ti_3Si_4$ and $DyTi_{0.3}Si_{1.7}$ were found. Analysis of the powder X-ray diffractograms shows that the $Dy_2Ti_3Si_4$ and $DyTi_{0.3}Si_{1.7}$ compounds crystallize in the tetragonal $Sc_2Re_3Si_4$-type structure (space group $P4_12_12$) and hexagonal AlB_2-type structure (space group *P6/mmm*), respectively (Table 2). The atomic coordinates for the $Dy_2Ti_3Si_4$ compound are given in Table 3.

The reliability factors in Tables 1 and 2 are $R_F = 100 \cdot \left[\Sigma_k |(I_k^{obs})^{1/2} - (I_k^{cal})^{1/2}|\right] / \Sigma_k |(I_k^{obs})^{1/2}|$ % (I_k^{obs} is the inte-

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Table 1
Crystallographic data of compounds in the binary Dy–Si and Ti–Si systems

No.	Compound	Space group	Structure type	*a* (nm)	*b* (nm)	*c* (nm)	R_F (%)	Refs.
1	Si^a	$Fd3m$	C	0.54307				[1,2]
2	Ti (LT)[a]	$P6_3/mmc$	Mg	0.29511		0.46843		[1,2]
	Ti (HT)	$Im3m$	W	0.33065				[1,2]
3	Dy (LT1)	$Cmcm$		0.3595	0.6183	0.5677		[1,2]
	Dy (LT2)[a]	$P6_3/mmc$	Mg	0.35903		0.56475		[1,2]
	Dy (LT2)[a]	$P6_3/mmc$	Mg	0.3588(2)		0.5646(3)	7.9	This work[b]
	Dy (HT)	$Im3m$	W	0.398				[1,2]
4	Ti_3Si^a	$P4_2/n$	Ti_3P	1.0196		0.5097		[2,4]
	Ti_3Si^a	$P4_2/n$	Ti_3P	1.0159(4)		0.5085(2)	4.1	This work[b]
5	$Ti_5Si_3^a$	$P6_3/mcm$	Mn_5Si_3	0.7429		0.5139		[2,4]
	Ti_5Si_3	$P6_3/mcm$	Mn_5Si_3	0.7482(9)		0.5153(4)	4.7	This work[b]
6	$Ti_5Si_4^a$	$P4_12_12$	Zr_5Si_4	0.6702		1.2174		[2,4]
7	$TiSi^a$	$Pnma$	MnP	0.6544	0.3638	0.4997		[2,4]
	$TiSi^a$	$Pnma$	MnP	0.6609(2)	0.3593(1)	0.5006(1)	2.7	This work[b]
	TiSi	$Pmm2$	TiSi	0.3618	0.6492	0.4973		[2,4]
8	$TiSi_2^a$	$Fddd$	$TiSi_2$	0.8267	0.4800	0.8551		[2,4]
	$TiSi_2^a$	$Fddd$	$TiSi_2$	0.8258(2)	0.4796(1)	0.8543(2)	3.7	This work[b]
	$TiSi_2$	$Cmcm$	$ZrSi_2$	0.360	1.376	0.360		[2,4]
9	$Dy_5Si_3^a$	$P6_3/mcm$	Mn_5Si_3	0.837		0.626		[2,3]
	$Dy_5Si_3^a$	$P6_3/mcm$	Mn_5Si_3	0.8371(4)		0.6284(2)	6.0	This work[b]
10	$Dy_5Si_4^a$	$Pnma$	Sm_5Ge_4	0.736	1.448	0.765		[2,3]
	$Dy_5Si_4^a$	$Pnma$	Sm_5Ge_4	0.7317(8)	1.451(2)	0.779(1)	5.0	This work[b]
11	DySi (HT)	$Pnma$	FeB	0.787	0.380	0.565		[2,3]
	DySi (LT)[a]	$Cmcm$	CrB	0.4237	1.0494	0.3818		[2,3]
	DySi (LT)[a]	$Cmcm$	CrB	0.4235(1)	1.0470(3)	0.3810(1)	3.1	This work[b]
12	$DySi_{1.67}^a$	$P6/mmm$	AlB_2	0.383		0.411		[2,3]
	$DySi_{1.67}^a$	$P6/mmm$	AlB_2	0.3830(1)		0.4116(1)	3.9	This work[b]
13	$DySi_2$ (HT)	$I4_1/amd$	$ThSi_2$	0.403		1.338		[2,3]
	$DySi_2$ (LT)[a]	$Imma$	$GdSi_2$	0.404	0.394	1.334		[2,3]
	$DySi_2$ (LT)[a]	$Imma$	$GdSi_2$	0.4027(1)	0.3934(1)	1.3335(4)	3.8	This work[b]

[a] Compounds belongs to the isothermal cross-section at 1200 K.

[b] Data for compounds from X-ray phase analysis of the three-component samples.

grated intensity evaluated from summation of contribution of the kth peaks to net observed intensity, I_k^{cal} is the integrated intensity calculated from refined structural parameters).

It was found that the system contains an extended region of ternary solid solution based on the DyTiSi ternary compound ($DyTiSi_{1\ldots0.9}$). However, DyTiSi does not demonstrate a transformation of the CeFeSi structure type to the CeScSi structure type within this homogeneity area, like the GdTiGe compound [8].

It is obvious that the $DyTi_{0.3}Si_{1.7}$ compound belongs to an extended region of the AlB_2-type $DySi_{1.56}$-based solid solution. The other binary compounds do not show any visible solubility.

4. Conclusions

We have confirmed the known CeFeSi-type DyTiSi compound and found the new $Sc_2Re_3Si_4$-type $Dy_2Ti_3Si_4$ and AlB_2-type $DyTi_{0.3}Si_{1.7}$ compounds in the Dy–Ti–Si isothermal cross-section. It is obvious that the isothermal

Table 2
Crystallographic data of compounds in the ternary Dy–Ti–Si system

No.	Compound	Space group	Structure type	*a* (nm)	*c* (nm)	R_F (%)	Ref.
1	DyTiSi	$P4/nmm$	CeFeSi	0.4004	0.7512		[5]
	$DyTiSi_{1\ldots0.9}$	$P4/nmm$	CeFeSi	0.4014(1) . . . 0.4017(1)	0.7525(1) . . . 0.7530(1)	5.7 6.0	This work
2	$Dy_2Ti_3Si_4$	$P4_12_12$	Zr_5Si_4	0.6977(1)	1.2814(2)	1.5	This work
3	$DyTi_{0.3}Si_{1.7}$	$P6/mmm$	AlB_2	0.3824(1)	0.4119(1)	2.9	This work

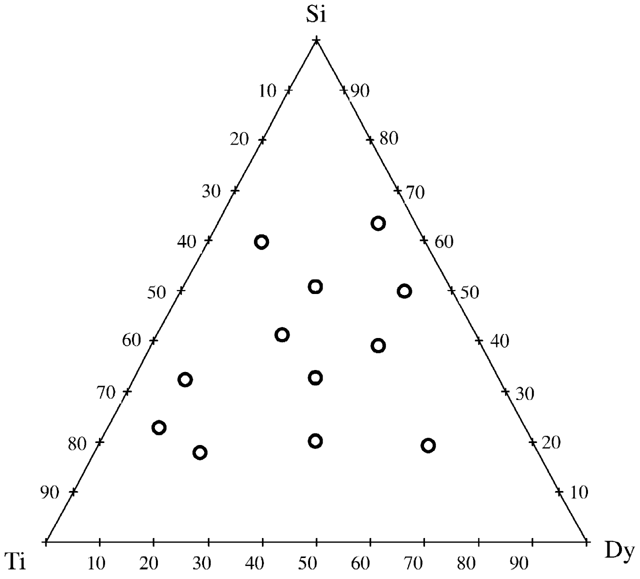

Fig. 1. Composition of samples investigated in the Dy–Ti–Si system.

Table 3
Atomic position parameters of the $Sc_2Re_3Si_4$-type $Dy_2Ti_3Si_4$ compound (space group $P4_12_12$)

Atom	Type position	x/a	y/b	z/c	Occupation factor
Dy	8(b)	0.341(2)	0.005(2)	0.4678(4)	1
Ti1	4(a)	0.321(5)	x	0	1
Ti2	8(b)	0.153(4)	−0.002(4)	0.871(3)	1
Si1	8(b)	0.209(8)	0.137(5)	0.684(3)	1
Si2	8(b)	0.288(5)	0.963(6)	0.052(2)	1

sections of the R–Ti–Si systems are similar to the Dy–Ti–Si isothermal section when R=Gd, Tb, Ho, Er, Tm.

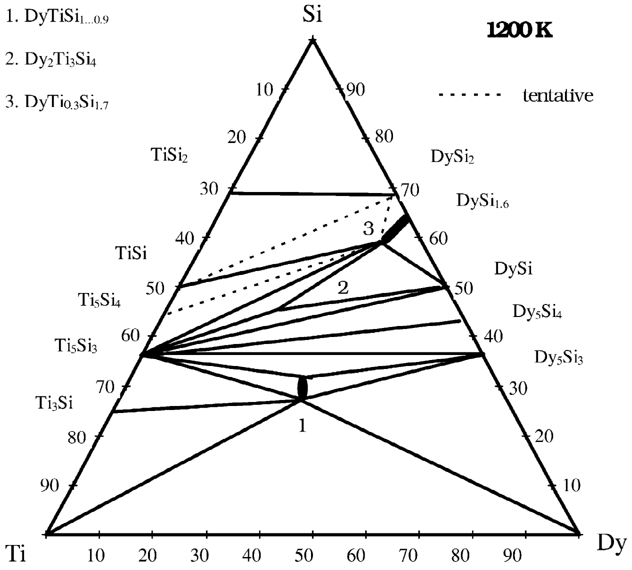

Fig. 2. Isothermal section of the Dy–Ti–Si system at 1200 K.

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