The crystal structural of the $Er_{10}Ga_3Si_3$ ternary compounds

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Abstracts. A ternary compound $Er_{10}Ga_3Si_3$ was synthesized and studied by means of X-ray powder diffraction technique using Rietveld methods. The ternary compound $Er_{10}Ga_3Si_3$ crystallizes in the hexagonal structure, space group *P6₃/mcm* (N_0.193) with the Mn_5Si_3 structure type and lattice parameters a= 8.3595(1)Å, c=6.3095(1)Å, V = 381.84Å^3, z=1 and ρ_x=8.55 g/cm^3.

Introduction

Searching for novel compounds, especially rare earth compounds, with excellent properties is very important for developing new potential function materials. Compounds with the Mn_5Si_3-type structure have been sources of useful chemical instruction as well as of significant experimental errors, both deriving from a remarkable flexibility of this particular structure type to accommodate a great range of host substitutions as well as to bind diverse interstitials [1-2]. In the R-Ga-Si ternary system, the crystal structures of $REGa_xSi_{2-x-y}$ (RE=Ho, Er, Tm; $0.33\leq x \leq 0.40$, $0.10\leq y \leq 0.18$) [3], EuGaSi [4], $Ga_{1.34}NdSi_{0.66}$ and $NdGa_{0.86}Si_{1.14}$ [5] have been reported. To the best of our knowledge, ternary intermetallic compound $Er_{10}Ga_3Si_3$ have not been reported in literature. This work reports on the crystal structure of $Er_{10}Ga_3Si_3$.

Experimental details

The sample of $Er_{10}Ga_3Si_3$ 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. Erbium (purity of 99.9%), gallium (purity of 99.9%), and silicon (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. The weight loss during melting was less than 1%. Following the melting, the ingot was wrapped in a tantalum foil, sealed under vacuum in a silica tube and annealed at 1123 K for 4 weeks, then cooled down at a rate of 10 K/h to room temperature. The sample was ground in an agate mortars and pestled to particle sizes of no larger than 45 μm. High-quality powder X-ray diffraction patterns of the sample were collected at room temperature using a Rigaku Smart Lab 2006 powder diffractometer equipped with a Cu Kα radiation (40kV, 150mA) and a graphite monochromator. The scan range was from 10.00 ^{o} to 100.00 ^{o} (2θ) with a step size of 0.02 ^{o} and a count time of 1 s per step.

Results and discussion

The powder X-ray diffraction pattern of $Er_{10}Ga_3Si_3$ was successfully indexed using the Jade 5.0 [6] program in a hexagonal unit cell with the lattice parameters a= 8.3595(1)Å, c=6.3095(1)Å. Reflection conditions ($\bar{h}$ *h0l : l = 2n, 000l : l = 2n*) pointed to 3 space groups *P6₃/mcm* (No. 193), $\bar{p}$ *6c2* (No. 188) *and P6₃cm* (No. 185) [7]. By comparing crystallographic characteristics of the $Er_{10}Ga_3Si_3$ compound with those presented in the structure type database, it was found that $Er_{10}Ga_3Si_3$ and Mn_5Si_3 [8] have the same structure type (space group *P6₃/mcm*). So the space group *P6₃/mcm* (No.193) and the atomic position parameters of Mn_5Si_3 were taken as the starting

values to refine the structural parameters of $Er_{10}Ga_3Si_3$. Structure refinement of $Er_{10}Ga_3Si_3$ was then performed using the DBWS9807 program [9]. The Er sites corresponded to the Mn sites, and both Ga and Si occupied the Si site in Mn_5Si_3. When the 6 (g) site occupied by 50% Ga and 50% Si, the goodness-of-fit parameters of these refinements led to the best values: R_p=8.97%, R_{wp}=12.03%, R_B=6.42%, R_F=4.27%. The details of the Rietveld refinement of $Er_{10}Ga_3Si_3$ are summarized in Table 1, and the atomic positions and thermal displacement factors are presented in Table 2. The observed, calculated, and residuals X-ray powder diffraction patterns of $Er_{10}Ga_3Si_3$ are shown in Figure. 1. A set of interatomic distances in $Er_{10}Ga_3Si_3$ are given in Table 3. The crystal structure of the $Er_{10}Ga_3Si_3$ compound is shown in Figure 2.

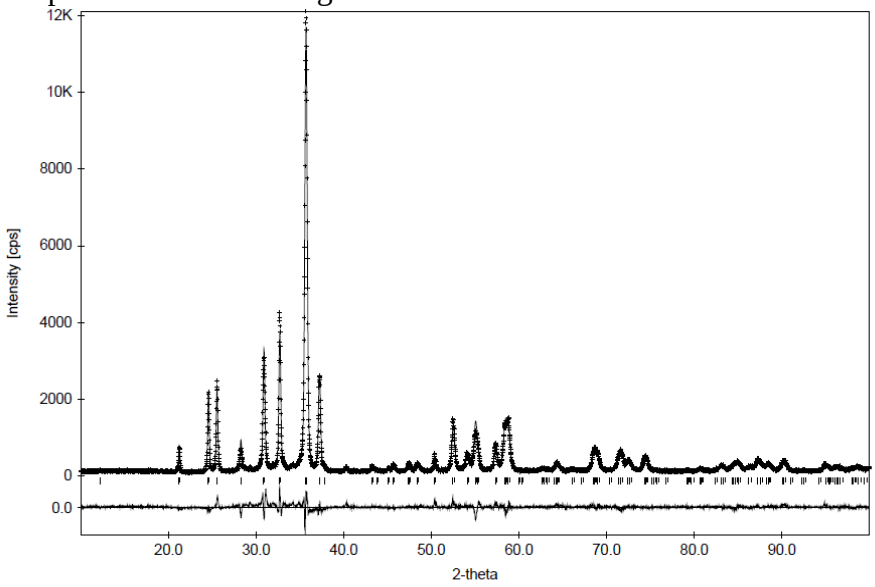

Fig.1. Observed, calculated and residuals X-ray powder diffraction patterns of $Er_{10}Ga_3Si_3$

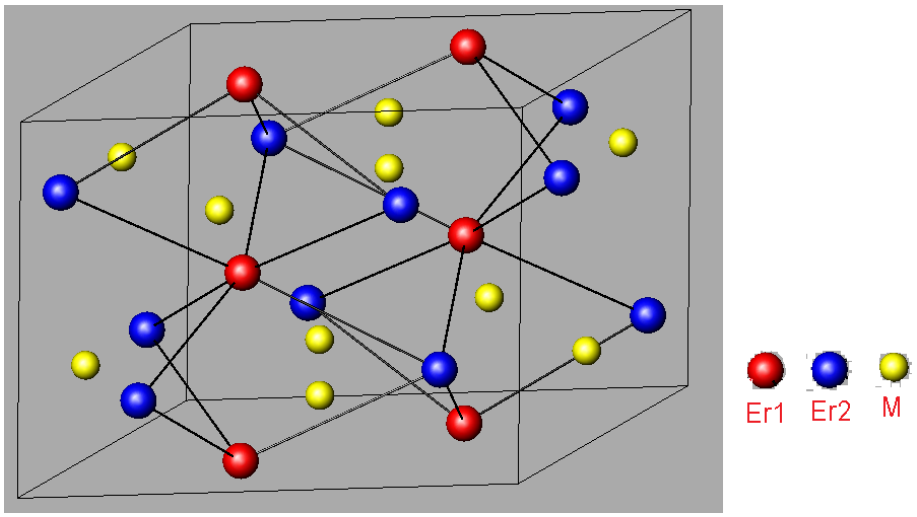

Fig.2. Crystal structure of the $Er_{10}Ga_3Si_3$ compound (M=50% Ga+50% Si)

Table 1. Rietveld refinement data of $Er_{10}Ga_3Si_3$

Formula	$Er_{10}Ga_3Si_3$
Space group	*P6₃/mcm* (No.193)
Radiation wavelength Cu $K\alpha_1$ (Å)	1.54056
Unit cell parameters (Å)	a= 8.3595(1), c=6.3095(1)
Unit-cell volume ($Å^3$)	381.84
Calculated density (g/cm^3)	8.55
Formula units per unit cell	*Z*= 1
Scan range	$10^o \leq 2\theta \leq 100^o$
Residual values	
R_p	0.0897
R_{wp}	0.1203
R_B	0.0642
R_F	0.0427

$$R_P = \frac{\sum |Y_i(obs) - Y_i(calc)|}{\sum Y_i(obs)} \qquad R_{WP} = \left\{ \frac{\sum \omega_i [Y_i(obs) - Y_i(calc)]^2}{\sum \omega_i [Y_i(obs)]^2} \right\}^{1/2}$$

$$R_B = \frac{\sum |I_H(obs) - I_H(calc)|}{\sum I_H(obs)} \qquad R_F = \frac{\sum |[I_H(obs)]^{1/2} - [I_H(calc)]^{1/2}|}{\sum (I_H(obs))^{1/2}}$$

Table 2 Atomic coordinates and thermal parameters for $Er_{10}Ga_3Si_3$

Atom	position	X	Y	Z	Occ.	B ($Å^2$)
Er1	4d	1/3	2/3	0	1	0.76 (7)
Er2	6g	0.2400(2)	0	0.25	1	0.47 (5)
Ga	6g	0.6020(5)	0	0.25	0.50(1)	0.59 (10)
Si	6g	0.6020(5)	0	0.25	0.50(1)	0.59 (10)

Table 3 Selected interatomic distances (Å) for $Er_{10}Ga_3Si_3$

Atom-atom		Distance(Å)	multiplicity	Atom-atom		distance(Å)	multiplicity
M	-Er1	3.006(1)	×4	Er_2	-M	2.902(5)	×2
	-Er2	2.902(5)	×2		- M	3.026(2)	×1
	- M	3.596(1)	×3		$-Er_1$	3.611(5)	×4
	- Er_2	3.026(2)	×1		-Er2	3.475(3)	×2
Er_1	-Er1	3.155(2)	×2				
	-Er2	3.611(5)	×6				
	- M	3.006(1)	×3				

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