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Letter

Crystallographic data of new ternary Sm_5Ge_4-type $Gd_2Sc_3Ge_4$ and $R_2Sc_3Si_4$ compounds (R=Sm, Gd–Tm)

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Abstract

Investigations made by powder X-ray diffraction on eight new ternary $Gd_2Sc_3Ge_4$ and $R_2Sc_3Si_4$ compounds (R=Gd–Tm) are reported. The following compounds were observed to crystallize in the orthorhombic Sm_5Ge_4-type structure (space group *Pnma*): $Gd_2Sc_3Ge_4$ (a=0.7211(2) nm, b=1.4050(6) nm, c=0.7453(3) nm), $Sm_2Sc_3Si_4$ (a=0.7094(1) nm, b=1.3992(4) nm, c=0.7402(2) nm), $Gd_2Sc_3Si_4$ (a=0.7092(2) nm, b=1.4012(4) nm, c=0.7412(2) nm), $Tb_2Sc_3Si_4$ (a=0.7078(1) nm, b=1.3982(3) nm, c=0.7395(2) nm), $Dy_2Sc_3Si_4$ (a=0.7060(1) nm, b=1.3951(4) nm, c=0.7380(2) nm), $Ho_2Sc_3Si_4$ (a=0.7042(1) nm, b=1.3921(4) nm, c=0.7362(2) nm), $Er_2Sc_3Si_4$ (a=0.7028(1) nm, b=1.3894(4) nm, c=0.7343(2) nm) and $Tm_2Sc_3Si_4$ (a=0.7011(2) nm, b=1.3852(5) nm, c=0.7324(2) nm).

Keywords: Ternary rare earths compounds; Silicides; Germanides; Structure type

This paper reports on the structural data of eight new compounds using powder X-ray diffraction analysis.

In the present investigation the compounds were made in an electric arc furnace under an argon atmosphere using a non-consumable tungsten electrode and a water-cooled copper tray. Silicon (purity, 99.99%), germanium (purity, 99.99%), scandium (purity, 99.99%), samarium (purity 99.99%), gadolinium (purity, 99.99%), terbium (purity, 99.99%), dysprosium (purity, 99.99%), holmium (purity, 99.98%), erbium (purity, 99.98%) and thulium (purity 99.99%) were used as the starting components. Titanium was used as a getter during the melting process. The compounds were annealed at 1070 K for 200 h in argon atmosphere with titanium chips and quenched in ice-cold water.

X-ray powder diffraction analyses were obtained on an DRON-3.0 (Cu Kα-radiation, $2\theta=20\ldots70°$). The obtained diffractograms were identified via calculated X-ray patterns which were obtained in the isotropic approximation using the Rietan-programs [1].

Eight new compounds have been detected: $Gd_2Sc_3Ge_4$, $Sm_2Sc_3Si_4$, $Gd_2Sc_3Si_4$, $Tb_2Sc_3Si_4$, $Dy_2Sc_3Si_4$, $Ho_2Sc_3Si_4$, $Er_2Sc_3Si_4$ and $Tm_2Sc_3Si_4$. Analysis of the powder X-ray diffractograms shows that these compounds crystallize in the orthorhombic Sm_5Ge_4-type structure (*Pnma*) [2] (Table 1). The lattice parameters of the compounds, refined at room temperature, and the reliability factor R_F resulting from the refinements are given in Table 2. The Sc atoms occupy the atomic positions of Sm2 and Sm3 in the Sm_5Ge_4-type structure.

The dependencies of the lattice parameters of the $\{Sm,Gd–Tm\}_2Sc_3Si_4$ compounds of the Sm_5Ge_4 type on the crystallographic radii R of the low temperature modification of the corresponding rare-earth metals [3] are presented in Fig. 1.

Table 1
Atomic position parameters of $Ce_2Sc_3Si_4$ (Sm_5Ge_4 structure type; space group *Pnma*) [2,4]

Atom	Type position	x/a	y/b	z/c
Ce	8(d)	0.1040	0.0971	0.8879
Sc1	4(c)	0.3392	1/4	0.9984
Sc2	8(d)	0.1716	0.1240	0.3248
Si1	4(c)	0.2123	1/4	0.6191
Si2	4(c)	0.9673	1/4	0.1241
Si3	8(d)	0.1533	0.9611	0.5367

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Table 2
Lattice parameters *a*, *b*, *c* (nm) and unit cell volume *V* (nm^3) of the $Gd_2Sc_3Ge_4$ and $R_2Sc_3Si_4$ (R=Sm, Gd–Tm) compounds[a]

Compound	Structure	*a*	*b*	*c*	*V*	R_F
$Sm_2Sc_3Si_4$	Sm_5Ge_4	0.7094(1)	1.3992(4)	0.7402(2)	0.73472	8.1
$Gd_2Sc_3Si_4$	Sm_5Ge_4	0.7092(2)	1.4012(4)	0.7412(2)	0.73683	6.7
$Tb_2Sc_3Si_4$	Sm_5Ge_4	0.7078(1)	1.3982(3)	0.7395(2)	0.73183	7.9
$Dy_2Sc_3Si_4$	Sm_5Ge_4	0.7060(1)	1.3951(4)	0.7380(2)	0.72690	8.6
$Ho_2Sc_3Si_4$	Sm_5Ge_4	0.7042(1)	1.3921(4)	0.7362(2)	0.72173	9.5
$Er_2Sc_3Si_4$	Sm_5Ge_4	0.7028(1)	1.3894(4)	0.7343(2)	0.71700	8.5
$Tm_2Sc_3Si_4$	Sm_5Ge_4	0.7011(2)	1.3852(5)	0.7324(2)	0.71121	8.6
$Gd_2Sc_3Ge_4$	Sm_5Ge_4	0.7211(2)	1.4050(6)	0.7453(3)	0.75504	8.4

[a] The R_F factor is given in %.

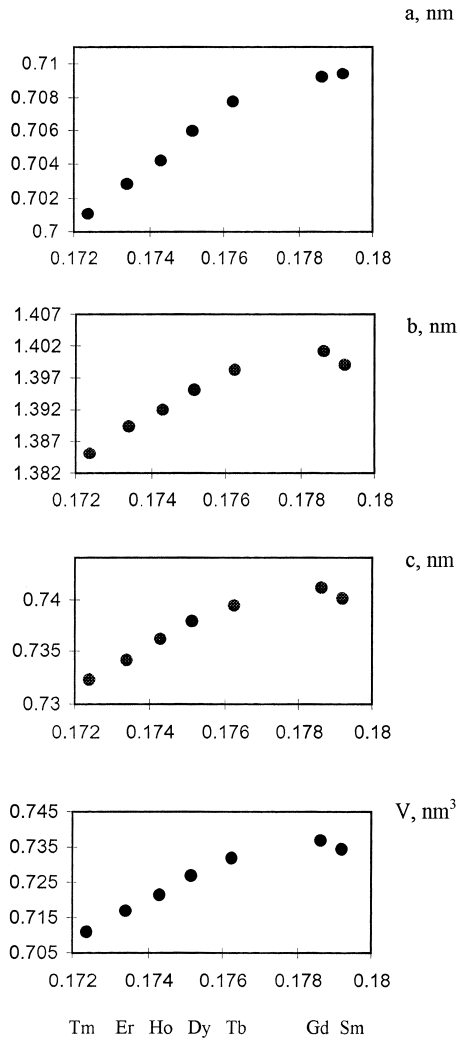

Fig. 1. Dependence of the cell parameters of the $\{Sm, Gd–Tm\}_2Sc_3Si_4$ compounds on the *R* crystallographic radius.

The lattice parameters *a*, *b*, *c* and the cell volume *V* are proportional to the crystallographic radius of the rare earth metals for all rare earths excepting Sm.

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