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Lanthanum iron trigermanide, $LaFeGe_3$

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(Ge–Fe) = 0.002 Å
R factor = 0.031
wR factor = 0.075
Data-to-parameter ratio = 16.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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Lanthanum iron trigermanide, $LaFeGe_3$, adopts the $BaNiSn_3$-type structure, which consists of square nets of Ge atoms, with Fe and Ge atoms positioned alternately above or below each square. Between these layers reside the La atoms.

Comment

A class of ternary rare-earth iron trigermanides, (RE)$FeGe_3$, with the $BaNiSn_3$-type structure (Dörrscheidt & Schäfer, 1978), has been identified for RE = La, Ce and Pr (Fedyna *et al.*, 1987; Fedyna *et al.*, 1993; Yamamoto *et al.*, 1994; Salamakha *et al.*, 1996). Interest in these compounds stems from the discovery that $CeFeGe_3$ is a heavy-fermion material with an unusually high Kondo temperature (Yamamoto *et al.*, 1994; Yamamoto *et al.*, 1995). For the solid solution $Ce_{1-x}La_xFeGe_3$ and its end members, extensive investigations of physical properties such as magnetic susceptibility, electrical resistivity, heat capacity, thermoelectric power and magnetoresistance have been carried out (Yamamoto & Ishikawa, 1996; Sampathkumaran & Das, 1996; Bud'ko *et al.*, 1998; Bud'ko *et al.*, 1999). All crystallographic studies have apparently been limited to powder samples. Refinements on powder data suggested a fully stoichiometric structure for $CeFeGe_3$ (Yamamoto *et al.*, 1994; Yan *et al.*, 1998) and, interestingly, a partial occupancy of the Fe site in $PrFe_{0.54}Ge_3$ (Fedyna *et al.*, 1987). The crystal structure of $LaFeGe_3$ determined from single-crystal data is presented here. The cell parameters are close to those previously reported from refinements of powder data [a = 4.368 Å and c = 9.985 Å (Yamamoto *et al.*, 1994), or a = 4.365 Å and c = 9.972 Å (Bud'ko *et al.*, 1998)].

The structure of $LaFeGe_3$ is shown in Fig. 1. If an ionic formulation is assumed, it consists of La^{3+} ions residing in the cavities between $[FeGe_3]^{3-}$ layers stacked along the c axis. These layers are made up of square nets of Ge2 atoms, with half of the squares capped on one side by Fe atoms and half on the other side by Ge1 atoms. Atoms Ge2 are thus tetrahedrally coordinated by two Fe and two Ge1 atoms. A short Fe—Ge1 contact [2.299 (3) Å] between the $[FeGe_3]^{3-}$ layers results in atoms Fe and Ge1 adopting a square-pyramidal coordination. The structures of $LaFeGe_3$ ($BaNiSn_3$-type, space group $I4mm$) and $LaFe_2Ge_2$ ($ThCr_2Si_2$-type, space group $I4/mmm$) (Rossi *et al.*, 1978; Venturini & Malaman, 1996) are closely related, both being ternary ordered variants of the $BaAl_4$-type structure. The ordering of Fe and Ge atoms is reversed in the square nets and the capping sites on one side of the squares, so that the layers consist of $GeFe_{2/4}Ge_{2/4}$ tetrahedra in $LaFeGe_3$ but $FeGe_{4/4}$ tetrahedra in $LaFe_2Ge_2$. Because the layers are held by stronger heteroatomic Fe—Ge1 interactions [2.299 (3) Å] in $LaFeGe_3$ compared with homoatomic Ge—Ge interactions [2.706 (4) Å] in $LaFe_2Ge_2$

(Venturini & Malaman, 1996), the *c* parameter is considerably more contracted in the former [9.9726 (10) Å *versus* 10.562 (1) Å, respectively].

Experimental

A mixture of La powder (Alfa–Aesar, 99.9%), Fe powder (Cerac, 99.9%) and Ge powder (Cerac, 99.999%) in a 1:1:4 molar ratio was reacted in an evacuated fused-silica tube. The tube was heated at 973 K for 1 d, heated to 1273 K over a period of 1 d, kept at that temperature for 2 d, and then cooled slowly to room temperature at a rate of 6 K h^{-1}. Silver plate-shaped crystals were obtained, which were found by semiquantitative energy-dispersive X-ray analysis to have a composition (at%) of 22 (2)% La, 21 (2)% Fe and 57 (3)% Ge, in good agreement with the expected values of 20% La, 20% Fe and 60% Ge.

Crystal data

$LaFeGe_3$	Mo $K\alpha$ radiation
M_r = 412.53	Cell parameters from 889 reflections
Tetragonal, *I*4*mm*	θ = 5.1–32.9°
a = 4.3660 (5) Å	μ = 37.91 mm^{-1}
c = 9.9726 (10) Å	*T* = 295 (2) K
V = 190.10 (4) $Å^3$	Plate, silver
Z = 2	0.10 × 0.08 × 0.01 mm
D_x = 7.207 Mg m^{-3}	

Data collection

Bruker Platform/SMART 1000 CCD diffractometer	248 independent reflections
ω scans	244 reflections with $I > 2\sigma(I)$
Absorption correction: numerical (*SHELXTL*; Sheldrick, 2001)	R_{int} = 0.046
T_{min} = 0.084, T_{max} = 0.650	θ_{max} = 32.9°
1248 measured reflections	*h* = −6 → 6
	k = −6 → 6
	l = −15 → 15

Refinement

Refinement on F^2	$(\Delta/\sigma)_{max}$ < 0.001
$R[F^2 > 2\sigma(F^2)]$ = 0.031	$\Delta\rho_{max}$ = 1.95 e $Å^{-3}$
$wR(F^2)$ = 0.075	$\Delta\rho_{min}$ = −1.98 e $Å^{-3}$
S = 1.08	Absolute structure: Flack (1983), 117 Friedel pairs
248 reflections	Flack parameter = 0.58 (6)
15 parameters	
$w = 1/[\sigma^2(F_o^2) + (0.0523P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$	

Table 1
Selected geometric parameters (Å, °).

La—Ge1^{i}	3.1586 (5)	Fe—Ge1	2.299 (3)
La—Ge2^{i}	3.2627 (13)	Fe—Ge2^{iii}	2.3728 (9)
La—Fe^{ii}	3.355 (3)	Ge1—Ge2	2.8024 (16)
La—Ge2	3.3656 (13)	Ge2—Ge2^{iv}	3.0872 (4)
La—Fe^{i}	3.4918 (12)		

Symmetry codes: (i) $\frac{1}{2}+x, y-\frac{1}{2}, z-\frac{1}{2}$; (ii) $x, y, z-1$; (iii) $\frac{1}{2}+x, y-\frac{1}{2}, \frac{1}{2}+z$; (iv) $-y, x, z$.

The value of the Flack parameter suggests an inversion twin. The structure was thus refined as a twin with components in the ratio 0.58 (6):0.42 (6). The maximum peak and deepest hole are located 0.86 Å and 0.64 Å, respectively, from La.

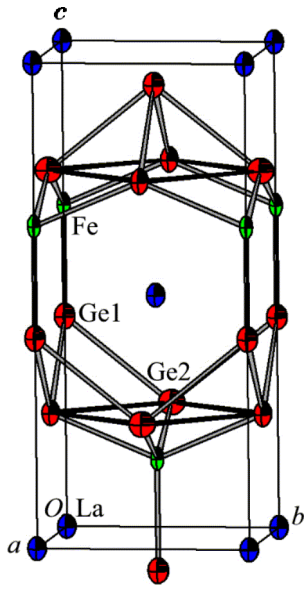

Figure 1
Projection of $LaFeGe_3$ approximately along the *a* axis. Displacement ellipsoids are drawn at the 90% probability level. Colour key: La blue, Fe green, Ge red.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *ATOMS* (Dowty, 1999); software used to prepare material for publication: *SHELXTL*.

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