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Erbium nickel disilicide, $ErNiSi_2$

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(Ni–Si) = 0.001 Å
R factor = 0.025
wR factor = 0.057
Data-to-parameter ratio = 15.6

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

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Single crystals of $ErNiSi_2$ were synthesized from the corresponding elements by arc melting. The ternary intermetallic compound crystallizes in the orthorhombic space group *Cmcm* and adopts the $CeNiSi_2$ structure type [Bodak & Gladyshevskii (1969). *Kristallografiya*, **14**, 990–994], with all four crystallographically unique atoms in special positions of site symmetry *m*2*m*.

Comment

Ternary intermetallics of rare earth metals with the general formula $RETX_2$ (where RE is a rare earth metal, T is a transition metal and X is a *p*-block element) crystallize mostly in 23 structure types (Parthé *et al.*, 1993–1994), *viz*. monoclinic $NdRuSi_2$, $CeCoC_2$ and $LaCuS_2$, orthorhombic $CeNiSi_2$, $YIrGe_2$, $LuMnGe_2$, $ZrCrSi_2$, $CeRhGe_2$, $TbFeSi_2$, $LaTmIr_2Ge_4$, $LuNiSn_2$, $NdAgAs_2$, $MgCuAl_2$, $NdNiGa_2$, $CeRhSn_2$ (Niepmann *et al.*, 1999), $ScRhSi_2$, $ScFeSi_2$, $CeNiC_2$, $ScCoC_2$ and $LuRuB_2$, and tetragonal $HfCuSi_2$, $ScCoC_2$ and $LaRhC_2$.

The $RETX_2$ phases have been the focus of special attention due to their interesting magnetic and electrical properties, *e.g.* the Kondo effect. An accurate determination of the crystal structure for phases of this composition is a basic requirement for the better understanding of their physical properties. The existence of the phase $ErNiSi_2$ was first reported by Bodak & Gladyshevskii (1969) who, on the basis of X-ray powder diffraction data, established that the crystal structure adopts the orthorhombic $CeNiSi_2$ structure type. Analogous results were obtained by Gil *et al.* (1994). In these investigations, information about structural data (atomic coordinates, displacement parameters) was not presented. Thus, it seemed appropriate to determine completely the crystal structure of $ErNiSi_2$, and we present these results here.

$ErNiSi_2$ adopts the $CeNiSi_2$ structure type (Bodak & Gladyshevskii, 1969). A clinographic projection of the unit-cell contents is shown in Fig. 1. The coordination around Er (site symmetry *m*2*m*) consists of 21 atoms, if bonding interactions are considered for distances < 4.0 Å, resulting in an $[ErSi_4Ni_4Si_6NiEr_6]$ polyhedron (Fig. 2*a*). The coordination polyhedron around the Ni atom (site symmetry *m*2*m*) is a monocapped tetragonal antiprism, $[NiSi_5Er_4]$, made up of 4 Er atoms in one basal plane with a capping Si atom, and 4 Si atoms in the second basal plane, if bonding interactions are considered for distances < 3.1 Å (Fig. 2*b*). The coordination polyhedron around atom Si1 (site symmetry *m*2*m*, bonding interactions < 3.1 Å) is a tricapped trigonal prism, $[Si1Ni-Si_2Er_6]$, with one additional Ni and two Er atoms as capping atoms (Fig. 2*c*). The coordination polyhedron around atom Si2 (site symmetry *m*2*m*, bonding interactions < 3.1 Å) is a distorted cuboctahedron, $[Si2Ni_4Si_4Er_4]$ (Fig. 2*d*).

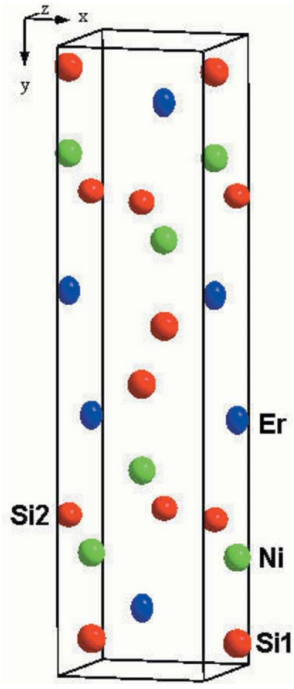

Figure 1
A clinographic projection of the $ErNiSi_2$ unit-cell contents, with displacement ellipsoids drawn at the 95% probability level.

The interatomic distances (Table 1) are in good agreement with the sums of the atomic radii (Emsley, 1991). The shortest distance with the highest deviation (93% of the sum of the atomic radii) is observed between Ni and Si atoms, with an Ni—Si distance of 2.255 (3) Å.

Experimental

The single crystal used in this work was extracted from an alloy with nominal composition $Er_{23}Ni_{27}Si_{50}$, which was prepared by arc melting of the initial components (purity better than 99.9%) in an electric arc furnace with a water-cooled copper bottom (Ti-getter) under an argon atmosphere, and annealed at 870 K. A preliminary crystallographic investigation was performed using Laue and rotation methods (RKV-86 and RGNS-2 chambers, Mo $K\alpha$ radiation).

Crystal data

$ErNiSi_2$
M_r = 282.15
Orthorhombic, *Cmcm*
a = 3.9423 (9) Å
b = 16.502 (3) Å
c = 3.9319 (9) Å
V = 255.79 (9) Å^3
Z = 4
D_x = 7.327 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1017 reflections
θ = 4.9–32.7°
μ = 40.49 mm^{-1}
T = 295 (2) K
Plate, metallic light grey
0.21 × 0.19 × 0.04 mm

Data collection

Oxford Diffraction Xcalibur3 CCD area-detector diffractometer
ω scans
Absorption correction: analytical *CrysAlis RED* (Oxford Diffraction, 2005)
T_{min} = 0.002, T_{max} = 0.199
1025 measured reflections
281 independent reflections
280 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 32.7°
$h = -5 \rightarrow 4$
$k = -24 \rightarrow 23$
$l = -5 \rightarrow 5$

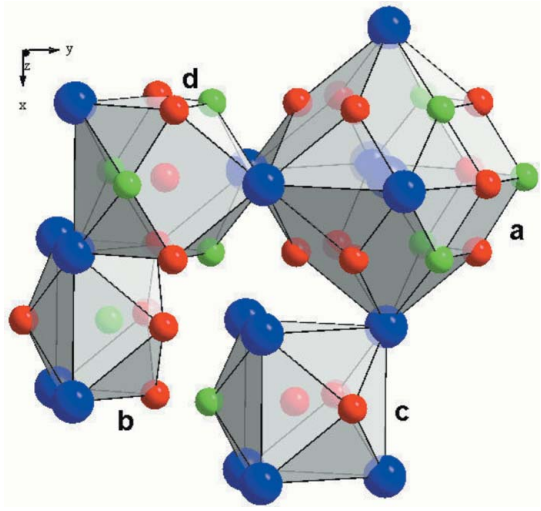

Figure 2
The coordination polyhedra around (*a*) the Er atom, (*b*) the Ni atom, and (*c*) and (*d*) the Si atoms. Er atoms are blue, Ni atoms green and Si atoms red.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.057
S = 1.33
281 reflections
18 parameters
$w = 1/[\sigma^2(F_o^2) + (0.023P)^2 + 5.5174P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 4.29 e Å^{-3}
$\Delta\rho_{min}$ = −2.85 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.0048 (7)

Table 1
Selected interatomic distances (Å).

Er—Si1^{i}	2.9899 (10)	Ni—Si1	2.255 (3)
Er—Ni^{ii}	3.0178 (6)	Ni—Si2^{vii}	2.3110 (15)
Er—Si2^{iii}	3.090 (2)	Ni—Si2^{iv}	2.3202 (15)
Er—Si1^{iv}	3.100 (2)	Si1—Si1^{viii}	2.358 (3)
Er—Er^{v}	3.9319 (9)	Si2—Si2^{ix}	2.7840 (5)
Er—Er^{vi}	3.9423 (9)		

Symmetry codes: (i) $-x-\frac{1}{2}, -y+\frac{1}{2}, -z$; (ii) $-x+\frac{1}{2}, -y+\frac{1}{2}, -z+1$; (iii) $x+\frac{1}{2}, y-\frac{1}{2}, z$; (iv) $x-\frac{1}{2}, y-\frac{1}{2}, z$; (v) $x, y, z-1$; (vi) $x-1, y, z$; (vii) $-x, -y+1, -z$; (viii) $-x, -y+1, -z+1$; (ix) $-x+\frac{1}{2}, -y+\frac{3}{2}, -z+1$.

Atomic coordinates were standardized using the *STRUCTURE-TIDY* program (Gelato & Parthé, 1987). The highest maximum residual electron density is 1.06 Å from atom Si1 and the deepest hole is 0.65 Å from the Er atom.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2004); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXL97* (Sheldrick, 1997).

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