Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Erbium dinickel disilicide, $ErNi_2Si_2$

Joanna Kończyk,[a] Bernard Marciniak,[a] Pavlo Demchenko,[b] Oksana Bodak[a,b] and Volodymyr Pavlyuk[a,b]*

[a]Institute of Chemistry and Environment Protection, Jan Dlugosz University, al. Armii Krajowej 13/15, 42-200 Czestochowa, Poland, and [b]Department of Inorganic Chemistry, Ivan Franko Lviv University, Kyryla and Mefodiya Street 6-8, 79005 Lviv, Ukraine

Correspondence e-mail: j.konczyk@ajd.czest.pl

Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(Ni–Si) = 0.004 Å
R factor = 0.014
wR factor = 0.036
Data-to-parameter ratio = 10.9

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

Erbium dinickel disilicide, $ErNi_2Si_2$, crystallizes in the tetragonal $ThCr_2Si_2$ structure type, which is an ordered superstucture of the $BaAl_4$ type. The coordination numbers are 22 for Er (2a site), 12 for Ni (4d site), and 9 for Si (4e site).

Received 10 October 2006
Accepted 26 October 2006

In memory of Professor Dr Oksana Bodak.

Comment

The ternary intermetallics $RENi_2Si_2$ (where RE is a rare earth) belong to a large group of compounds crystallizing in the tetragonal $ThCr_2Si_2$ type structure (a ternary derivative of the $BaAl_4$ type, also called $CeGa_2Al_2$ type) in space group $I4/mmm$. All atoms are located at special positions: RE at 2a (0, 0, 0), Ni at 4d (0, $\frac{1}{2}$, $\frac{1}{4}$) and Si at 4e (0, 0, z), with z ranging from 0.350 for $CeNi_2Si_2$ (Bodak *et al.*, 1966) and $TmNi_2Si_2$ (Barandiaran *et al.*, 1987) to 0.390 for $PrNi_2Si_2$ (Barandiaran *et al.*, 1986). These compounds show interesting physical properties and present different types of magnetic structures, *e.g.* those containing Pr, Nd, Ho, Er and Tm have a complex incommensurate antiferromagnetic structure.

The structure of $ErNi_2Si_2$ has been determined previously from powder samples by X-ray (Bodak *et al.*, 1966) and neutron diffraction measurements (Yakinthos & Ikonomou, 1980; Barandiaran *et al.*, 1987; Yan *et al.*, 1998). However, in some of these studies, only the cell parameters and the isotypism with the $ThCr_2Si_2$ type structure were reported (Bodak *et al.*, 1966; Yakinthos & Ikonomou, 1980). In other

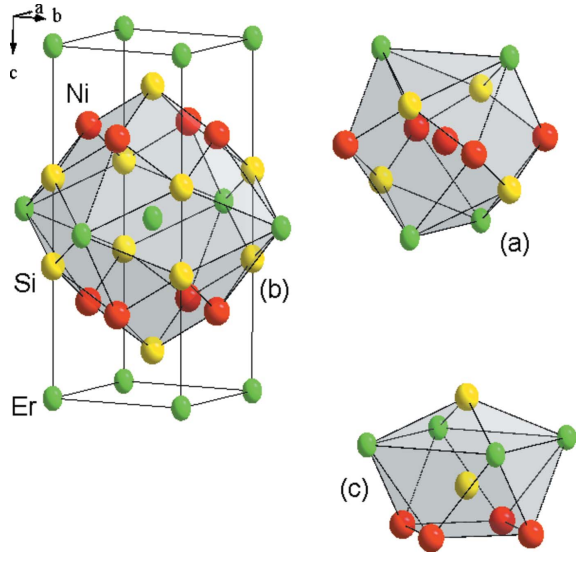

Figure 1
Clinographic projections of $ErNi_2Si_2$, with displacement ellipsoids drawn at the 95% probability level, showing the coordination polyhedra of (*a*) Ni, (*b*) Er and (*c*) Si atoms.

studies, the structural refinements were conducted without anisotropic displacement parameters and gave unsatisfactory reliability factors of about 0.10 (Barandiaran *et al.*, 1987; Yan *et al.*, 1998). Bearing in mind also the close relationship of the $ThCr_2Si_2$ (*I*4/*mmm*) and $CaBe_2Ge_2$ (*P*4/*nmm*) structure types, it is necessary to determine precisely the structure type for the $ErNi_2Si_2$ phase and to perform a complete structural investigation on the basis of single-crystal X-ray diffraction data, as reported here.

$ErNi_2Si_2$ adopts the $ThCr_2Si_2$ type structure (Fig. 1), and is isotypic with $ErCo_2Si_2$ (Demchenko *et al.*, 2005) and many other 1:2:2 silicides containing rare earths and transition metals. The Er atom (site symmetry 4/*mmm*) is at the centre of a 22-atom polyhedron, $[ErSi_8Ni_8Si_2Er_4]$ (Fig. 1*b*), the Ni atom (site symmetry $\overline{4}m2$) is at the centre of a distorted cuboctahedron, $[NiSi_4Ni_4Er_4]$ (Fig. 1*a*), and the Si atom (site symmetry 4*mm*) is at the centre of a monocapped tetragonal antiprism, $[SiNi_4Si_1Er_4]$ (Fig. 1*c*). The interatomic distances agree well with the sums of the atomic radii (Emsley, 1991). The shortest distance of 2.3020 (13) Å, found between Ni and Si atoms (Table 1), corresponds to 95% of the sum of the atomic radii.

Experimental

A needle-shaped single crystal of the title compound was extracted from an alloy with nominal composition $Er_{27}Ni_{37}Si_{36}$, which was prepared by arc-melting of the component elements (purity >99.9%) under an argon atmosphere followed by annealing at 870 K. A preliminary crystallographic investigation was performed using Laue and rotation methods (RKV-86 and RGNS-2 chambers, Mo Kα radiation).

Crystal data

$ErNi_2Si_2$
M_r = 340.86
Tetragonal, *I*4/*mmm*
a = 3.9431 (9) Å
c = 9.543 (2) Å
V = 148.37 (6) Å^3
Z = 2
D_x = 7.629 Mg m^{-3}
Mo Kα radiation
μ = 41.06 mm^{-1}
T = 295 (2) K
Needle, metallic light grey
0.17 × 0.05 × 0.02 mm

Data collection

Oxford Diffraction Xcalibur3 CCD area-detector diffractometer
ω scans
Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2005)
T_{min} = 0.094, T_{max} = 0.432
603 measured reflections
87 independent reflections
87 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 30.1°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.014
$wR(F^2)$ = 0.037
S = 1.25
87 reflections
8 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0158P)^2 + 2.224P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.63 e Å^{-3}
$\Delta\rho_{min}$ = −1.35 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.0042 (10)

Table 1
Selected bond lengths (Å).

Er—Si^{i}	3.0344 (11)	Ni—Ni^{iii}	2.7882 (6)
Er—Ni	3.0950 (5)	Si—Si^{iv}	2.395 (5)
Ni—Si^{ii}	2.3020 (13)		

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

The structure refinement of $ErNi_2Si_2$ clearly indicated that this phase crystallizes in the tetragonal crystal system in space group *I*4/*mmm*, adopting the $ThCr_2Si_2$ structure type, with satisfactory reliability factors, values of refined parameters and geometric values. Refinements in space group *P*4/*nmm* ($CaBe_2Ge_2$ structure type) were less satisfactory and resulted in higher values of the *R* factors and atomic displacement factors. The deepest hole is located 1.346 Å from Er.

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*.

References

Barandiaran, J. M., Gignoux, D., Schmitt, D. & Gomez Sal, J. C. (1986). *Solid State Commun.* **57**, 941–945.
Barandiaran, J. M., Gignoux, D., Schmitt, D., Gomez Sal, J. C. & Rodriguez Fernandez, J. (1987). *J. Magn. Magn. Mater.* **69**, 61–70.
Bodak, O. I., Gladyshevskii, E. I. & Krypyakevich, P. I. (1966). *Izv. Akad. Nauk SSSR Neorg. Mater.* **2**, 2151–2155. (In Russian.)
Brandenburg, K. (1999). *DIAMOND*. Release 2.1c. Crystal Impact GbR, Bonn, Germany.
Demchenko, P., Kończyk, J., Bodak, O., Marciniak, B. & Matvijishyn, R. (2005). *Acta Cryst.* E**61**, i218–i220.
Emsley, J. (1991). *The Elements*, 2nd ed., pp. 63–178. Oxford: Clarendon Press.
Oxford Diffraction (2004). *CrysAlis CCD*. Version 1.170. Oxford Diffraction Ltd., Abingdon, Oxfordshire, England.
Oxford Diffraction (2005). *CrysAlis RED*. Version 1.171. Oxford Diffraction Ltd., Abingdon, Oxfordshire, England.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Yakinthos, J. K. & Ikonomou, P. F. (1980). *Solid State Commun.* **34**, 777–778.
Yan, J., Ou, X., Zeng, L. & Hao, J. (1998). *Trans. Nonferrous Met. Soc. China*, **8**, 622–625.