

Redetermination of iron dialuminide, FeAl₂

Ihor Chumak,^{a*} Klaus W. Richter^b and Helmut Ehrenberg^a

^aInstitute for Complex Materials, IFW Dresden, Helmholtzstrasse 20, 01069 Dresden, Germany, and ^bDepartment of Inorganic Chemistry/Materials Chemistry, University of Vienna, Waehringerstrasse 42, A-1090 Vienna, Austria
Correspondence e-mail: i.chumak@ifw-dresden.de

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The crystal structure of iron dialuminide [Corby & Black (1973). *Acta Cryst.* **B29**, 2669–2677] has been redetermined on a single crystal synthesized from the elements by arc melting. The compound crystallizes in the triclinic space group $P\bar{1}$ with 19 atoms per unit cell, one Fe site being on an inversion centre. The crystal structure can be described as an inclusion-plus-deformation derivative of the orthorhombic YPd₂Si structure type.

Comment

The crystal structure of FeAl₂ was first described by Corby & Black (1973). Single-crystal data were collected at Mo $K\alpha$, Fe $K\alpha$ and Cr $K\alpha$ wavelengths using integrated Weissenberg photographs. The authors solved the structure by use of the anomalous dispersion technique in a triclinic model with 18 atoms per unit cell: space group $P1$ (No. 1), Pearson symbol

$aP18$, $a = 4.878$ (1) Å, $b = 6.461$ (2) Å and $c = 8.800$ (3) Å, and $\alpha = 91.75$ (5)°, $\beta = 73.27$ (5)° and $\gamma = 96.89$ (3)°.

For the present work, single crystals of FeAl₂ were isolated during an investigation of the Ni–Fe–Al ternary system between 50 and 100 at% of Al (Chumak *et al.*, 2007). Our single-crystal investigations confirm the triclinic crystal system, but with one additional atom per unit cell (Pearson symbol $aP19$) and an additional inversion symmetry according to space group $P\bar{1}$ (No. 2). The unit cell contains three Fe sites, six Al sites and one statistically occupied Fe/Al (M) site (71:29%). A graphical representation of the FeAl₂ structure and the various coordination polyhedra is given in Fig. 1. The coordination number (CN) of Fe/Al is 11 and the coordination polyhedron is a distorted trigonal prism with five additional vertices. The coordination polyhedra of Al are: a trigonal prism with five additional vertices (Al1, CN = 11), a distorted trigonal prism with four additional vertices (Al4, CN = 10), a nearly regular icosahedron (Al2, CN = 12), a distorted icosahedron with one additional vertex (Al3, CN = 13) and distorted bicapped pentagonal prisms (Al5 and Al6, CN = 12). The coordination polyhedra of Fe are: a trigonal prism with five additional vertices (Fe1, CN = 11), a distorted tetragonal prism with two additional vertices (Fe2, CN = 10) and a nearly regular icosahedron (Fe3, CN = 12).

The shortest interatomic distances (Table 1) indicate metallic-type bonding (the shortest Fe–Al distance of 2.424 (3) Å is 97.3% of the sum of the atomic radii (Shannon, 1976).

The FeAl₂ structure is derived from the orthorhombic YPd₂Si structure (Moreau *et al.*, 1982) [an ordered Fe₃C type in the space group $Pnma$ (No. 62), Pearson symbol $oP16$, $a = 7.303$ (2) Å, $b = 6.918$ (2) Å and $c = 5.489$ (1) Å] by including three additional atoms per unit cell and strong deformation. Both structures can be represented as an arrangement of trigonal prisms, with significant distortions in the case of FeAl₂ (Fig. 2). Examples of similar deformations are realised in the

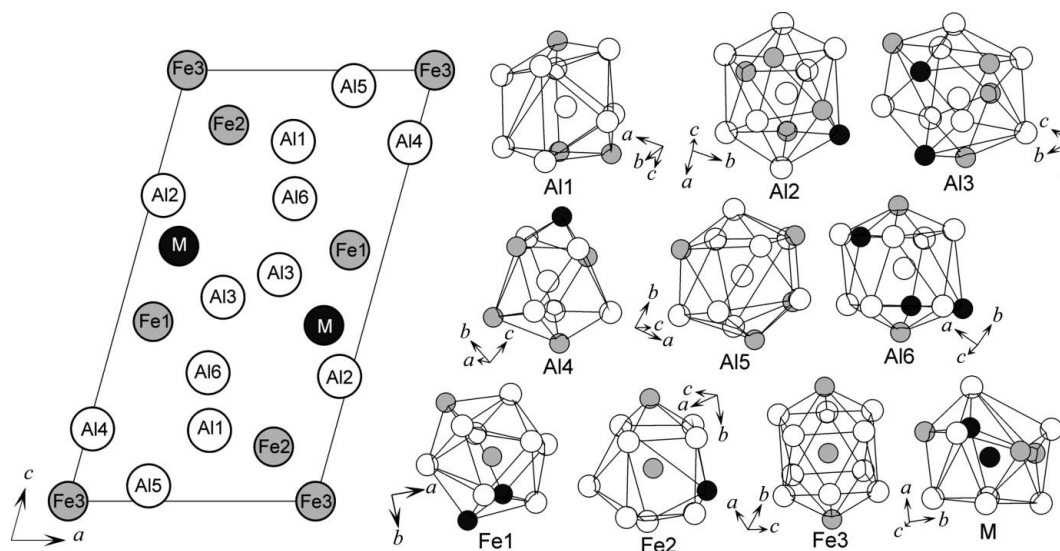


Figure 1

The unit cell and the coordination polyhedra of the atoms in the structure of FeAl₂. Generic atom labels without symmetry codes have been used for all symmetry-related atom sites.

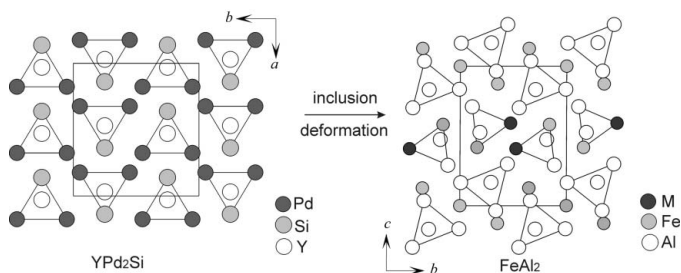


Figure 2
The arrangement of the trigonal prisms in the YPd_2Si and $FeAl_2$ structures.

$MgCuAl_2$ and $CaRhIn_2$ structures, which can be interpreted as inclusion-plus-deformation derivatives of $CaIn_2$ (Hoffmann & Poettgen, 2000, 2001).

Experimental

The single crystal used for structure determination was separated from an $FeAl_2$ single-phase alloy, prepared from the elements by arc melting under an argon atmosphere. The composition of the phase, determined by electron-probe microanalysis (EPMA) on a Cameca SX electron probe 100 (Cameca, Courbevoie, France) using wavelength-dispersive spectroscopy (WDS) for quantitative analyses and employing pure aluminium and iron as standard materials, is in very good agreement with the final composition from the crystal structure refinement, viz. $Fe_{33.6}Al_{66.4}$ from EPMA and $Fe_{33.7}Al_{66.3}$ from refinement.

Crystal data

$Fe_{6.41}Al_{12.59}$ $\gamma = 83.062 (9)^\circ$
 $M_r = 697.68$ $V = 262.79 (5) \text{ \AA}^3$
 Triclinic, $P\bar{1}$ $Z = 1$
 $a = 4.8745 (6) \text{ \AA}$ Mo $K\alpha$ radiation
 $b = 6.4545 (8) \text{ \AA}$ $\mu = 9.61 \text{ mm}^{-1}$
 $c = 8.7361 (10) \text{ \AA}$ $T = 296 \text{ K}$
 $\alpha = 87.930 (9)^\circ$ $0.04 \times 0.03 \times 0.02 \text{ mm}$
 $\beta = 74.396 (9)^\circ$

Table 1
Selected bond lengths (\AA).

Fe1—Fe4A	2.6057 (18)	Fe4A—Al4 ⁱⁱⁱ	2.532 (3)
Fe2—Al6 ⁱ	2.424 (3)	Fe4A—Fe4A ⁱⁱⁱ	2.533 (3)
Fe2—Fe3 ⁱⁱ	2.7258 (13)	Al5—Al5 ^{iv}	2.606 (5)

Symmetry codes: (i) $-x + 1, -y + 1, -z + 1$; (ii) $x, y, z + 1$; (iii) $-x, -y + 1, -z + 1$; (iv) $-x + 1, -y + 1, -z$.

Data collection

Bruker Kappa APEXII CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2004)
 $T_{\min} = 0.715, T_{\max} = 0.825$
 4139 measured reflections
 1560 independent reflections
 1004 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.043$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.052$
 $wR(F^2) = 0.136$
 $S = 1.05$
 1560 reflections
 90 parameters
 $\Delta\rho_{\max} = 1.71 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -1.10 \text{ e \AA}^{-3}$

The data were refined with anisotropic displacement parameters for all atoms. The atomic coordinates were standardized using the *STRUCTURE TIDY* program (Gelato & Parthé, 1987). The Fe/Al atoms constituting the *M* site were constrained to have identical coordinates and displacement parameters. Their site-occupation factors were refined while restraining their sum to unity and yielded values of 0.705 (1) and 0.295 (1) for atoms Fe4A and Al4B, respectively.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Version 6.12; Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: KU3029). Services for accessing these data are described at the back of the journal.

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