Redetermination of the crystal structure of iron silicide, FeSi

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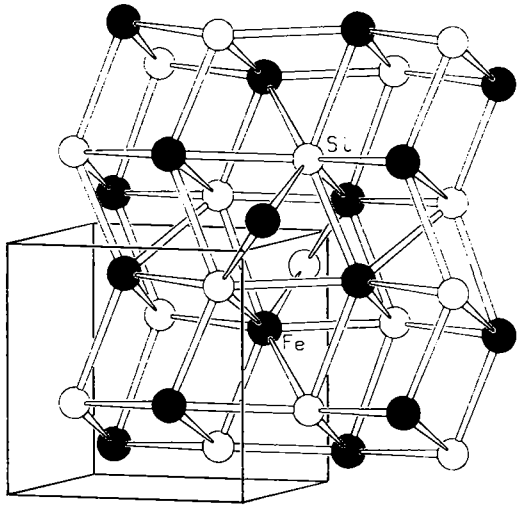

Source of material: FeSi single crystals can be prepared by means of chemical vapor transport using iodine as transport agent. FeSi is deposited at 1073 K. The temperature gradients during our experiments were 1073 K-1273 K (Fe) and 1003-1073 K (Si) using a 3-T-technique (see ref. 1).

The shape of the crystal is a distorted octahedron. The octahedron decomposes in two tetrahedra. The $\{\bar{1},\bar{1},\bar{1}\}$-tetrahedron has larger faces than the $\{1,1,1\}$-tetrahedron. The Flack x-parameter is 0.08(2) The lattice constant of the crystal was determined in three ways: 1) From the orienting matrix, which was based on 50 reflections in the 2θ range 27.4°-30.4°, using λ =0.71073 Å, it follows a =4.495(2) Å. 2) The double ω scan with 20 reflections in the 2θ range 27.4°-29.0° using λ =0.71073 Å yields a = 4.491(1) Å. 3) From the orienting matrix using the α1 peaks from 14 reflections in the 2θ range 104.4°-110.5° and λ =0.7093 Å it follows a =4.487(2) Å. The atomic coordinates of this work do not differ much from those of earlier investigations (see ref. 2-4). The sevenfold coordination of Fe by Si and Si by Fe with one short Fe–Si distance (2.288(1) Å) is confirmed. Taking into account the next nearest neighbours and following O'Keeffe's definition of a weighted coordination number Z* (see ref. 5) one gets Z*(Fe) =8.53 and Z*(Si) =8.88.

FeSi, cubic, $P2_13$ (No. 198), a =4.495(2) Å, V =90.8 Å^3, Z =4, $R(F)$ =0.014, $R_w(F^2)$ =0.030.

Table 1. Parameters used for the X-ray data collection

Crystal:	octahedral shape, metallic grey, size 0.22 x 0.23 x 0.25 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	161.60 cm^{-1}
Diffractometer:	Siemens-Stoe
Scan mode:	ω/2θ
$T_{measurement}$:	298 K
$2\theta_{max}$:	111.3°
$N(hkl)_{unique}$:	408
Criterion for I_o:	$I_o > 2\,\sigma(I_o)$
$N(param)_{refined}$:	8
Programs:	SHELX-76, SHELXL-93, STRUX, X-RED, X-SHAPE, PLATON, BLOKJE, SCHAKAL

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Table 2. Final atomic coordinates and displacement parameters (in Å^2)

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Fe(1)	4a	0.13650(2)	x	x	0.00421(3)	U_{11}	U_{11}	−0.00001(2)	U_{12}	U_{12}
Si(1)	4a	0.84262(5)	x	x	0.00531(5)	U_{11}	U_{11}	−0.00048(4)	U_{12}	U_{12}