Refinement of the crystal structure of scandium diiron disilicide, $ScFe_2Si_2$

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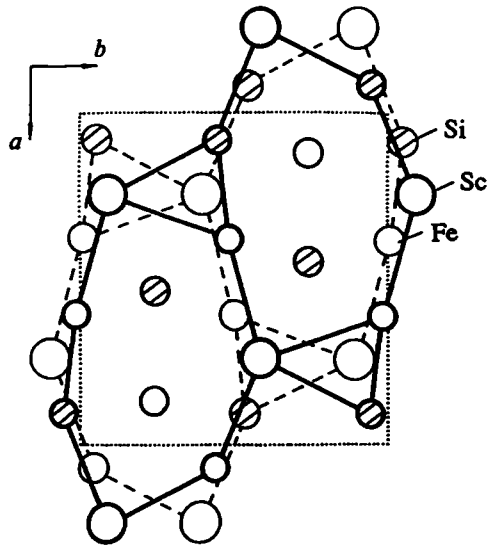

Source of material: Pieces of scandium, iron and silicon were arc melted in argon atmosphere. A single crystal of prismatic shape was extracted from the alloy which was homogenated in an evacuated quartz tube at 1073 K during 15 days.

Fe_2ScSi_2, orthorhombic, *Pbcm* (No. 57), a =7.5002(9) Å, b =7.1375(9) Å, c =5.0224(4) Å, V =268.9 Å^3, Z =4, $R(F)$ =0.040, $R_w(F)$ =0.023.

The synthesis and X-ray structure of $ScFe_2Si_2$ was reported before (see ref. 3). The compound was found to crystallize with the $HfFe_2Si_2$ structure type (see ref. 5). Both structures were established on single crystals from photographic data. Here we report the first single crystal counter data on that structure type. As shown in the figure, the structure of $ScFe_2Si_2$ can be described in terms of nets which connect Sc, Fe1 and Si1 atoms at z=1/4 (dashed lines), and at z=3/4 (full lines), and of additional Fe2 and Si2 atoms which are both situated at the heights z=0 and z=0.5. Scandium is the only rare earth element which participates in the formation of that structure type for which the two above compounds are the only known members to date.

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

Crystal:	grey prism, size 0.016 x 0.032 x 0.112 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	136.28 cm^{-1}
Diffractometer:	Philips PW1100
Scan mode:	$\omega/2\theta$
$T_{measurement}$:	293 K
$2\theta_{max}$:	59.9°
N(hkl)$_{unique}$:	338
Criterion for F_o:	$F_o > 2\,\sigma(F_o)$
N($param$)$_{refined}$:	30
Program:	Xtal3.2

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}
Sc	4*d*	0.2511(3)	0.4028(3)	1/4	0.0027(7)	0.0047(7)	0.0047(8)	0.0008(6)	0	0
Fe(1)	4*d*	0.3843(2)	0.0115(2)	1/4	0.0036(6)	0.0033(6)	0.0041(7)	–0.0008(6)	0	0
Fe(2)	4*c*	0.8824(2)	1/4	0	0.0043(6)	0.0042(5)	0.0042(6)	0	0	0.0005(5)
Si(1)	4*d*	0.0832(3)	0.0500(4)	1/4	0.005(1)	0.006(1)	0.006(1)	–0.001(1)	0	0
Si(2)	4*c*	0.5479(3)	1/4	0	0.003(1)	0.006(1)	0.006(1)	0	0	–0.001(1)

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