Low Temperature $FeSi_2$ Structure: AB2_oC48_64_df_2g-001

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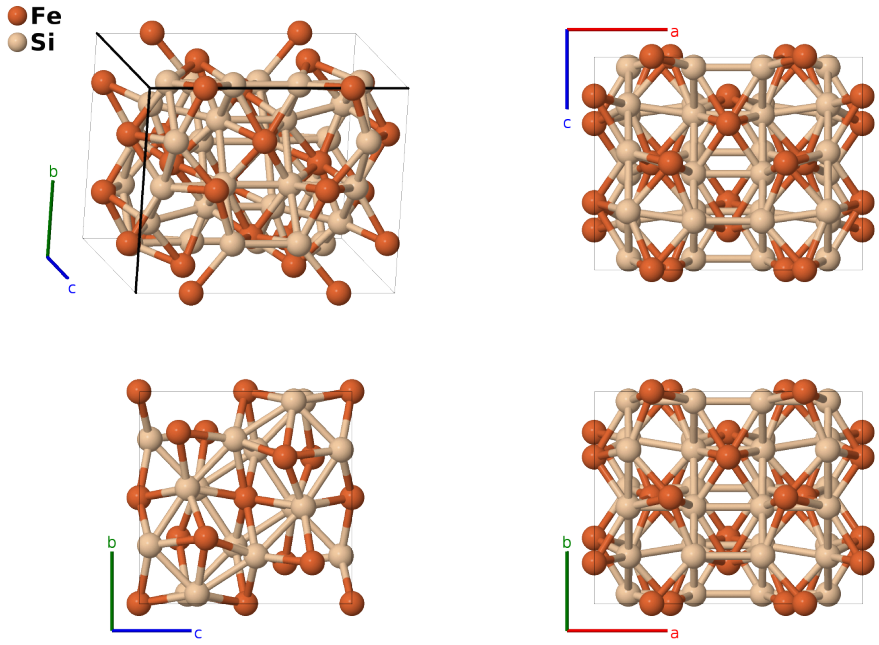
https://aflow.org/p/MR28

https://aflow.org/p/AB2_oC48_64_df_2g-001

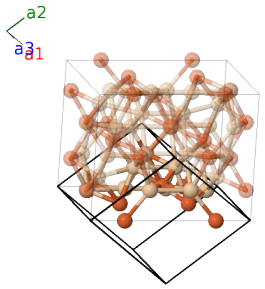


Prototype	$FeSi_2$
AFLOW prototype label	AB2_oC48_64_df_2g-001
ICSD	9119
Pearson symbol	oC48
Space group number	64
Space group symbol	*Cmce*
AFLOW prototype command	`aflow --proto=AB2_oC48_64_df_2g-001 --params=`$a, b/a, c/a, x_1, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4$

- This is the low temperature structure of $FeSi_2$. This transforms to the tetragonal high temperature structure above 962-1000K, with the exact temperature dependent up on the iron concentration in the high temperature phase. (Villars, 2018)

Base-centered Orthorhombic primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\,\hat{\mathbf{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2$	=	$ax_1\,\hat{\mathbf{x}}$	(8d)	Fe I
$\mathbf{B_2}$	=	$-\left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8d)	Fe I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2$	=	$-ax_1\,\hat{\mathbf{x}}$	(8d)	Fe I
$\mathbf{B_4}$	=	$\left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8d)	Fe I
$\mathbf{B_5}$	=	$-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8f)	Fe II
$\mathbf{B_6}$	=	$\left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Fe II
$\mathbf{B_7}$	=	$-\left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Fe II
$\mathbf{B_8}$	=	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-by_2\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(8f)	Fe II
$\mathbf{B_9}$	=	$(x_3 - y_3)\,\mathbf{a}_1 + (x_3 + y_3)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(16g)	Si I
$\mathbf{B_{10}}$	=	$\left(-x_3 + y_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_3 + y_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16g)	Si I
$\mathbf{B_{11}}$	=	$-\left(x_3 + y_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(-x_3 + y_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16g)	Si I
$\mathbf{B_{12}}$	=	$(x_3 + y_3)\,\mathbf{a}_1 + (x_3 - y_3)\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(16g)	Si I
$\mathbf{B_{13}}$	=	$-(x_3 - y_3)\,\mathbf{a}_1 - (x_3 + y_3)\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(16g)	Si I
$\mathbf{B_{14}}$	=	$\left(x_3 - y_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_3 + y_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16g)	Si I
$\mathbf{B_{15}}$	=	$\left(x_3 + y_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_3 - y_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16g)	Si I
$\mathbf{B_{16}}$	=	$-(x_3 + y_3)\,\mathbf{a}_1 - (x_3 - y_3)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(16g)	Si I
$\mathbf{B_{17}}$	=	$(x_4 - y_4)\,\mathbf{a}_1 + (x_4 + y_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(16g)	Si II
$\mathbf{B_{18}}$	=	$\left(-x_4 + y_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_4 + y_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16g)	Si II
$\mathbf{B_{19}}$	=	$-\left(x_4 + y_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(-x_4 + y_4 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16g)	Si II

$\mathbf{B_{20}}$	=	$(x_4+y_4)\,\mathbf{a}_1+(x_4-y_4)\,\mathbf{a}_2-z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}}-by_4\,\hat{\mathbf{y}}-cz_4\,\hat{\mathbf{z}}$	(16g)	Si II
$\mathbf{B_{21}}$	=	$-(x_4-y_4)\,\mathbf{a}_1-(x_4+y_4)\,\mathbf{a}_2-z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}}-by_4\,\hat{\mathbf{y}}-cz_4\,\hat{\mathbf{z}}$	(16g)	Si II
$\mathbf{B_{22}}$	=	$\left(x_4-y_4+\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_4+y_4+\frac{1}{2}\right)\,\mathbf{a}_2-\left(z_4-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{x}}+by_4\,\hat{\mathbf{y}}-c\left(z_4-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16g)	Si II
$\mathbf{B_{23}}$	=	$\left(x_4+y_4+\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_4-y_4+\frac{1}{2}\right)\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{x}}-by_4\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16g)	Si II
$\mathbf{B_{24}}$	=	$-(x_4+y_4)\,\mathbf{a}_1-(x_4-y_4)\,\mathbf{a}_2+z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}}+by_4\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(16g)	Si II

References

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[2] P. Villars, H. Okamoto, and K. Cenzual, eds., *ASM Alloy Phase Diagram Database* (ASM International, 2018), chap. Iron-Silicon Binary Phase Diagram (1997 Lindholm M.). Copyright ©2006-2018 ASM International.

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