Bainite (Fe_3C) Structure: AB3_hP8_182_c_g-001

This structure originally had the label `AB3_hP8_182_c_g`. Calls to that address will be redirected here.

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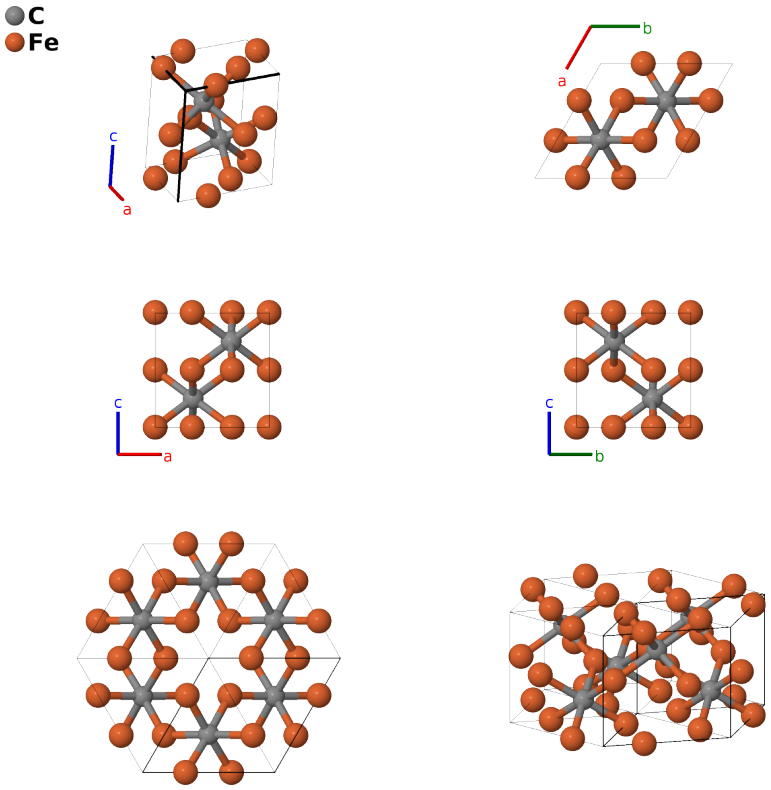
https://aflow.org/p/JRHU

https://aflow.org/p/AB3_hP8_182_c_g-001



Prototype	Fe_3C
AFLOW prototype label	AB3_hP8_182_c_g-001
Mineral name	bainite
ICSD	none
Pearson symbol	hP8
Space group number	182
Space group symbol	$P6_322$
AFLOW prototype command	`aflow --proto=AB3_hP8_182_c_g-001 --params=`$a, c/a, x_2$

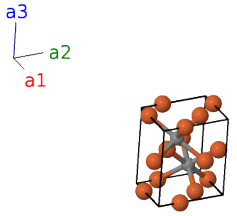
Other compounds with this structure

ϵ-Fe_3N

- Strictly speaking, bainite is a microstructure. However, (Villars, 1991) Vol. II, p. 1894, refers to this crystal structure as upper bainite, and (Villars, 2014) refers to this as bainite.

Hexagonal primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(2c)	C I
$\mathbf{B_2}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(2c)	C I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1$	=	$\frac{1}{2}ax_2\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}}$	(6g)	Fe I
$\mathbf{B_4}$	=	$x_2\,\mathbf{a}_2$	=	$\frac{1}{2}ax_2\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}}$	(6g)	Fe I
$\mathbf{B_5}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2$	=	$-ax_2\,\hat{\mathbf{x}}$	(6g)	Fe I
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_2\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(6g)	Fe I
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_2\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(6g)	Fe I
$\mathbf{B_8}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(6g)	Fe I

References

[1] M. Reibold, A. A. Levin, D. C. Meyer, P. Paufler, and W. Kochmann, *Microstructure of a Damascene sabre after annealing*, Int. J. Mater. Res. **97**, 1172–1182 (2006), doi:10.3139/ijmr-2006-0184.

[2] P. Villars and L. Calvert, *Pearson's Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OH, 1991), 2nd edn.

Found in

[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.