η-Fe$_2$Al$_5$ Structure: A5B_oC24_63_afg_c-001

https://aflow.org/p/US2Q

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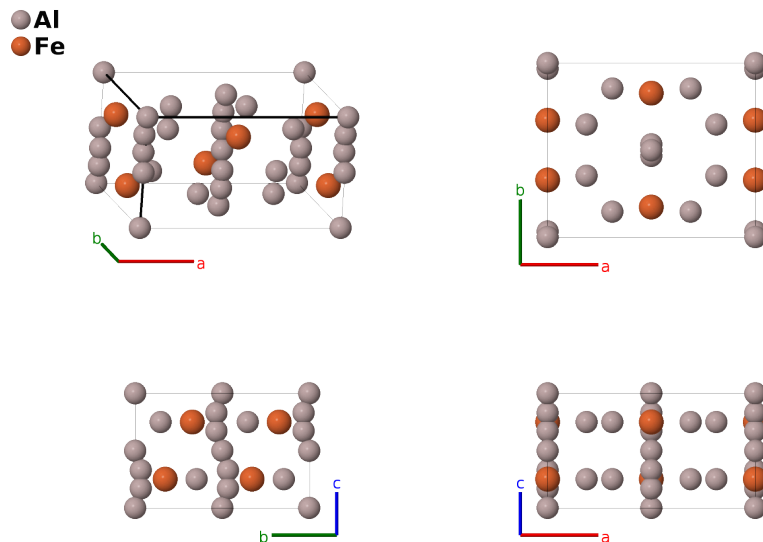
Prototype	Al$_5$Fe$_2$
AFLOW prototype label	A5B_oC24_63_afg_c-001
ICSD	105132
Pearson symbol	oC24
Space group number	63
Space group symbol	$Cmcm$
AFLOW prototype command	aflow --proto=A5B_oC24_63_afg_c-001 --params=$a, b/a, c/a, y_2, y_3, z_3, x_4, y_4$

- The Al-I (4a) sites are occupied 34% of the time, while the Al-III (8g) sites are 24% occupied, giving a stoichiometry near Fe$_2$Al$_5$.

- We have shifted the origin to move the Al-I atom from the (4b) site in (Burkhardt, 1994) to the (4a) site.

Base-centered Orthorhombic primitive vectors

$$\mathbf{a_1} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$
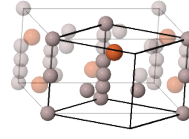
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	0	$=$	0	(4a)	Al I
$\mathbf{B_2}$	$=$	$\tfrac{1}{2}\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}c\,\hat{\mathbf{z}}$	(4a)	Al I
$\mathbf{B_3}$	$=$	$-y_2\,\mathbf{a_1} + y_2\,\mathbf{a_2} + \tfrac{1}{4}\,\mathbf{a_3}$	$=$	$by_2\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Fe I
$\mathbf{B_4}$	$=$	$y_2\,\mathbf{a_1} - y_2\,\mathbf{a_2} + \tfrac{3}{4}\,\mathbf{a_3}$	$=$	$-by_2\,\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	Fe I
$\mathbf{B_5}$	$=$	$-y_3\,\mathbf{a_1} + y_3\,\mathbf{a_2} + z_3\,\mathbf{a_3}$	$=$	$by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8f)	Al II
$\mathbf{B_6}$	$=$	$y_3\,\mathbf{a_1} - y_3\,\mathbf{a_2} + \left(z_3 + \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$-by_3\,\hat{\mathbf{y}} + c\left(z_3 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(8f)	Al II
$\mathbf{B_7}$	$=$	$-y_3\,\mathbf{a_1} + y_3\,\mathbf{a_2} - \left(z_3 - \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$by_3\,\hat{\mathbf{y}} - c\left(z_3 - \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(8f)	Al II
$\mathbf{B_8}$	$=$	$y_3\,\mathbf{a_1} - y_3\,\mathbf{a_2} - z_3\,\mathbf{a_3}$	$=$	$-by_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8f)	Al II
$\mathbf{B_9}$	$=$	$(x_4 - y_4)\,\mathbf{a_1} + (x_4 + y_4)\,\mathbf{a_2} + \tfrac{1}{4}\,\mathbf{a_3}$	$=$	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(8g)	Al III
$\mathbf{B_{10}}$	$=$	$-(x_4 - y_4)\,\mathbf{a_1} - (x_4 + y_4)\,\mathbf{a_2} + \tfrac{3}{4}\,\mathbf{a_3}$	$=$	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(8g)	Al III
$\mathbf{B_{11}}$	$=$	$-(x_4 + y_4)\,\mathbf{a_1} - (x_4 - y_4)\,\mathbf{a_2} + \tfrac{1}{4}\,\mathbf{a_3}$	$=$	$-ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(8g)	Al III
$\mathbf{B_{12}}$	$=$	$(x_4 + y_4)\,\mathbf{a_1} + (x_4 - y_4)\,\mathbf{a_2} + \tfrac{3}{4}\,\mathbf{a_3}$	$=$	$ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(8g)	Al III

References

[1] U. Burkhardt, Y. Grin, M. Ellner, and K. Peters, *Structure refinement of the iron-aluminium phase with the approximate composition Fe$_2$Al$_5$*, Acta Crystallogr. Sect. B **50**, 313–316 (1994), doi:10.1107/S0108768193013989.

Found in

[1] T. Tsukahara, N. Takata, S. Kobayashi, and M. Takeyama, *Mechanical Properties of Fe$_2$Al$_5$ and FeAl$_3$ Intermetallic Phases at Ambient Temperature*, Tetsu-to-Hagane **102**, 29–35 (2016), doi:10.2355/tetsutohagane.TETSU-2015-063.