Model of Austenite Structure (cI32): AB12C3_cI32_229_a_h_b-001

This structure originally had the label `AB12C3_cI32_229_a_h_b`. Calls to that address will be redirected here.

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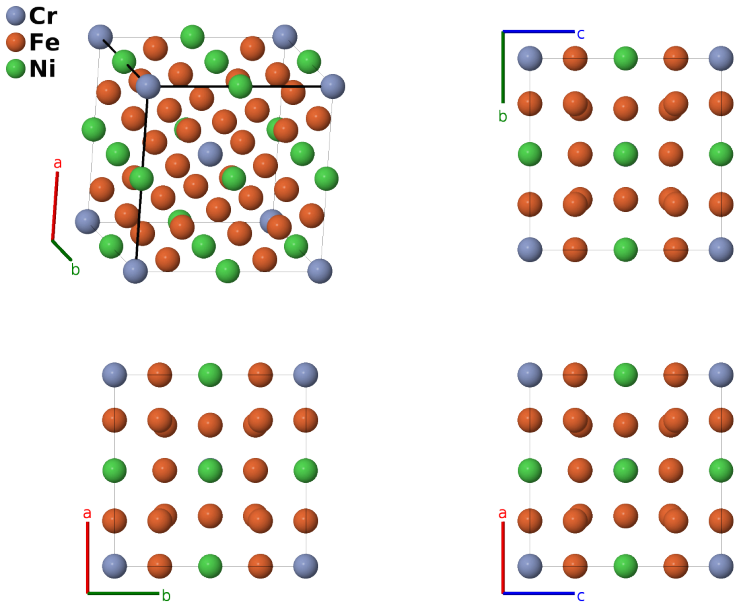
https://aflow.org/p/L6PB

https://aflow.org/p/AB12C3_cI32_229_a_h_b-001

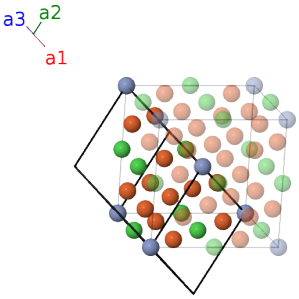


Prototype	$CrFe_{12}Ni_3$
AFLOW prototype label	AB12C3_cI32_229_a_h_b-001
ICSD	none
Pearson symbol	cI32
Space group number	229
Space group symbol	$Im\bar{3}m$
AFLOW prototype command	`aflow --proto=AB12C3_cI32_229_a_h_b-001 --params=`a, y_3

- Austenitic steels are alloys of iron and other metals with an averaged face-centered cubic structure. This model represents one approximation for an austenite steel. If we set $y_3 = 1/4$, the atoms are on the sites of an fcc lattice.

Body-centered Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Cr I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(6b)	Ni I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}}$	(6b)	Ni I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{z}}$	(6b)	Ni I
$\mathbf{B_5}$	=	$2y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + y_3\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{y}} + ay_3\,\hat{\mathbf{z}}$	(24h)	Fe I
$\mathbf{B_6}$	=	$y_3\,\mathbf{a}_2 - y_3\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{y}} + ay_3\,\hat{\mathbf{z}}$	(24h)	Fe I
$\mathbf{B_7}$	=	$-y_3\,\mathbf{a}_2 + y_3\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{y}} - ay_3\,\hat{\mathbf{z}}$	(24h)	Fe I
$\mathbf{B_8}$	=	$-2y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - y_3\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{y}} - ay_3\,\hat{\mathbf{z}}$	(24h)	Fe I
$\mathbf{B_9}$	=	$y_3\,\mathbf{a}_1 + 2y_3\,\mathbf{a}_2 + y_3\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{z}}$	(24h)	Fe I
$\mathbf{B_{10}}$	=	$-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{z}}$	(24h)	Fe I
$\mathbf{B_{11}}$	=	$y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{z}}$	(24h)	Fe I
$\mathbf{B_{12}}$	=	$-y_3\,\mathbf{a}_1 - 2y_3\,\mathbf{a}_2 - y_3\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{z}}$	(24h)	Fe I
$\mathbf{B_{13}}$	=	$y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + 2y_3\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}}$	(24h)	Fe I
$\mathbf{B_{14}}$	=	$y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2$	=	$-ay_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}}$	(24h)	Fe I
$\mathbf{B_{15}}$	=	$-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2$	=	$ay_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}}$	(24h)	Fe I
$\mathbf{B_{16}}$	=	$-y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - 2y_3\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}}$	(24h)	Fe I

References

[1] M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW library of crystallographic prototypes: part 1*, Comput. Mater. Sci. **136**, S1–S828 (2017), doi:10.1016/j.commatsci.2017.01.017.