Model of Austenite Structure (cF108): AB18C8_cF108_225_a_eh_f-001

This structure originally had the label `AB18C8_cF108_225_a_eh_f`. Calls to that address will be redirected here.

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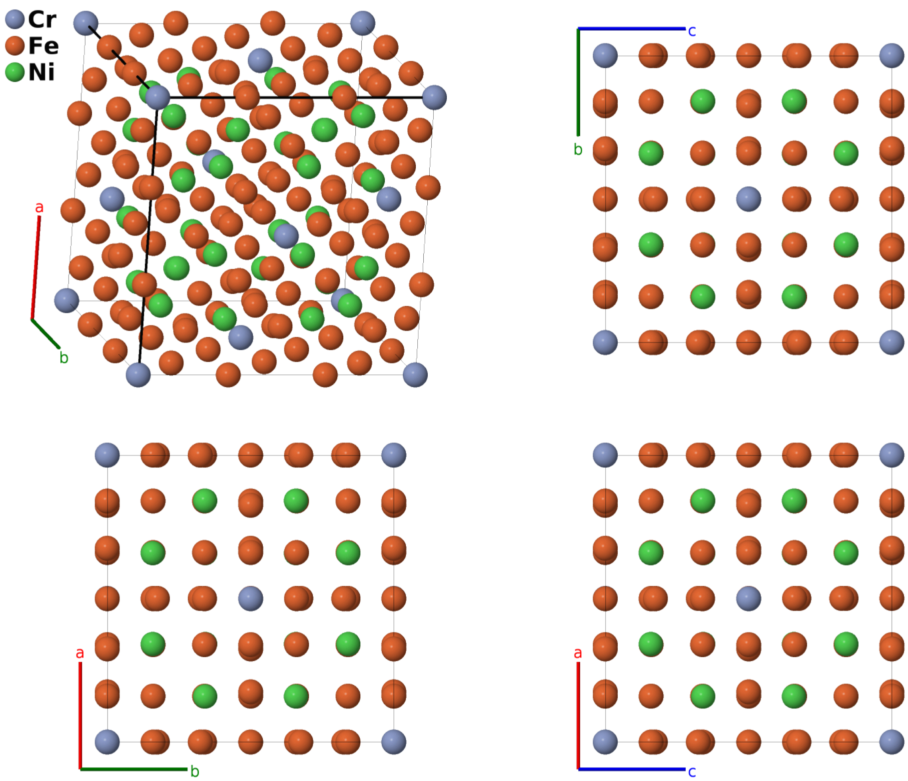
https://aflow.org/p/VR5Q

https://aflow.org/p/AB18C8_cF108_225_a_eh_f-001

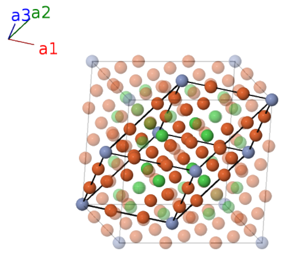


Prototype	$CrFe_{18}MoNi_8$
AFLOW prototype label	AB18C8_cF108_225_a_eh_f-001
ICSD	none
Pearson symbol	cF108
Space group number	225
Space group symbol	$Fm\overline{3}m$
AFLOW prototype command	`aflow --proto=AB18C8_cF108_225_a_eh_f-001` `--params=`a, x_2, x_3, y_4

- 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 $x_2 = 1/3$, $x_3 = 2/3$, and $y_4 = 2/3$, the atoms are on the sites of an fcc lattice with lattice constant $a_{fcc} = a/3$.

Face-centered Cubic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$ =	0	=	0	(4a)	Cr I
$\mathbf{B_2}$ =	$-x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\mathbf{\hat{x}}$	(24e)	Fe I
$\mathbf{B_3}$ =	$x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\mathbf{\hat{x}}$	(24e)	Fe I
$\mathbf{B_4}$ =	$x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\mathbf{\hat{y}}$	(24e)	Fe I
$\mathbf{B_5}$ =	$-x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\mathbf{\hat{y}}$	(24e)	Fe I
$\mathbf{B_6}$ =	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$ax_2\,\mathbf{\hat{z}}$	(24e)	Fe I
$\mathbf{B_7}$ =	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$-ax_2\,\mathbf{\hat{z}}$	(24e)	Fe I
$\mathbf{B_8}$ =	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\mathbf{\hat{x}} + ax_3\,\mathbf{\hat{y}} + ax_3\,\mathbf{\hat{z}}$	(32f)	Ni I
$\mathbf{B_9}$ =	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - 3x_3\,\mathbf{a}_3$	=	$-ax_3\,\mathbf{\hat{x}} - ax_3\,\mathbf{\hat{y}} + ax_3\,\mathbf{\hat{z}}$	(32f)	Ni I
$\mathbf{B_{10}}$ =	$x_3\,\mathbf{a}_1 - 3x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-ax_3\,\mathbf{\hat{x}} + ax_3\,\mathbf{\hat{y}} - ax_3\,\mathbf{\hat{z}}$	(32f)	Ni I
$\mathbf{B_{11}}$ =	$-3x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\mathbf{\hat{x}} - ax_3\,\mathbf{\hat{y}} - ax_3\,\mathbf{\hat{z}}$	(32f)	Ni I
$\mathbf{B_{12}}$ =	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + 3x_3\,\mathbf{a}_3$	=	$ax_3\,\mathbf{\hat{x}} + ax_3\,\mathbf{\hat{y}} - ax_3\,\mathbf{\hat{z}}$	(32f)	Ni I
$\mathbf{B_{13}}$ =	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\mathbf{\hat{x}} - ax_3\,\mathbf{\hat{y}} - ax_3\,\mathbf{\hat{z}}$	(32f)	Ni I
$\mathbf{B_{14}}$ =	$-x_3\,\mathbf{a}_1 + 3x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$ax_3\,\mathbf{\hat{x}} - ax_3\,\mathbf{\hat{y}} + ax_3\,\mathbf{\hat{z}}$	(32f)	Ni I
$\mathbf{B_{15}}$ =	$3x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\mathbf{\hat{x}} + ax_3\,\mathbf{\hat{y}} + ax_3\,\mathbf{\hat{z}}$	(32f)	Ni I
$\mathbf{B_{16}}$ =	$2y_4\,\mathbf{a}_1$	=	$ay_4\,\mathbf{\hat{y}} + ay_4\,\mathbf{\hat{z}}$	(48h)	Fe II
$\mathbf{B_{17}}$ =	$2y_4\,\mathbf{a}_2 - 2y_4\,\mathbf{a}_3$	=	$-ay_4\,\mathbf{\hat{y}} + ay_4\,\mathbf{\hat{z}}$	(48h)	Fe II
$\mathbf{B_{18}}$ =	$-2y_4\,\mathbf{a}_2 + 2y_4\,\mathbf{a}_3$	=	$ay_4\,\mathbf{\hat{y}} - ay_4\,\mathbf{\hat{z}}$	(48h)	Fe II
$\mathbf{B_{19}}$ =	$-2y_4\,\mathbf{a}_1$	=	$-ay_4\,\mathbf{\hat{y}} - ay_4\,\mathbf{\hat{z}}$	(48h)	Fe II
$\mathbf{B_{20}}$ =	$2y_4\,\mathbf{a}_2$	=	$ay_4\,\mathbf{\hat{x}} + ay_4\,\mathbf{\hat{z}}$	(48h)	Fe II
$\mathbf{B_{21}}$ =	$-2y_4\,\mathbf{a}_1 + 2y_4\,\mathbf{a}_3$	=	$ay_4\,\mathbf{\hat{x}} - ay_4\,\mathbf{\hat{z}}$	(48h)	Fe II
$\mathbf{B_{22}}$ =	$2y_4\,\mathbf{a}_1 - 2y_4\,\mathbf{a}_3$	=	$-ay_4\,\mathbf{\hat{x}} + ay_4\,\mathbf{\hat{z}}$	(48h)	Fe II
$\mathbf{B_{23}}$ =	$-2y_4\,\mathbf{a}_2$	=	$-ay_4\,\mathbf{\hat{x}} - ay_4\,\mathbf{\hat{z}}$	(48h)	Fe II
$\mathbf{B_{24}}$ =	$2y_4\,\mathbf{a}_3$	=	$ay_4\,\mathbf{\hat{x}} + ay_4\,\mathbf{\hat{y}}$	(48h)	Fe II
$\mathbf{B_{25}}$ =	$2y_4\,\mathbf{a}_1 - 2y_4\,\mathbf{a}_2$	=	$-ay_4\,\mathbf{\hat{x}} + ay_4\,\mathbf{\hat{y}}$	(48h)	Fe II
$\mathbf{B_{26}}$ =	$-2y_4\,\mathbf{a}_1 + 2y_4\,\mathbf{a}_2$	=	$ay_4\,\mathbf{\hat{x}} - ay_4\,\mathbf{\hat{y}}$	(48h)	Fe II
$\mathbf{B_{27}}$ =	$-2y_4\,\mathbf{a}_3$	=	$-ay_4\,\mathbf{\hat{x}} - ay_4\,\mathbf{\hat{y}}$	(48h)	Fe II

References

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