Model of Austenite Structure (cP32): AB27CD3_cP32_221_a_dij_b_c-001

This structure originally had the label `AB27CD3_cP32_221_a_dij_b_c`. Calls to that address will be redirected here.

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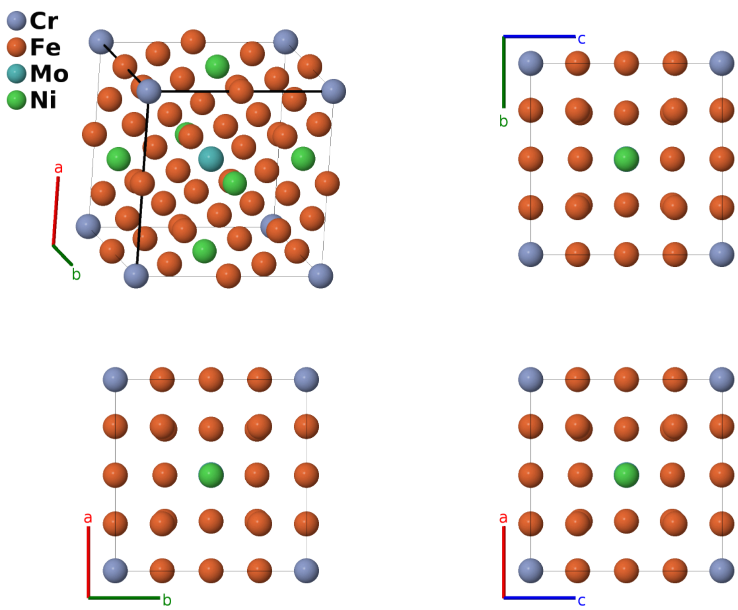
https://aflow.org/p/3F7M

https://aflow.org/p/AB27CD3_cP32_221_a_dij_b_c-001

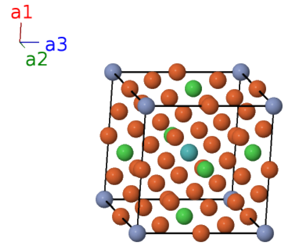


Prototype	$CrFe_{27}MoNi_3$
AFLOW prototype label	AB27CD3_cP32_221_a_dij_b_c-001
ICSD	none
Pearson symbol	cP32
Space group number	221
Space group symbol	$Pm\bar{3}m$
AFLOW prototype command	`aflow --proto=AB27CD3_cP32_221_a_dij_b_c-001 --params=`a, y_5, y_6

- 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. It is not meant to represent a real steel, and the selection of atom types for each Wyckoff position is arbitrary. When $y_5 = y_6 = 1/4$ all the atoms are on sites of a bcc lattice.

Simple Cubic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = a\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Cr I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(1b)	Mo I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(3c)	Ni I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(3c)	Ni I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(3c)	Ni I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(3d)	Fe I
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{y}}$	(3d)	Fe I
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{z}}$	(3d)	Fe I
$\mathbf{B_9}$	=	$y_5\,\mathbf{a}_2 + y_5\,\mathbf{a}_3$	=	$ay_5\,\hat{\mathbf{y}} + ay_5\,\hat{\mathbf{z}}$	(12i)	Fe II
$\mathbf{B_{10}}$	=	$-y_5\,\mathbf{a}_2 + y_5\,\mathbf{a}_3$	=	$-ay_5\,\hat{\mathbf{y}} + ay_5\,\hat{\mathbf{z}}$	(12i)	Fe II
$\mathbf{B_{11}}$	=	$y_5\,\mathbf{a}_2 - y_5\,\mathbf{a}_3$	=	$ay_5\,\hat{\mathbf{y}} - ay_5\,\hat{\mathbf{z}}$	(12i)	Fe II
$\mathbf{B_{12}}$	=	$-y_5\,\mathbf{a}_2 - y_5\,\mathbf{a}_3$	=	$-ay_5\,\hat{\mathbf{y}} - ay_5\,\hat{\mathbf{z}}$	(12i)	Fe II
$\mathbf{B_{13}}$	=	$y_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_3$	=	$ay_5\,\hat{\mathbf{x}} + ay_5\,\hat{\mathbf{z}}$	(12i)	Fe II
$\mathbf{B_{14}}$	=	$y_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_3$	=	$ay_5\,\hat{\mathbf{x}} - ay_5\,\hat{\mathbf{z}}$	(12i)	Fe II
$\mathbf{B_{15}}$	=	$-y_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_3$	=	$-ay_5\,\hat{\mathbf{x}} + ay_5\,\hat{\mathbf{z}}$	(12i)	Fe II
$\mathbf{B_{16}}$	=	$-y_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_3$	=	$-ay_5\,\hat{\mathbf{x}} - ay_5\,\hat{\mathbf{z}}$	(12i)	Fe II
$\mathbf{B_{17}}$	=	$y_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2$	=	$ay_5\,\hat{\mathbf{x}} + ay_5\,\hat{\mathbf{y}}$	(12i)	Fe II
$\mathbf{B_{18}}$	=	$-y_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2$	=	$-ay_5\,\hat{\mathbf{x}} + ay_5\,\hat{\mathbf{y}}$	(12i)	Fe II
$\mathbf{B_{19}}$	=	$y_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2$	=	$ay_5\,\hat{\mathbf{x}} - ay_5\,\hat{\mathbf{y}}$	(12i)	Fe II
$\mathbf{B_{20}}$	=	$-y_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2$	=	$-ay_5\,\hat{\mathbf{x}} - ay_5\,\hat{\mathbf{y}}$	(12i)	Fe II
$\mathbf{B_{21}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + y_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + ay_6\,\hat{\mathbf{y}} + ay_6\,\hat{\mathbf{z}}$	(12j)	Fe III
$\mathbf{B_{22}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + y_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - ay_6\,\hat{\mathbf{y}} + ay_6\,\hat{\mathbf{z}}$	(12j)	Fe III
$\mathbf{B_{23}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 - y_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + ay_6\,\hat{\mathbf{y}} - ay_6\,\hat{\mathbf{z}}$	(12j)	Fe III
$\mathbf{B_{24}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - y_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - ay_6\,\hat{\mathbf{y}} - ay_6\,\hat{\mathbf{z}}$	(12j)	Fe III
$\mathbf{B_{25}}$	=	$y_6\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + y_6\,\mathbf{a}_3$	=	$ay_6\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + ay_6\,\hat{\mathbf{z}}$	(12j)	Fe III
$\mathbf{B_{26}}$	=	$y_6\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - y_6\,\mathbf{a}_3$	=	$ay_6\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - ay_6\,\hat{\mathbf{z}}$	(12j)	Fe III
$\mathbf{B_{27}}$	=	$-y_6\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + y_6\,\mathbf{a}_3$	=	$-ay_6\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + ay_6\,\hat{\mathbf{z}}$	(12j)	Fe III
$\mathbf{B_{28}}$	=	$-y_6\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - y_6\,\mathbf{a}_3$	=	$-ay_6\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - ay_6\,\hat{\mathbf{z}}$	(12j)	Fe III
$\mathbf{B_{29}}$	=	$y_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ay_6\,\hat{\mathbf{x}} + ay_6\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(12j)	Fe III
$\mathbf{B_{30}}$	=	$-y_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ay_6\,\hat{\mathbf{x}} + ay_6\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(12j)	Fe III

$\mathbf{B_{31}}$	$=$	$y_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	$=$	$ay_6\,\hat{\mathbf{x}} - ay_6\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(12j)	Fe III
$\mathbf{B_{32}}$	$=$	$-y_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	$=$	$-ay_6\,\hat{\mathbf{x}} - ay_6\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(12j)	Fe III

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.