Model of Ferrite Structure (cF128): A9B16C7_cF128_225_acd_2f_be-001

This structure originally had the label `A9B16C7_cF128_225_acd_2f_be`. Calls to that address will be redirected here.

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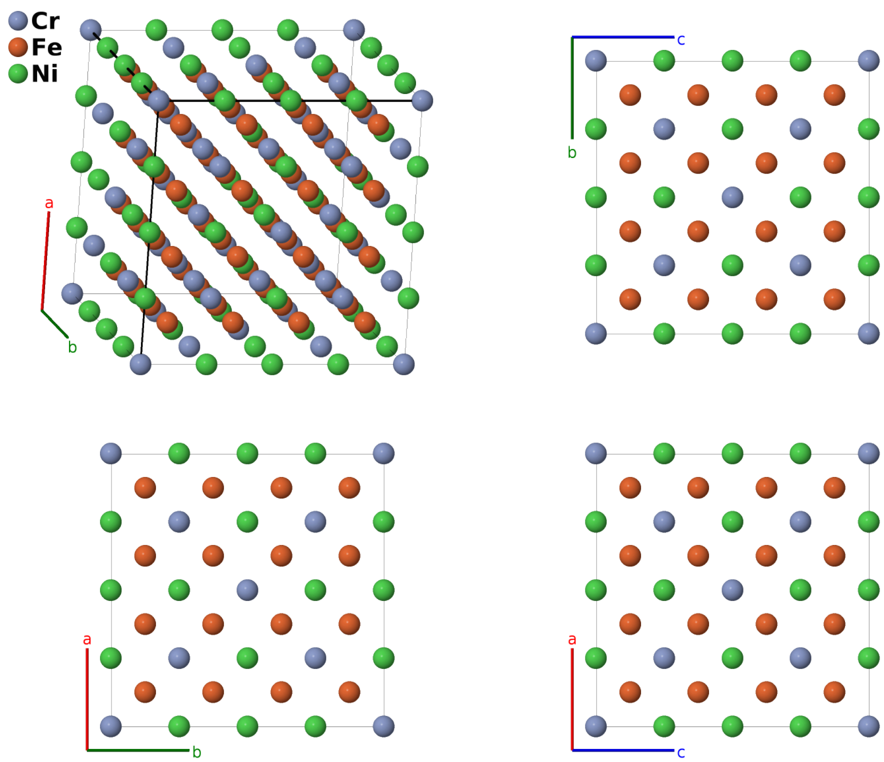
https://aflow.org/p/FENM

https://aflow.org/p/A9B16C7_cF128_225_acd_2f_be-001



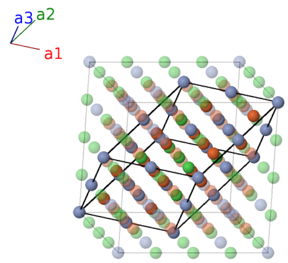
Prototype	$Cr_9Fe_{16}Ni_7$
AFLOW prototype label	A9B16C7_cF128_225_acd_2f_be-001
ICSD	none
Pearson symbol	cF128
Space group number	225
Space group symbol	$Fm\bar{3}m$
AFLOW prototype command	`aflow --proto=A9B16C7_cF128_225_acd_2f_be-001` `--params=`a, x_5, x_6, x_7

- Ferritic steels are alloys of iron and other metals with an averaged body-centered cubic structure. This model represents one approximation for a ferritic steel. It is not meant to represent a real steel, and the selection of atom types for each Wyckoff position is arbitrary.

- If we set $x_5 = 1/4, x_6 = 1/8$, and $x_7 = 3/8$ and replace the nickel atoms by chromium, this structure reverts to CsCl ($B2$) with $a_{B2} = 1/4a$.
- If we replace both the nickel and chromium atoms by iron the structure becomes a body-centered cubic lattice ($A2$) again with $a_{A2} = 1/4a$.

Face-centered Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	Cr I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(4b)	Ni I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(8c)	Cr II
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} + \frac{3}{4}a\,\hat{\mathbf{z}}$	(8c)	Cr II
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(24d)	Cr III
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(24d)	Cr III
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(24d)	Cr III
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(24d)	Cr III
$\mathbf{B_9}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}}$	(24d)	Cr III
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(24d)	Cr III
$\mathbf{B_{11}}$	=	$-x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}}$	(24e)	Ni II
$\mathbf{B_{12}}$	=	$x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}}$	(24e)	Ni II
$\mathbf{B_{13}}$	=	$x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{y}}$	(24e)	Ni II
$\mathbf{B_{14}}$	=	$-x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{y}}$	(24e)	Ni II
$\mathbf{B_{15}}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{z}}$	(24e)	Ni II
$\mathbf{B_{16}}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{z}}$	(24e)	Ni II
$\mathbf{B_{17}}$	=	$x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}} + ax_6\,\hat{\mathbf{z}}$	(32f)	Fe I
$\mathbf{B_{18}}$	=	$x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 - 3x_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}} + ax_6\,\hat{\mathbf{z}}$	(32f)	Fe I
$\mathbf{B_{19}}$	=	$x_6\,\mathbf{a}_1 - 3x_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}} - ax_6\,\hat{\mathbf{z}}$	(32f)	Fe I
$\mathbf{B_{20}}$	=	$-3x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}} - ax_6\,\hat{\mathbf{z}}$	(32f)	Fe I
$\mathbf{B_{21}}$	=	$-x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + 3x_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}} - ax_6\,\hat{\mathbf{z}}$	(32f)	Fe I
$\mathbf{B_{22}}$	=	$-x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 - x_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}} - ax_6\,\hat{\mathbf{z}}$	(32f)	Fe I
$\mathbf{B_{23}}$	=	$-x_6\,\mathbf{a}_1 + 3x_6\,\mathbf{a}_2 - x_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}} + ax_6\,\hat{\mathbf{z}}$	(32f)	Fe I
$\mathbf{B_{24}}$	=	$3x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 - x_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}} + ax_6\,\hat{\mathbf{z}}$	(32f)	Fe I
$\mathbf{B_{25}}$	=	$x_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} + ax_7\,\hat{\mathbf{z}}$	(32f)	Fe II

$\mathbf{B_{26}}$	=	$x_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 - 3x_7\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} + ax_7\,\hat{\mathbf{z}}$	(32f)	Fe II
$\mathbf{B_{27}}$	=	$x_7\,\mathbf{a}_1 - 3x_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} - ax_7\,\hat{\mathbf{z}}$	(32f)	Fe II
$\mathbf{B_{28}}$	=	$-3x_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} - ax_7\,\hat{\mathbf{z}}$	(32f)	Fe II
$\mathbf{B_{29}}$	=	$-x_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 + 3x_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} - ax_7\,\hat{\mathbf{z}}$	(32f)	Fe II
$\mathbf{B_{30}}$	=	$-x_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 - x_7\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} - ax_7\,\hat{\mathbf{z}}$	(32f)	Fe II
$\mathbf{B_{31}}$	=	$-x_7\,\mathbf{a}_1 + 3x_7\,\mathbf{a}_2 - x_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} + ax_7\,\hat{\mathbf{z}}$	(32f)	Fe II
$\mathbf{B_{32}}$	=	$3x_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 - x_7\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} + ax_7\,\hat{\mathbf{z}}$	(32f)	Fe II

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.