Ga_4Ni Structure: A4B_cI40_197_cde_c-001

This structure originally had the label `A4B_cI40_197_cde_c`. Calls to that address will be redirected here.

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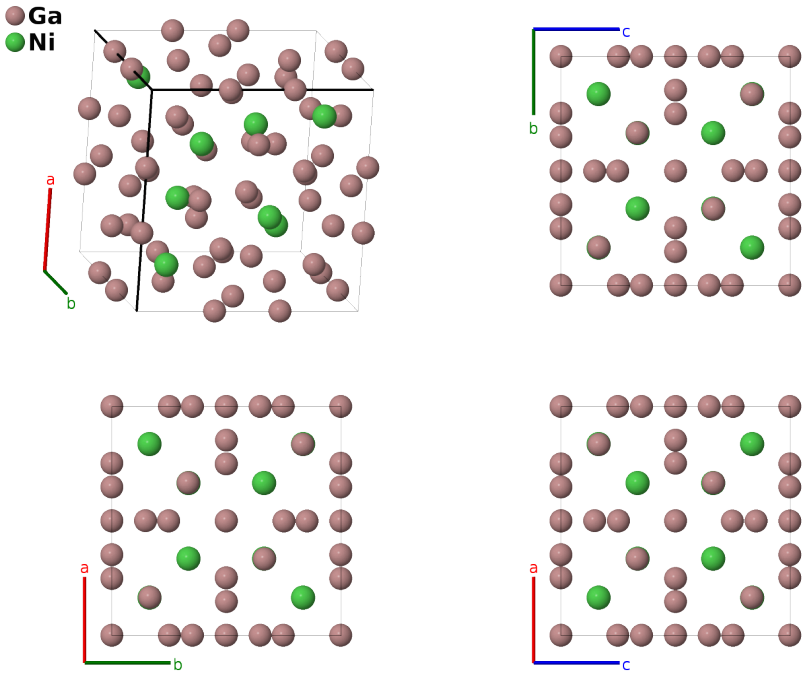
https://aflow.org/p/PBV9

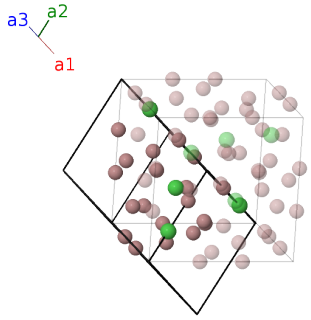
https://aflow.org/p/A4B_cI40_197_cde_c-001



Prototype	Ga_4Ni
AFLOW prototype label	A4B_cI40_197_cde_c-001
ICSD	103863
Pearson symbol	cI40
Space group number	197
Space group symbol	$I23$
AFLOW prototype command	`aflow --proto=A4B_cI40_197_cde_c-001 --params=`a, x_1, x_2, x_3, x_4

Body-centered Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$2x_1\,\mathbf{a}_1 + 2x_1\,\mathbf{a}_2 + 2x_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}} + ax_1\,\hat{\mathbf{z}}$	(8c)	Ga I
$\mathbf{B_2}$	=	$-2x_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} - ax_1\,\hat{\mathbf{y}} + ax_1\,\hat{\mathbf{z}}$	(8c)	Ga I
$\mathbf{B_3}$	=	$-2x_1\,\mathbf{a}_2$	=	$-ax_1\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}} - ax_1\,\hat{\mathbf{z}}$	(8c)	Ga I
$\mathbf{B_4}$	=	$-2x_1\,\mathbf{a}_1$	=	$ax_1\,\hat{\mathbf{x}} - ax_1\,\hat{\mathbf{y}} - ax_1\,\hat{\mathbf{z}}$	(8c)	Ga I
$\mathbf{B_5}$	=	$2x_2\,\mathbf{a}_1 + 2x_2\,\mathbf{a}_2 + 2x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(8c)	Ni I
$\mathbf{B_6}$	=	$-2x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(8c)	Ni I
$\mathbf{B_7}$	=	$-2x_2\,\mathbf{a}_2$	=	$-ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(8c)	Ni I
$\mathbf{B_8}$	=	$-2x_2\,\mathbf{a}_1$	=	$ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(8c)	Ni I
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}}$	(12d)	Ga II
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}}$	(12d)	Ga II
$\mathbf{B_{11}}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{y}}$	(12d)	Ga II
$\mathbf{B_{12}}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{y}}$	(12d)	Ga II
$\mathbf{B_{13}}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2$	=	$ax_3\,\hat{\mathbf{z}}$	(12d)	Ga II
$\mathbf{B_{14}}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{z}}$	(12d)	Ga II
$\mathbf{B_{15}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(12e)	Ga III
$\mathbf{B_{16}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(12e)	Ga III
$\mathbf{B_{17}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(12e)	Ga III
$\mathbf{B_{18}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(12e)	Ga III
$\mathbf{B_{19}}$	=	$x_4\,\mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{z}}$	(12e)	Ga III
$\mathbf{B_{20}}$	=	$-x_4\,\mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{z}}$	(12e)	Ga III

References

[1] L. Jingkui and X. Sishen, *The Structure of $NiGa_4$ Crystal – A New Vacancy Controlled γ-Brass Phase*, Scientia Sinica, Series A **26**, 1305–1313 (1983).

Found in

[1] P. Villars and L. Calvert, *Pearson's Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OH, 1991), 2nd edn.