Y-MgNiSn Structure: A7B7C2_tP32_101_ade_bde_d-001

This structure originally had the label `A7B7C2_tP32_101_bde_ade_d`. Calls to that address will be redirected here.

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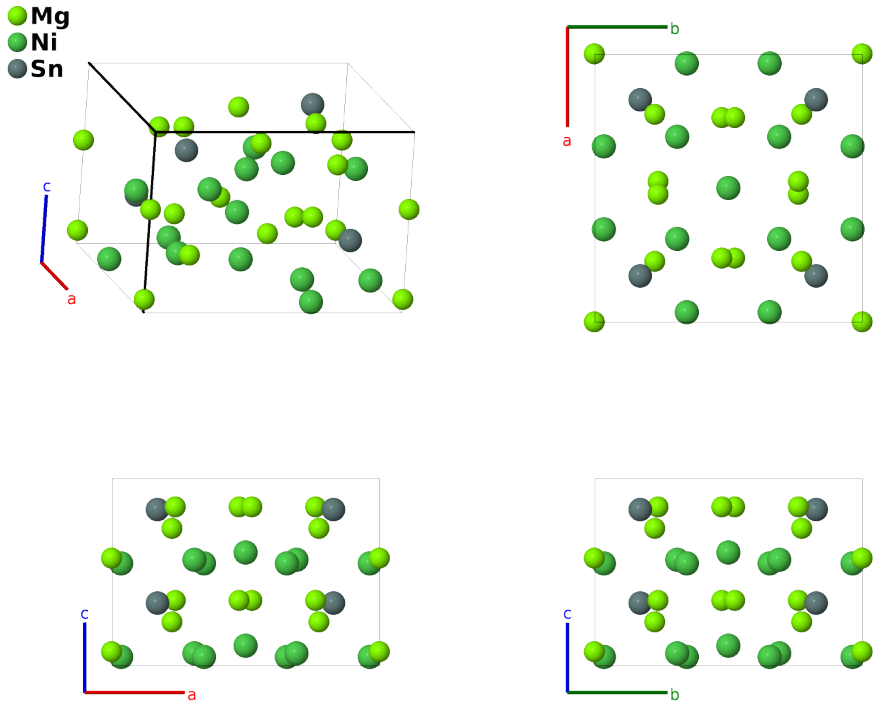
https://aflow.org/p/LR8K

https://aflow.org/p/A7B7C2_tP32_101_ade_bde_d-001



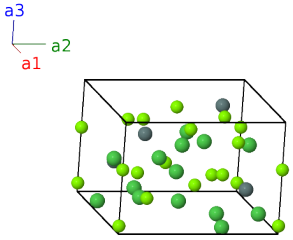
Prototype	MgNiSn
AFLOW prototype label	A7B7C2_tP32_101_ade_bde_d-001
ICSD	99208
Pearson symbol	tP32
Space group number	101
Space group symbol	$P4_2cm$
AFLOW prototype command	`aflow --proto=A7B7C2_tP32_101_ade_bde_d-001 --params=`$a, c/a, z_1, z_2, x_3, z_3, x_4, z_4, x_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7$

- This is the Y-phase of the Mg-Ni-Sn ternary system. The (2b), (4d) and (8e) Wyckoff positions are partially occupied and are represented by the labels M-I, M-II, and M-III, respectively. Here, M-I is $Mg_{0.88}Ni_{0.12}$, which we label "Ni", M-II is $Sn_{0.88}Mg_{0.12}$ labeled "Sn", and M-III is $Mg_{0.95}Ni_{0.05}$, labeled "Ni", with the supposed element names picked to highlight the different Wyckoff positions.

- We previously referred to this as the γ-phase, but Y-phase is the proper terminology (Boudard, 2004).

Simple Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(2a)	Mg I
$\mathbf{B_2}$	=	$\left(z_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(z_1+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	Mg I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1+\frac{1}{2}\,\mathbf{a}_2+z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{1}{2}a\,\hat{\mathbf{y}}+cz_2\,\hat{\mathbf{z}}$	(2b)	Ni I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1+\frac{1}{2}\,\mathbf{a}_2+\left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{1}{2}a\,\hat{\mathbf{y}}+c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	Ni I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1+x_3\,\mathbf{a}_2+z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}}+ax_3\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(4d)	Mg II
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1-x_3\,\mathbf{a}_2+z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}}-ax_3\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(4d)	Mg II
$\mathbf{B_7}$	=	$-x_3\,\mathbf{a}_1+x_3\,\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}}+ax_3\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4d)	Mg II
$\mathbf{B_8}$	=	$x_3\,\mathbf{a}_1-x_3\,\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}}-ax_3\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4d)	Mg II
$\mathbf{B_9}$	=	$x_4\,\mathbf{a}_1+x_4\,\mathbf{a}_2+z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}}+ax_4\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(4d)	Ni II
$\mathbf{B_{10}}$	=	$-x_4\,\mathbf{a}_1-x_4\,\mathbf{a}_2+z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}}-ax_4\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(4d)	Ni II
$\mathbf{B_{11}}$	=	$-x_4\,\mathbf{a}_1+x_4\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}}+ax_4\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4d)	Ni II
$\mathbf{B_{12}}$	=	$x_4\,\mathbf{a}_1-x_4\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}}-ax_4\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4d)	Ni II
$\mathbf{B_{13}}$	=	$x_5\,\mathbf{a}_1+x_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}}+ax_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(4d)	Sn I
$\mathbf{B_{14}}$	=	$-x_5\,\mathbf{a}_1-x_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}}-ax_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(4d)	Sn I
$\mathbf{B_{15}}$	=	$-x_5\,\mathbf{a}_1+x_5\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}}+ax_5\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4d)	Sn I
$\mathbf{B_{16}}$	=	$x_5\,\mathbf{a}_1-x_5\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}}-ax_5\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4d)	Sn I
$\mathbf{B_{17}}$	=	$x_6\,\mathbf{a}_1+y_6\,\mathbf{a}_2+z_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}}+ay_6\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}}$	(8e)	Mg III
$\mathbf{B_{18}}$	=	$-x_6\,\mathbf{a}_1-y_6\,\mathbf{a}_2+z_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}}-ay_6\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}}$	(8e)	Mg III
$\mathbf{B_{19}}$	=	$-y_6\,\mathbf{a}_1+x_6\,\mathbf{a}_2+\left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_6\,\hat{\mathbf{x}}+ax_6\,\hat{\mathbf{y}}+c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8e)	Mg III
$\mathbf{B_{20}}$	=	$y_6\,\mathbf{a}_1-x_6\,\mathbf{a}_2+\left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ay_6\,\hat{\mathbf{x}}-ax_6\,\hat{\mathbf{y}}+c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8e)	Mg III
$\mathbf{B_{21}}$	=	$x_6\,\mathbf{a}_1-y_6\,\mathbf{a}_2+\left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}}-ay_6\,\hat{\mathbf{y}}+c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8e)	Mg III
$\mathbf{B_{22}}$	=	$-x_6\,\mathbf{a}_1+y_6\,\mathbf{a}_2+\left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}}+ay_6\,\hat{\mathbf{y}}+c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8e)	Mg III
$\mathbf{B_{23}}$	=	$-y_6\,\mathbf{a}_1-x_6\,\mathbf{a}_2+z_6\,\mathbf{a}_3$	=	$-ay_6\,\hat{\mathbf{x}}-ax_6\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}}$	(8e)	Mg III
$\mathbf{B_{24}}$	=	$y_6\,\mathbf{a}_1+x_6\,\mathbf{a}_2+z_6\,\mathbf{a}_3$	=	$ay_6\,\hat{\mathbf{x}}+ax_6\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}}$	(8e)	Mg III
$\mathbf{B_{25}}$	=	$x_7\,\mathbf{a}_1+y_7\,\mathbf{a}_2+z_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}}+ay_7\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}}$	(8e)	Ni III
$\mathbf{B_{26}}$	=	$-x_7\,\mathbf{a}_1-y_7\,\mathbf{a}_2+z_7\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}}-ay_7\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}}$	(8e)	Ni III
$\mathbf{B_{27}}$	=	$-y_7\,\mathbf{a}_1+x_7\,\mathbf{a}_2+\left(z_7+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_7\,\hat{\mathbf{x}}+ax_7\,\hat{\mathbf{y}}+c\left(z_7+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8e)	Ni III

$\mathbf{B_{28}}$	=	$y_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ay_7\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8e)	Ni III
$\mathbf{B_{29}}$	=	$x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} - ay_7\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8e)	Ni III
$\mathbf{B_{30}}$	=	$-x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} + ay_7\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8e)	Ni III
$\mathbf{B_{31}}$	=	$-y_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$-ay_7\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8e)	Ni III
$\mathbf{B_{32}}$	=	$y_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$ay_7\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8e)	Ni III

References

[1] M. Boudard, P. Bordet, H. Vincent, and F. Audebert, *The structure of the Y-phase in the Mg-Ni-Sn system*, J. Alloys Compd. **372**, 121–128 (2004), doi:10.1016/j.jallcom.2003.09.142.

Found in

[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.