NiTi Structure: AB_mP4_11_e_e-001

This structure originally had the label `AB_mP4_11_e_e`. Calls to that address will be redirected here.

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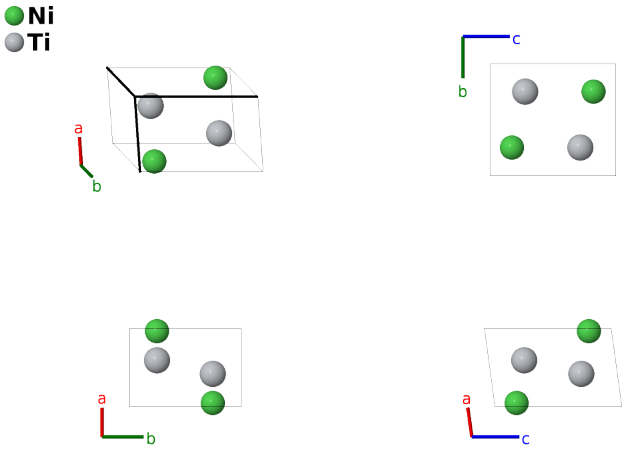
https://aflow.org/p/WBFX

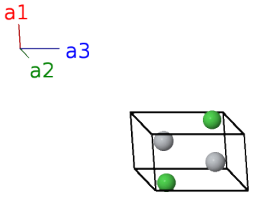
https://aflow.org/p/AB_mP4_11_e_e-001



Prototype	NiTi
AFLOW prototype label	AB_mP4_11_e_e-001
ICSD	157983
Pearson symbol	mP4
Space group number	11
Space group symbol	$P2_1/m$
AFLOW prototype command	`aflow --proto=AB_mP4_11_e_e-001 --params=`$a, b/a, c/a, \beta, x_1, z_1, x_2, z_2$

- (Sitepu, 2002) give the coordinates in the unique-axis c setting of space group $P2_1/m$ #11. We used FINDSYM to transform this to the standard unique-axis b setting. In our original version of this work we inadvertantly used 180° - β rather than β, and moved the nickel atoms by 1/2 c along the z-axis. These errors have been corrected here.

Simple Monoclinic primitive vectors



$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$

Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_1\sin\beta\,\hat{\mathbf{z}}$	(2e)	Ni I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_1\sin\beta\,\hat{\mathbf{z}}$	(2e)	Ni I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(2e)	Ti I
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_2\sin\beta\,\hat{\mathbf{z}}$	(2e)	Ti I

References

[1] H. Sitepu, W. W. Schmal, and J. K. Stalick, *Correction of intensities for preferred orientation in neutron-diffraction data of NiTi shape-memory alloy using the generalized spherical-harmonic description*, Appl. Phys. A **74**, S1719–S1721 (2002), doi:10.1007/s003390201840.

[2] 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.

Found in

[1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).