$TaTi_3$-I (BCC SQS-16) Structure: AB3_mC32_8_4a_12a-001

This structure originally had the label `AB3_mC32_8_4a_12a`. Calls to that address will be redirected here.

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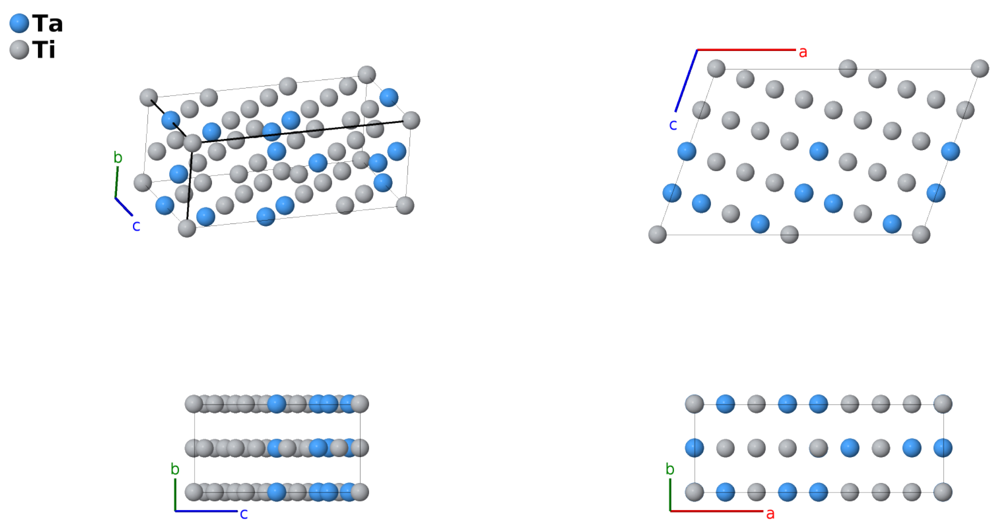
https://aflow.org/p/QVN8

https://aflow.org/p/AB3_mC32_8_4a_12a-001



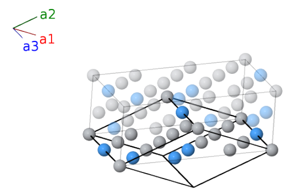
Prototype	$TaTi_3$
AFLOW prototype label	AB3_mC32_8_4a_12a-001
ICSD	none
Pearson symbol	mC32
Space group number	8
Space group symbol	Cm
AFLOW prototype command	`aflow --proto=AB3_mC32_8_4a_12a-001` `--params=`$a, b/a, c/a, \beta, x_1, z_1, x_2, z_2, x_3, z_3, x_4, z_4, x_5, z_5, x_6, z_6, x_7, z_7, x_8, z_8, x_9, z_9, x_{10}, z_{10}, x_{11}, z_{11}, x_{12}, z_{12}, x_{13}, z_{13}, x_{14}, z_{14}, x_{15}, z_{15}, x_{16}, z_{16}$

- This is a special quasirandom structure with 16 atoms per unit cell (SQS-16) for a bcc binary substitutional alloy A_xB_{1-x} (Jiang, 2004; Chakraborty, 2016)).
- Several compositions are available:
  - $TaTi_7$ (AB7_hR16_166_c_c2h),
  - Ta_3Ti_{13} (A3B13_oC32_38_ac_a2bcdef),
  - $TaTi_3$-I (AB3_mC32_8_4a_12a) (this structure),
  - $TaTi_3$-II (AB3_mC32_8_4a_4a4b) ,

– Ta_5Ti_{11} (A5B11_mP16_6_2abc_2a3b3c) ,
– Ta_3Ti_8 (A3B5_oC32_38_abce_abcdf) ,
– TaTi (AB_aP16_2_4i_4i).

Base-centered Monoclinic primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} + cz_1\sin\beta\,\hat{\mathbf{z}}$	(2a)	Ta I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(2a)	Ta II
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(2a)	Ta III
$\mathbf{B_4}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(2a)	Ta IV
$\mathbf{B_5}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(2a)	Ti I
$\mathbf{B_6}$	=	$x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(2a)	Ti II
$\mathbf{B_7}$	=	$x_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} + cz_7\sin\beta\,\hat{\mathbf{z}}$	(2a)	Ti III
$\mathbf{B_8}$	=	$x_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} + cz_8\sin\beta\,\hat{\mathbf{z}}$	(2a)	Ti IV
$\mathbf{B_9}$	=	$x_9\,\mathbf{a}_1 + x_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$(ax_9 + cz_9\cos\beta)\,\hat{\mathbf{x}} + cz_9\sin\beta\,\hat{\mathbf{z}}$	(2a)	Ti V
$\mathbf{B_{10}}$	=	$x_{10}\,\mathbf{a}_1 + x_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$(ax_{10} + cz_{10}\cos\beta)\,\hat{\mathbf{x}} + cz_{10}\sin\beta\,\hat{\mathbf{z}}$	(2a)	Ti VI
$\mathbf{B_{11}}$	=	$x_{11}\,\mathbf{a}_1 + x_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$(ax_{11} + cz_{11}\cos\beta)\,\hat{\mathbf{x}} + cz_{11}\sin\beta\,\hat{\mathbf{z}}$	(2a)	Ti VII
$\mathbf{B_{12}}$	=	$x_{12}\,\mathbf{a}_1 + x_{12}\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3$	=	$(ax_{12} + cz_{12}\cos\beta)\,\hat{\mathbf{x}} + cz_{12}\sin\beta\,\hat{\mathbf{z}}$	(2a)	Ti VIII
$\mathbf{B_{13}}$	=	$x_{13}\,\mathbf{a}_1 + x_{13}\,\mathbf{a}_2 + z_{13}\,\mathbf{a}_3$	=	$(ax_{13} + cz_{13}\cos\beta)\,\hat{\mathbf{x}} + cz_{13}\sin\beta\,\hat{\mathbf{z}}$	(2a)	Ti IX
$\mathbf{B_{14}}$	=	$x_{14}\,\mathbf{a}_1 + x_{14}\,\mathbf{a}_2 + z_{14}\,\mathbf{a}_3$	=	$(ax_{14} + cz_{14}\cos\beta)\,\hat{\mathbf{x}} + cz_{14}\sin\beta\,\hat{\mathbf{z}}$	(2a)	Ti X
$\mathbf{B_{15}}$	=	$x_{15}\,\mathbf{a}_1 + x_{15}\,\mathbf{a}_2 + z_{15}\,\mathbf{a}_3$	=	$(ax_{15} + cz_{15}\cos\beta)\,\hat{\mathbf{x}} + cz_{15}\sin\beta\,\hat{\mathbf{z}}$	(2a)	Ti XI
$\mathbf{B_{16}}$	=	$x_{16}\,\mathbf{a}_1 + x_{16}\,\mathbf{a}_2 + z_{16}\,\mathbf{a}_3$	=	$(ax_{16} + cz_{16}\cos\beta)\,\hat{\mathbf{x}} + cz_{16}\sin\beta\,\hat{\mathbf{z}}$	(2a)	Ti XII

References

[1] C. Jiang, C. Wolverton, J. Sofo, L.-Q. Chen, and Z.-K. Liu, *First-principles study of binary bcc alloys using special quasirandom structures*, Phys. Rev. B **69**, 214202 (2004), doi:10.1103/PhysRevB.69.214202.

[2] T. Chakraborty, J. Rogal, and R. Drautz, *Unraveling the composition dependence of the martensitic transformation temperature: A first-principles study of Ti-Ta alloys*, Phys. Rev. B **94**, 224104 (2016), doi:10.1103/PhysRevB.94.224104.