Al_3Ti ($D0_{22}$) Structure: A3B_tI8_139_ad_b-001

This structure originally had the label `A3B_tI8_139_bd_a`. Calls to that address will be redirected here.

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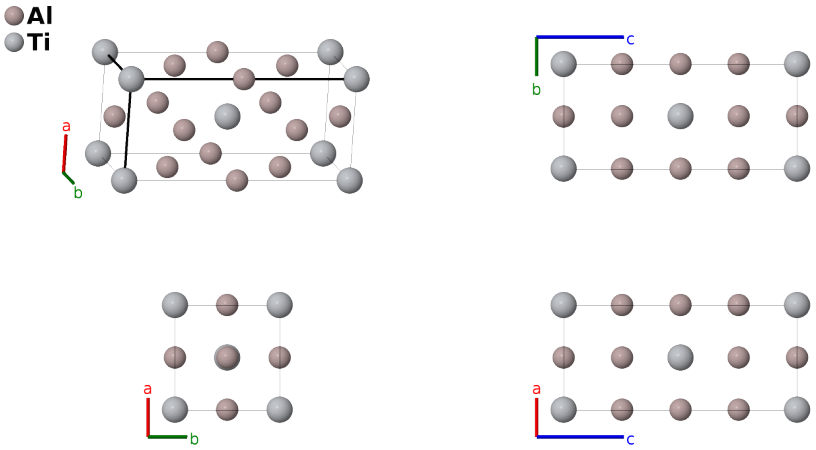
https://aflow.org/p/7W3W

https://aflow.org/p/A3B_tI8_139_ad_b-001



Prototype	Al_3Ti
AFLOW prototype label	A3B_tI8_139_ad_b-001
***Strukturbericht* designation**	$D0_{22}$
ICSD	58189
Pearson symbol	tI8
Space group number	139
Space group symbol	$I4/mmm$
AFLOW prototype command	`aflow --proto=A3B_tI8_139_ad_b-001 --params=`$a, c/a$

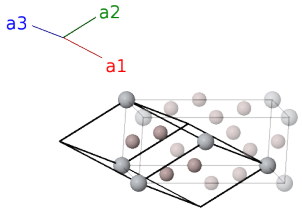
Other compounds with this structure

Al_3Hf, $Al_{3-x}Fe_xMo$, Al_3Nb, Al_3Sc, Al_3Ta, Al_3V, Ga_3Hf, Ga_3Nb, Ga_3Ti, α-$NbPd_3$, Ni_3V, Pd_3Nb, Pd_3Ta, Pd_3V, Pt_3V

- When $c = 2a$ the atoms are on the sites of a face-centered cubic lattice. When $c/a = 1/\sqrt{2}$, this becomes the cubic $D0_3$ structure.

Body-centered Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Al I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	Ti I
$\mathbf{B_3}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	Al II
$\mathbf{B_4}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	Al II

References

[1] P. Norby and N. Christensen, *Preparation and Structure of Al_3Ti*, Acta Chem. Scand. pp. 157–159 (1986), doi:10.3891/acta.chem.scand.40a-0157.

[2] J. Nic, S. Zhang, and D. Mikkola, *Observations on the systematic alloying of Al3Ti with fourth period elements to yield cubic phases*, Scripta Metallurgica et Materialia **24**, 1099–1104 (1990), doi:10.1016/0956-716X(90)90306-2.

Found in

[1] W. B. Pearson, *A Handbook of Lattice Spacings and Structures of Metals and Alloys, Volume 2*, *International Series of Monographs on Metal Physics and Physical Metallurgy*, vol. 8 (Pergamon Press, Oxford, London, Edinburgh, New York, Toronto, Sydney, Paris, Braunschweig, 1967).