γ-CuTi ($B11$) Structure: AB_tP4_129_c_c-001

This structure originally had the label `AB_tP4_129_c_c`. Calls to that address will be redirected here.

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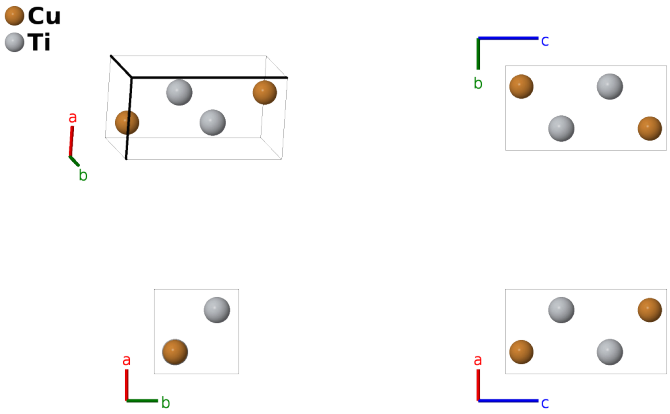
https://aflow.org/p/EKF2

https://aflow.org/p/AB_tP4_129_c_c-001



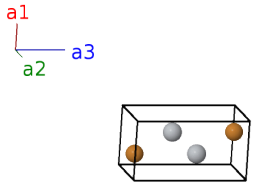
Prototype	CuTi
AFLOW prototype label	AB_tP4_129_c_c-001
***Strukturbericht* designation**	$B11$
ICSD	629389
Pearson symbol	tP4
Space group number	129
Space group symbol	$P4/nmm$
AFLOW prototype command	`aflow --proto=AB_tP4_129_c_c-001 --params=`$a, c/a, z_1, z_2$

Other compounds with this structure
AgZr, AlRe, AuCu, AuHf, AuMn, AuTi, HgPd, PdTa, SZr, TlF-I (high-temperature)

- When $c = 2a$, $z_1 = 1/8$, and $z_2 = 5/8$, the atoms are on the sites of a body-centered cubic lattice. If, on the other hand, $c = 2\sqrt{2a}$, with the same z_i, the atoms are on the site of a face-centered cubic lattice. This is the phase that (Lu, 1991) refer to as "Z2".

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
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(2c)	Cu I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(2c)	Cu I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2c)	Ti I
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(2c)	Ti I

References

[1] V. N. Eremenko, Y. I. Buyanov, and S. B. Prima, *Phase diagram of the system titanium-copper*, Soviet Powder Metallurgy and Metal Ceramics **5**, 494–502 (1966), doi:10.1007/BF00775543.

[2] Z. W. Lu, S.-H. Wei, and A. Zunger, *Long-Range Order in Binary Late-Transition-Metal Alloys*, Phys. Rev. Lett. **66**, 1753–1756 (1991), doi:10.1103/PhysRevLett.66.1753.

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.