Hypothetical BCT5 Si Structure: A_tI4_139_e-001

This structure originally had the label `A_tI4_139_e`. Calls to that address will be redirected here.

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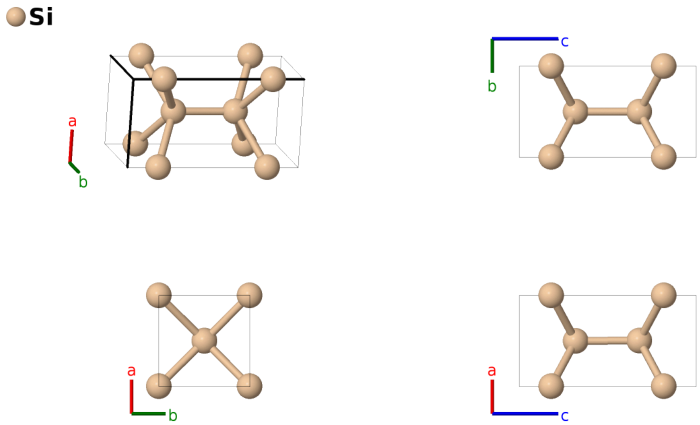
https://aflow.org/p/ZSDQ

https://aflow.org/p/A_tI4_139_e-001



Prototype Si

AFLOW prototype label A_tI4_139_e-001

ICSD none

Pearson symbol tI4

Space group number 139

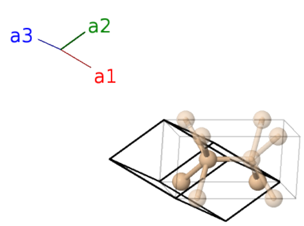
Space group symbol $I4/mmm$

AFLOW prototype command `aflow --proto=A_tI4_139_e-001 --params=`$a, c/a, z_1$

- The bct5 structure is a tetragonal analog of the diamond ($A4$) structure, with 5-fold coordination. It was proposed in (Boyer, 1991) as a low-energy metastable phase of silicon, based on first-principles calculations and model potentials. (Gerbig, 2012) found evidence of this structure in strained silicon.

Body-centered Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_1 + z_1\,\mathbf{a}_2$	=	$cz_1\,\hat{\mathbf{z}}$	(4e)	Si I
$\mathbf{B_2}$	=	$-z_1\,\mathbf{a}_1 - z_1\,\mathbf{a}_2$	=	$-cz_1\,\hat{\mathbf{z}}$	(4e)	Si I

References

[1] L. L. Boyer, E. Kaxiras, J. L. Feldman, J. Q. Broughton, and M. J. Mehl, *New low-energy crystal structure for silicon*, Phys. Rev. Lett. **67**, 715–718 (1991), doi:10.1103/PhysRevLett.67.715.

[2] Y. B. Gerbig, C. A. Michaels, A. M. Forster, and R. F. Cook, *In situ observation of the indentation-induced phase transformation of silicon thin films*, Phys. Rev. B **85**, 104102 (2012), doi:10.1103/PhysRevB.85.104102.