

Home Assignment 3

Group Theory 07

The diamond crystal structure belongs to the space group #227, i.e. a non-symmorphic group based on a face centered cubic (fcc) Bravais lattice (in Cartesian coordinates)

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}(\hat{x} + \hat{y})a \\ \mathbf{a}_2 &= \frac{1}{2}(\hat{y} + \hat{z})a \\ \mathbf{a}_3 &= \frac{1}{2}(\hat{z} + \hat{x})a,\end{aligned}$$

where a is the so-called lattice constant. In addition the diamond structure is defined through its basis that consists of two equivalent atomic sites,

$$\begin{aligned}\mathbf{b}_1 &= \mathbf{0} \\ \mathbf{b}_2 &= \frac{1}{4}(\mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3).\end{aligned}$$

- One of the generators of the space group is $\{c_4 | (-\frac{1}{4}, \frac{1}{4}, \frac{1}{4})\}$, where the non-trivial translation is expressed in terms of the unit vectors of the Bravais lattice ($\{\mathbf{a}_i\}$). Verify that this is a symmetry operation and describe where the screw axis is positioned in the crystal. Hint: it might be easier to visualize when the translation is expressed in Cartesian coordinates.
- Which is the isogonal point group? (Do not hesitate to study existing tables.)
- What is the little co-group and star of the wave vector $\Gamma \equiv (000)$ (Cartesian coordinates)?

d) What is the little co-group and star of the wave vector
(0.1777 0.2345 0.3678) (Cartesian coordinates)?