

Problem 3: Band structure of Antimony

Elemental antimony is a metal with a rhombohedral unit cell and two atoms per cell. In this exercise we plot the electronic band structure of metallic antimony using the empirical pseudopotential method of Cohen and Bergstresser (CB).

Antimony has the same structure as arsenic (see the text of the corresponding exercise) but here we describe it by a rhombohedral Bravais lattice whose three-fold symmetry axis is along z . The rhombohedral lattice has the following primitive vectors:

$$\begin{aligned}\mathbf{a}_1 &= a\left(\frac{\sqrt{3}}{2}\sin\theta, -\frac{1}{2}\sin\theta, \cos\theta\right), \\ \mathbf{a}_2 &= a(0, \sin\theta, \cos\theta), \\ \mathbf{a}_3 &= a\left(-\frac{\sqrt{3}}{2}\sin\theta, -\frac{1}{2}\sin\theta, \cos\theta\right),\end{aligned}$$

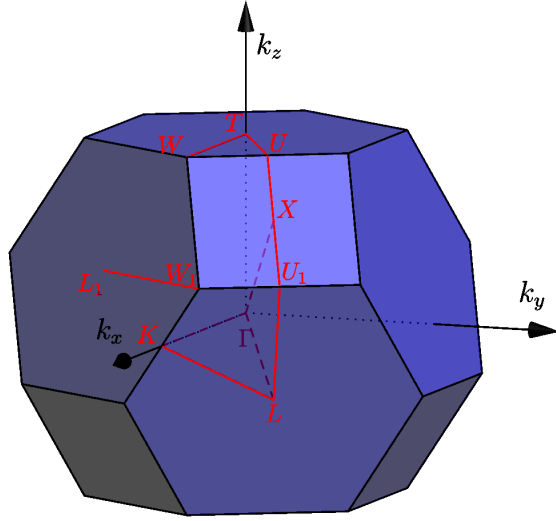
where $a = 8.486$ a.u., $\cos\theta = \frac{1}{\sqrt{3}}\sqrt{1+2\cos\alpha}$, $\sin\theta = \sqrt{\frac{2}{3}}\sqrt{1-\cos\alpha}$ and $\alpha = 57.23^\circ$. The atoms inside the unit cell are at $\mathbf{d}_{1,2} = \pm u\mathbf{d}$ where $\mathbf{d} = \mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3$ and $u = 0.2336$.

In order to apply the empirical pseudopotential method we need the form factors for arbitrary values of the reciprocal lattice vectors $|\mathbf{G}|^2$ and we can use the function:

$$U(|\mathbf{G}|^2) = \frac{A_1(|\mathbf{G}|^2 - A_2)}{e^{A_3(|\mathbf{G}|^2 - A_4)} + 1} \quad (1)$$

with $A_1 = 0.0782$, $A_2 = 2.367$, $A_3 = 3.260$, $A_4 = 2.803$. With these values of the parameters and \mathbf{G} vectors in atomic units (1/bohr), the form factors are in Hartree.

1. Show that the angle between any two vectors \mathbf{a}_1 , \mathbf{a}_2 , and \mathbf{a}_3 is α .
2. Modify the CB program in order to use Eq. 1 and to introduce the positions of the atoms in the unit cell of antimony.
3. Modify the CB program in order to calculate the reciprocal lattice vectors of the rhombohedral lattice of antimony. The Brillouin zone is shown in the figure. Find the coordinates of the points Γ , X , L , L_1 , T , W , W_1 , U , U_1 and K :



(Hint: The coordinates of each vertex of the BZ can be determined analytically as the solution of a 3×3 linear system, but you can also solve the linear system numerically using for instance the `Lapack` routine `DGESV`).

4. Show that only the hexagonal faces perpendicular to the k_z axis are regular and compute the side of the hexagon. The other hexagonal faces have sides of two different lengths that are also the sizes of the six rectangles. Find these two lengths.
5. To the points calculated before add the points $X_1 = (1.0127, 0, 0)$ and $H = (0.1542, -0.0890, 0.3534)$ (in units $\frac{2\pi}{a}$) and plot the band structure of antimony along the lines $X_1 - K - \Gamma - T - W \equiv W_1 - L$ and along the lines $U - X - \Gamma - L - U_1 \equiv U - T - H$.
6. Compare your results with Fig. 3 of Phys. Rev. **141**, 562 (1966).