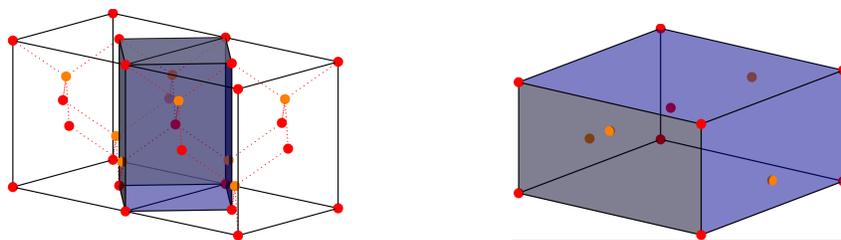


Problem 1: Band structure of white tin

Alpha tin (or gray tin), the low temperature structure of tin, has the diamond structure. You can find in the Cohen and Bergstresser (CB) paper the form factors of alpha tin and plot its electronic band structure using the code distributed in the lectures. At 13.6 °C the unit cell changes and tin becomes white tin, the room temperature phase. In this exercise we plot its band structure.

The structure of white tin (also known as beta tin) can be described by a centered tetragonal lattice with two atoms per cell. In order to visualize the unit cell, we can start from the tetragonal cell of alpha tin shown in the figure on the left:



The c/a ratio of this tetragonal cell is $c/a = \sqrt{2}$ ($a = a_{fcc}/\sqrt{2} = 4.59 \text{ \AA}$). Beta tin (shown in the figure on the right) can be obtained by decreasing c and increasing a until $c/a = 0.55$ and $a = 5.80 \text{ \AA}$. The simple tetragonal cell shown in the figure contains four atoms, but using a centered tetragonal Bravais lattice we can describe the structure with a unit cell with two atoms. The primitive lattice vectors are:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}(-a, a, c), \\ \mathbf{a}_2 &= \frac{1}{2}(a, -a, c), \\ \mathbf{a}_3 &= \frac{1}{2}(a, a, -c). \end{aligned}$$

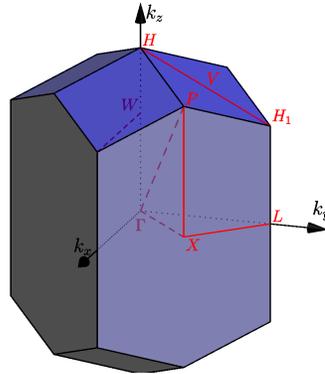
The position of the two atoms that in alpha tin were at $\mathbf{d}_{1,2} = \pm a_{fcc}(1/8, 1/8, 1/8)$ are strained uniformly and in beta tin are at $\mathbf{d}_{1,2} = \pm(a/4, 0, c/8)$ (with respect to the figure the origin is shifted in the center of the line that join the two atoms).

We can calculate the form factors for arbitrary values of the square modulus of the reciprocal lattice vectors $|\mathbf{G}|^2$, interpolating the form factors of alpha tin by an analytic 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 $A_1 = 0.0765$, $A_2 = 2.0997$, $A_3 = 2.9779$, $A_4 = 2.6524$, and using this function also for beta tin. These parameters, and \mathbf{G} vectors in atomic units (1/bohr), give the form factors in Hartree.

1. Plot the function $U(|\mathbf{G}|^2)$ and verify that, with these parameters A , it gives the same form factors of the CB paper at the corresponding $|\mathbf{G}|^2$ values.
2. Modify the program to calculate the energy bands with the CB empirical pseudopotentials to use Eq. 1. Check your changes by recalculating the band structure of alpha tin.
3. Modify the CB program and generate the reciprocal lattice vectors of the centered tetragonal lattice of beta tin. The Brillouin zone is shown in the figure. Find the coordinates of the high symmetry points Γ , X , L , H_1 , V , H , P , W :



4. Plot the band structure of beta tin along the lines $\Gamma-X-L-\Gamma-W-H-L$ and along the lines $X-P-V$.
5. Compare your results with Figs. 5 of Phys. Rev. **182**, 693 (1969).