Problem 4: Density of states of wurtzite CdS

CdS is a semiconductor with the wurtzite structure. This structure has four atoms in the unit cell. The Cd atoms occupy the hcp sites while the S atoms are in one half of the tetrahedral sites. Putting the origin in the middle of the bond the Cartesian coordinates of the atoms are:

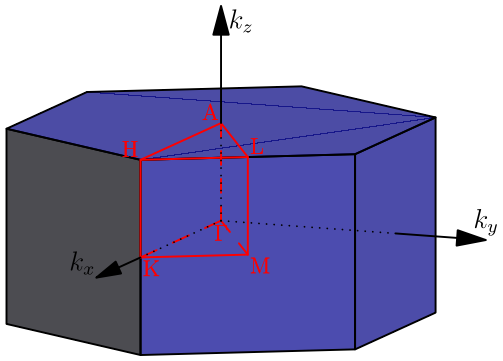
$$\begin{aligned} \mathbf{d}_{Cd_1} &= a(1/2, 1/(2\sqrt{3}), -7c/(16a)), \\ \mathbf{d}_{Cd_2} &= a(-1/2, -1/(2\sqrt{3}), c/(16a)), \\ \mathbf{d}_{S_1} &= a(1/2, 1/(2\sqrt{3}), c(u-7/16)/a), \\ \mathbf{d}_{S_2} &= a(-1/2, -1/(2\sqrt{3}), c(u-1/16)/a). \end{aligned} \quad (1)$$

where for u we take the ideal value $u = 3/8$. The size of the hexagonal Bravais lattice is $a = 7.823$ a.u., while for c/a we can take the ideal value $c/a = \sqrt{8/3}$.

The form factors for the wurtzite structure are given in Phys. Rev. **164**, 1069 (1967).

1. Modify the CB program in order to deal with the wurtzite structure and to use the form factors given in the above reference.

2. Modify the CB program in order to calculate the reciprocal lattice vectors of the hexagonal lattice of CdS. The Brillouin zone and a few high symmetry points are shown in the figure:



3. Compare your results with Fig. 7 of the above reference.

4. Compute the density of states of CdS as a function of energy and plot it.