Problem 9: Reflectivity of cubic ZnS and ZnSe

The imaginary part of the frequency dependent dielectric constant of a solid can be computed as a sum over the Brillouin zone. In c.g.s. units we have:

$$\epsilon_2(\omega) = \frac{e^2}{\pi m^2 \omega^2} \sum_{v,c} \int_{BZ} \delta(\epsilon_c(\mathbf{k}) - \epsilon_v(\mathbf{k}) - \hbar\omega) |p_{vc}|^2 d^3k \tag{1}$$

where $p_{vc} = -i\hbar\langle\psi_v(\mathbf{k})|\frac{d}{dz}|\psi_c(\mathbf{k})\rangle$ is the matrix element of the p_z operator between valence and conduction Bloch functions.

1. Consider the form factors for ZnSe given in Table I of Phys. Rev. **183**, 763 (1969) and use them to derive the band structure of this element. Compare the band structure with that obtained by the original CB parameters.

2. Modify the CB program in order to calculate the imaginary part of the dielectric constant and plot it for the frequency range 0 eV $< \hbar\omega <$ 15 eV and compare with Fig.10 of the above reference.

3. Put the analytical tail described in the above reference:

$$\varepsilon_2(\omega) = \frac{\beta\omega}{(\omega^2 + \gamma^2)^2} \tag{2}$$

   for frequency $\hbar\omega > 10.85$ eV. Here $\hbar\gamma = 4.5$ eV and β is determined so that $\varepsilon_2(\omega)$ is a continuous function. Using the following Kramers-Kröning relationship:

$$\varepsilon_1(\omega) = 1 + \frac{2}{\pi} P \int_0^\infty \frac{w' \varepsilon_2(\omega')}{\omega'^2 - \omega^2} d\omega' \tag{3}$$

   Find the real part of the dielectric function $\varepsilon_1(\omega)$.

4. The reflectivity of a solid, for normal incidence, can be written as:

$$R = \frac{(1-n)^2 + k^2}{(1+n)^2 + k^2} \tag{4}$$

   where $N = n + ik$ is the frequency dependent complex index of refraction such that $N(\omega) = \sqrt{\varepsilon(\omega)}$ where $\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$ is the complex dielectric constant. Using the real and imaginary part of the dielectric function compute the theoretical reflectivity of ZnSe and compare with Fig.11 of the above reference.

5. Repeat the calculation for ZnS with the parameters reported in the same reference and with those given in the CB table.