Optical properties of Tl_3TaSe_4 chalcogenide crystals

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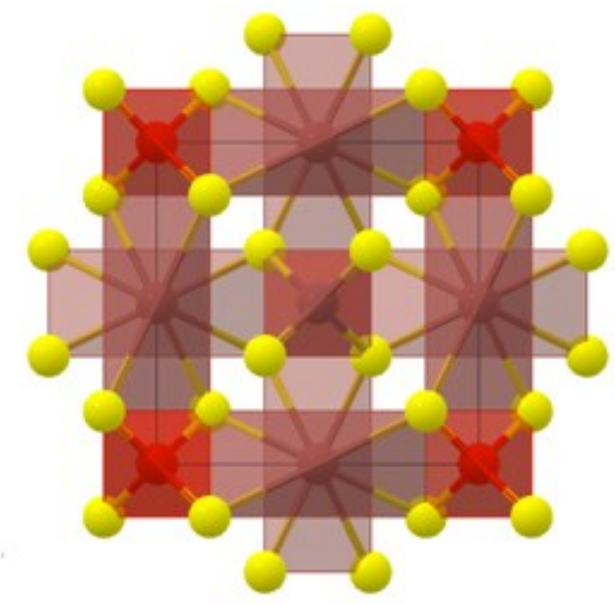

Fig. 1. Crystalline structure of Tl_3TaSe_4

The cluster consists of different states on each of the two neighbors. The individual bond polarizability [25] can be calculated as:

$$\alpha = \gamma \frac{(1-\alpha_p)\alpha_p e^2 d^2}{(1+\alpha_p)V_3}, \qquad (5)$$

where α_p is polarity and defines as:

$$\alpha_p = \frac{V_3}{\sqrt{V_2^2 + V_3^2}}, \qquad (6)$$

According to the special points method [20, 21, 25, 26], any average of any property over the electronic energy band is replaced by the values at a single special wave number, the Baldereschi point k. That wave number is chosen such that the first few sets of Fourier components of the band vanish, just as one would choose a point halfway to the Brillouin zone boundary in a one-dimensional crystal. As follows from the theory, the interaction between orbitals of cation and anion is described by the energy:

$$E_k = \frac{E_s + E_p}{2} \pm \sqrt{\left(\frac{E_s - E_p}{2}\right)^2 + f(k)^2 V_{sp\sigma}{}^2}, \qquad (1)$$

where $f(k)$ depending upon the relative phase and orientation of neighboring orbitals.

The optical dielectric susceptibility is calculated as the sum of polarizabilities of each bond type by their number per unit volume. Knowledge of susceptibility allows to predict the refractive index. The optical dielectric constant and refractive index are very important in determining the electric and optical properties of the materials. The imaginary part of the dielectric constant shows how a dielectric absorbs energy from an electric field caused by dipole motion. The real part of the dielectric function can be derived from the imaginary part by the Kramers–Kronig relationship. The refractive index $n(\omega)$ is given by Eq. (7):

$$n(\omega) = \left[\frac{\varepsilon_1(\omega)}{2} + \frac{\sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)}}{2}\right]^{1/2} \qquad (7)$$

Theoretical calculations of refractive index, optical dielectric constant, and reflection coefficient for Tl_3TaSe_4 crystal within the Harrison bonding orbitals model were carried out [1-3]. The calculations were performed for the spectral region far from the absorption edge, where the dispersion of the refractive index is absent. Our calculations show that the refractive index equals to 2.54 for Tl_3TaSe_4.The refractive index evaluation is of considerable importance for applications in integrated optic devices, where materials refractive index is the key parameter for device design.

A full set of analytical expressions are obtained for studies on the optical and dielectric properties of the crystal under investigation. The tight-binding point of view offers directly a way to describe localized charges since each of the orbitals in which the electronic states are expanded is associated with a particular atom. It should be noted that, in our current analysis, we are assuming that all matrix elements between the bonding and anti-bonding states are neglected. It was shown that Harrison's model allows analyzing the optical parameters of Tl_3XY_4 type compounds. Crystals under investigation are expected to contribute to the development of nanophysics and personalized medicine for health monitoring and prevention. The theoretical technique developed in this paper to use for the theoretical description of the optical properties of materials.

[1] W.A. Harrison, Tight-binding theory of the dielectric susceptibilities and transverse charges of insulators. Phys. Rew. B, 2006, 74, 205101.
[2] K. Hoang, S. Mohanti. Journ. of Science: Advanced Materials and Devices 1, (2016).
[3] O.V. Bokotey, Theoretical calculations of refractive properties for $Hg_3Te_2Cl_2$ crystals. Nanoscale Res. Lett. 2016, 11:251.