Dielectric properties of layer crystals and nanostructures based on them

Seredyuk B. O.[1], Karkulovska M. S.[2], Tovstyuk N.K.[2], Mykytiuk O.Y.[3]

[1]Dept. of Rocket Troops and Artillery, National Army Academy named after Hetman Petro Sahaidachnyi, Herojiv Majdany str. 32. Lviv-79032, Ukraine. E-mail: b.seredyuk@gmail.com

[2]Institute of Mathematics and Applied Physics, Lviv Polytechnic National University? Bandera str.,12, Lviv-79012, Ukraine

[3]Bukovinian State Medical University: Chernivtsi, UA

The effect of the degree of molecular bonding along the anisotropy axis of layer crystal on the dielectric constant, optical density, absolute index of refraction and transmittance is investigated. The case of low temperatures is considered, taking into account shielding effects caused by electron-electron interaction. The behavior of the dielectric function and its non-analyticity in the case of different dimensions of the system are investigated.

In the approximation of chaotic phases, real $\varepsilon_1(\vec{q},\Omega)$, and imaginary, $\varepsilon_2(\vec{q},\Omega)$, components $\varepsilon(\vec{q},\Omega)$ are connected to the polarization loop $\Pi(\vec{q},\Omega)$

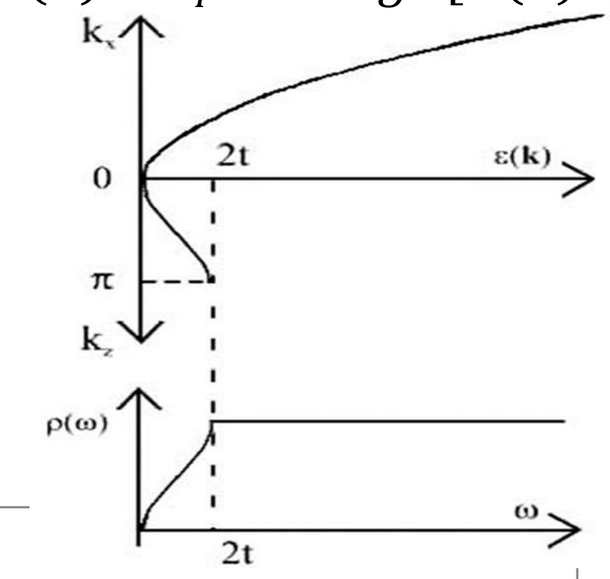
$$\Pi(q,\Omega) = i\int G_0\left(k+\frac{q}{2},\omega+\frac{\Omega}{2}\right)G_0\left(k-\frac{q}{2},\omega-\frac{\Omega}{2}\right)dkd\omega$$

$$G_0(k,\omega) = \{\omega - E(k) + \varepsilon_F + \iota\delta sign[E(k)-\varepsilon_F]\}^{-1}$$

The non-parabolic law of electron dispersion

$$E(\vec{k}) = \alpha\left(k_x^2 + k_y^2\right) + t(1 - cos\, d_z k_z)$$

where $\alpha\sim\frac{1}{m^*}$ and t energy parameters (in eV), in terms of electronic mixing, whereas $\alpha=1eV$, $t=0.1\ eV$, k_x, k_y – expressed in units of constant lattice and $\hbar=1$.



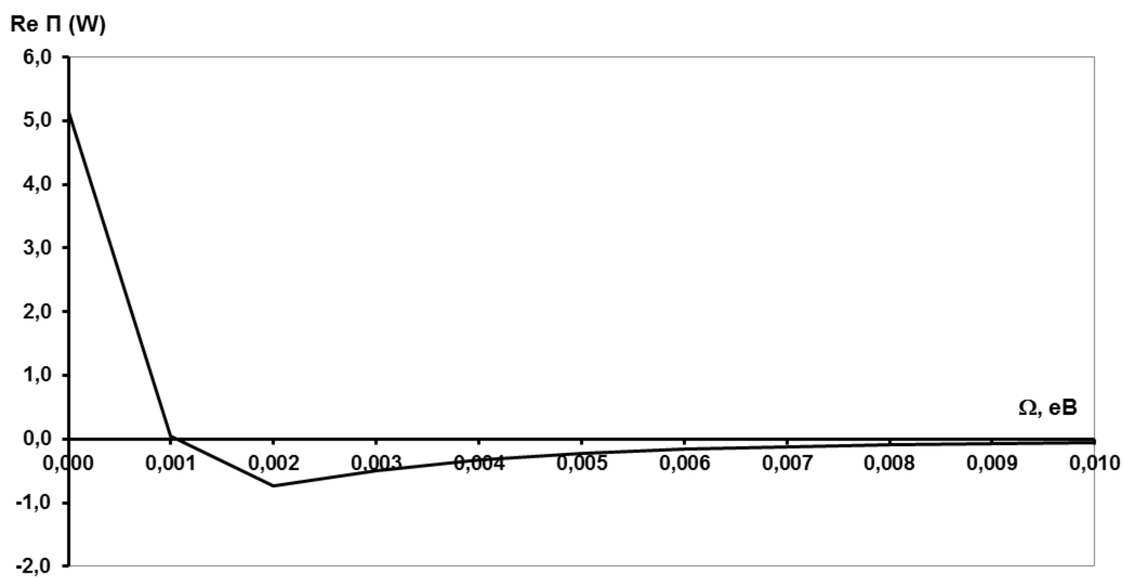


Fig. 2a. Frequency dependence of the real component of the polarization loop in 2D case at ε_F = *0,02eV*.

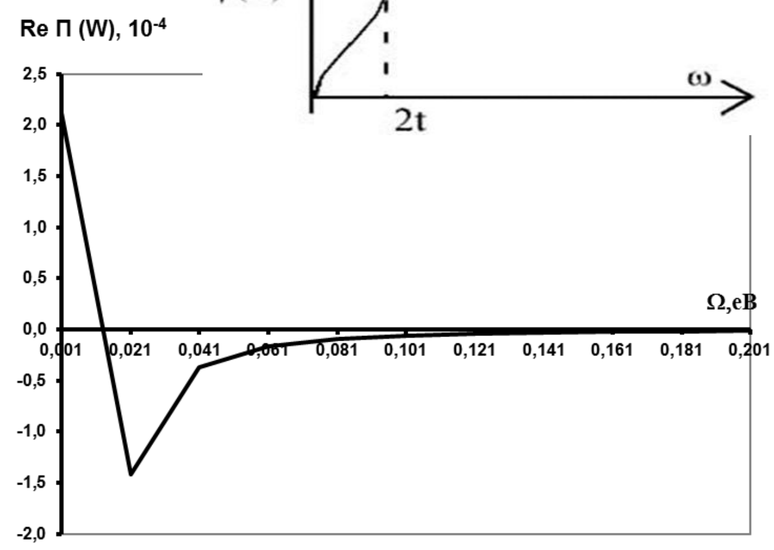


Fig. 2b. Frequency of dependence $Re\Pi$ in 3D anisotropic case for the energy parameters at ε_F *=0,001eV,*$\alpha = 1,0\ eV, t = 0,1eV$

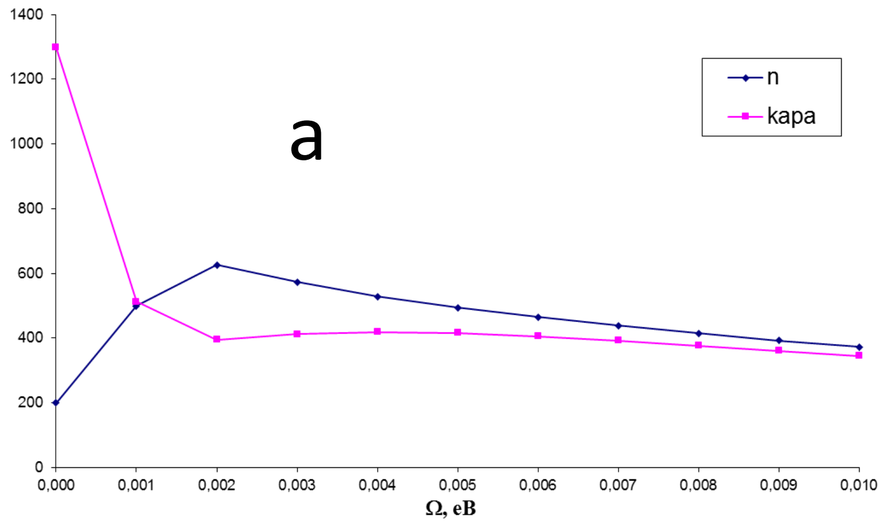
The dielectric constant are expressed as

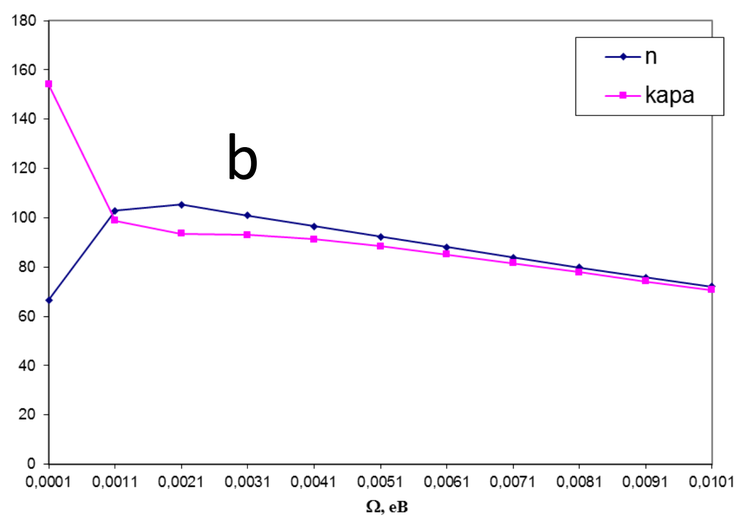
$$\varepsilon_1(\vec{q},\Omega) = 1 + \mathrm{Re}\,\Pi(\vec{q},\Omega)V_0(\vec{q})$$
$$\varepsilon_2(\vec{q},\Omega) = \mathrm{Im}\,\Pi(\vec{q},\Omega)V_0(\vec{q})$$

The absorption coefficient (χ) and the refractive index (n) are also analyzed

$$\chi = \sqrt{\frac{1}{2}\left(-\varepsilon_1 + \sqrt{\varepsilon_1^2+\varepsilon_2^2}\right)},\ n = \sqrt{\frac{1}{2}\left(\varepsilon_1 + \sqrt{\varepsilon_1^2+\varepsilon_2^2}\right)}$$

Fig. 3. Frequency dependences of absorption coefficient and refractive index for a) $\varepsilon_F = 0,02eV$ and b) $\varepsilon_F = 0,001eV$.





The change in the behavior of *n* as a function of frequency with decreasing dimensionality is explained by the frequency dependence of the average speed of the electromagnetic wave in the medium. The inverse problem can also be of interest: for example, based on the experimentally known ε_1 i ε_2 the initial potential of interelectron interaction can be estimated.

CONCLUSIONS

For various Ω the dispersion dependence of $Re\Pi(q_z,\Omega)$ has a completely different behavior, and even changes its sign. An increase in the Fermi level does not change the anisotropy, but it leads to the necessity to take into account (or neglect) the effects of non-parabolicity, and in layered crystals to make a transition from a 3D anisotropic case to a 2D one. Reduction from 3D to 2D increases by many times the numerical values of n, χ.