Optical Spectra Calculations in Layer Semiconductor 2H-PbI_2

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Abstract

Imaginary and real parts of the dielectric function of the layer semiconductor PbI_2 were found using the result of the pseudopotential method zone structure of electron energy spectra calculations. This enabled to calculate optical parameters of the crystal, in particular, absorption, and reflectivity and refraction spectra. There is a good agreement between the result of the reflectivity spectrum calculations and the experiment data.

Key words: layer crystal, lead iodide, optical spectra

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Results of the optical spectra calculations in the 2H-polytype layer semiconductor PbI_2 are presented in this article. Calculations were executed on the base of the electron energy spectra computing in the frame of the pseudopotential method using an '*ab initio'* nonsingular pseudopotential [1] the procedure of which has been given in [2].

Determination of the zone spectrum structure of the 2H-politype PbI_2 allow to realize the calculation of the imaginary part of the dielectric function [3]

$$\varepsilon_2(\omega) = \frac{e^2\hbar^2}{3\pi m^2\omega^2}\sum_{c,v}\int d^3k\,\delta(E_c(\vec{k}) - E_v(\vec{k}) - \hbar\omega)\,|<\varphi_{v\vec{k}}\,|\,\vec{\nabla}\cdot\vec{e}\,|\,\varphi_{c\vec{k}}>|^2, \qquad (1)$$

where $E_v(\vec{k})$, $Ec(\vec{k})$ and $\varphi_{v\vec{k}}$, $\varphi_{c\vec{k}}$ are the energies and wave functions of the electron from the state $\vec{k}$ in the valence or conduction bands accordingly, $\vec{e}$ is the polarization vector of incident light. Integral in (1) can be [4] recorded in the manner of the integral

$$\int\frac{dS}{|\vec{\nabla}_{\vec{k}}\omega(\vec{k})|}\,|<\varphi_{v\vec{k}}\,|\,\vec{\nabla}\cdot\vec{e}\,|\,\varphi_{c\vec{k}}>|^2\ , \qquad (2)$$

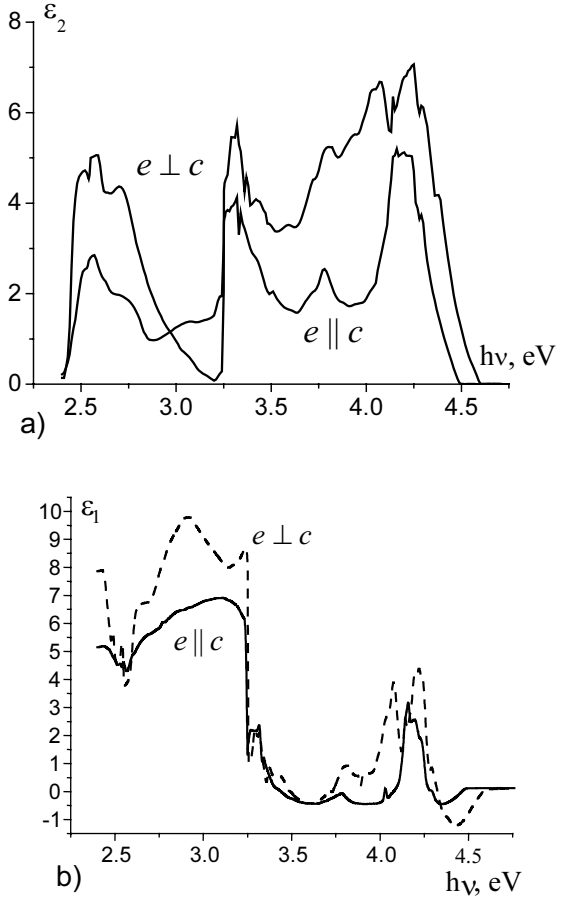


Fig. 1. Spectrum of the imaginary a) and real b) parts of dielectric function of PbI_2.

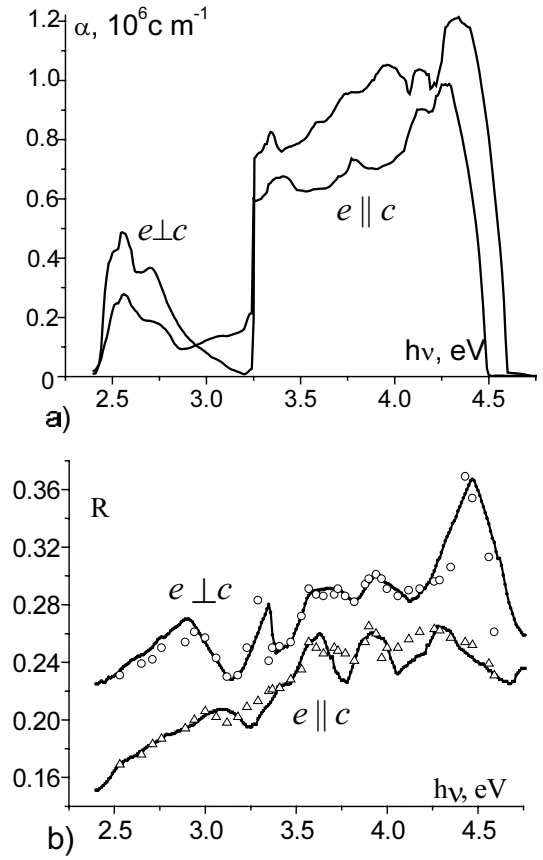


Fig. 2. Absorption (a) and reflectivity (b) spectra of PbI_2 (○ and Δ – experiment [6])

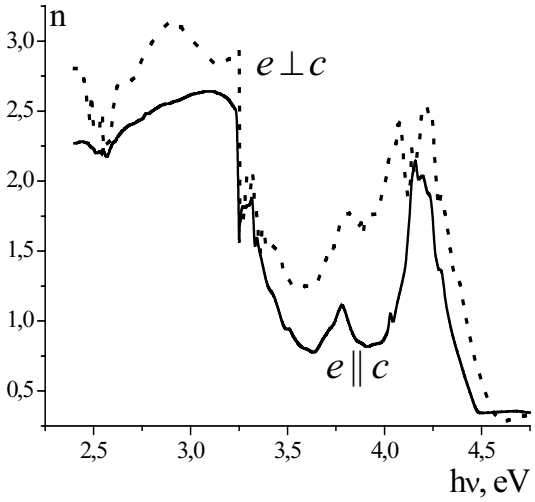
over the surface of constant energy $E_c(\vec{k}) - E_v(\vec{k}) = \hbar\omega$. The integration procedure was realized by the standard tetrahedron method [4] using 1000 points from the irreducible part of the Brillouin zone.

The real part of the dielectric function was found from the Kramers-Kronig correlation

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

using the computed relativities in the 2.4...8.5 eV energy region and tail function [5] $\beta\omega/(\omega^2 + \gamma^2)$ for higher energies (γ is an average energy and β is determined by continuity with $\varepsilon_2(\omega)$ at some cutoff energy E_c).

Results are shown in Fig. 1 for both polarizations of the light: $\vec{e} \perp c$ and $\vec{e} \parallel c$ where



Fug. 3. Refraction spectra of PbI_2.

c is the axis perpendicular to the layer packet plan.

Spectral dependences of ε_1 and ε_2 that were found allow making calculations of the spectrum of other optical parameters in the lead iodide (Fig.2 and Fig.3) together with experimental data at 4.2 K [6] for reflectivity. It can be seen, that essential anisotropy of optical parameters exists in PbI_2.

References

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