Abstract

Kohut Z.O. The electron polarizability of uniaxially stressed K_2ZnCL_4 crystals with the incommensurate phase. – Manuscript.

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The thesis is devoted to studies of spectral and temperature dependences of the refractive indices, birefringence, the piezooptic constants; the approximation $n_i(T, \lambda, \sigma)$ with the Selmeer formula, the calculations of the parameters of effective ultraviolet and infrared oscillators, electron polarizability, refraction, as well as the optical constants of both mechanically free and uniaxially stressed dielectric crystals K_2ZnCl_4. The methods for synthesizing crystals from aqueous solutions, measuring the effect of uniaxial mechanical stresses on the birefringent properties of crystals are also represented in the thesis.

The calculations on the basis of the first time *ab-initio* investigations of the band electronic structure, density of states and optical functions of K_2ZnCl_4 crystal for the orthorhombic space group of symmetry $Pna2_1$ were made. The valence-to-conduction band gap $E_g = 4.85$ *eV* of the crystal is found to be of the direct type in the Γ-point of Brillouin zone and to be formed by the electronic states of $ZnCl_4$ complexes only. One of the features of band structure of K_2ZnCl_4 is a presence of separated two groups of conduction bands, which are originated from different electrons: first group, at the bottom of conduction bands, is originated mainly from $ZnCl_4$ ions and second group of higher energies derives mainly from *d*-electrons of potassium.

It is revealed that the n_i values mainly increase under the action of uniaxial stresses, while the corresponding increments are the largest in the ultraviolet spectral range. These facts are caused by increment of the electron polarizability, the bonds refraction and the displacement of the absorption spectra to the longwave region. The uniaxial mechanical pressure along the principal crystallophysical axes is shown to give rise to shifting the PT points towards higher or lower temperatures, depending on the influence of uniaxial pressures upon the crystalline structure. The baric coefficients of the PT shift, $\partial T_c/\partial\sigma_m$, are determined for those crystals.

Keywords: refractive indices, birefringence, incommensurate phase, band energy structure, uniaxial pressure, phase transitions.