PECULIARITIES OF THE APPLICATION OF CLAUSIUS - MOSOTTI EQUATION TO THE CUBIC OXIDES

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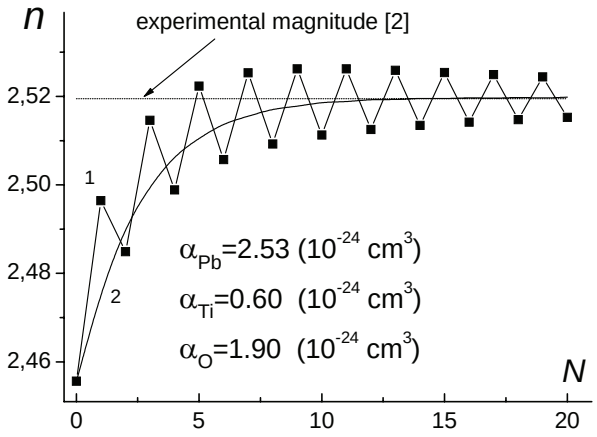
Clausius-Mosotti (CM) equation is widely used for the analysis of optical properties of glasses and cubic crystals. When a crystal with a cubic symmetry illuminated by linearly polarized light, the centres of gravity of external electronic shells of ions shall be displaced proportionally to the magnitude of local electric field $\mathbf{E}_{loc}$ on ions. Because dipole electronic polarizability (DEP) α of different ions is various, the system of induced electric dipole moments of ions in crystal may be considered as some cubic sublattices, displaced from each other and thus, application of CM equation can be wrongful [1].

Within the limits of this model we had been investigated optical properties of some cubic crystals with application of the Lorentz - Lorenz equation: $\frac{n^2-1}{n^2+2}=\frac{1}{3\varepsilon_o}\sum_{i=1}^{S}N_i\cdot b_i\cdot\alpha_i$, where n is a refractive index; α_i are DEP of i th sort of ion; b_i is the adjustment coefficient, defined by structure of a crystal and DEPs of all ions; N_i is the volume concentration of i th sort of ion. It is demonstrated, that for the crystals with rock-salt, cesium chloride and fluorite structure the coefficients b_i=1 and application to such objects CM equation of is quite true.



It is revealed, that for the crystals with perovskite structure (cubic phase of $BaTiO_3$ and $PbTiO_3$) the influence of the unequal displacement of dipole sublattices is very essential and, moreover, for the correct calculation of n magnitude it is need to execute not one, but series of iterations for the calculation of b_i magnitudes.

Results of the calculation of refractive index n of $PbTiO_3$ crystal (paraelectric phase) are presented in figure as a function of a quantity of iterations N for the one of possible combinations of DEPs of ions (see insert in figure). Thus, the cubic symmetry of an investigated crystal is not an applicability guarantee to the analysis of its optical properties by CM equation.

References

[1] Yatsenko A.A., Yatsenko A.V. // Cryst. Reports. 2009. V.54. P.518.
[2] Shannon R., Shannon R., Medenbach O., Fisher R. // J. Phys. Chem. Ref. Data. 2002. V.31. P.931.