MS15-P25 *B*3 and *B*20 compounds: pseudosymmetry and nonlinear optical properties

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In the present work, we have studied 111 crystals of AB type compounds belonging to two non-centrosymmetric structural types with cubic symmetry, namely, zinc blende (*B*3) and FeSi (*B*20) [1]. For selected crystals we have quantitatively estimated the degree of invariance with respect to the operation of inversion η (pseudoinversion) with a view to tracing the possible relationships between the nonlinear optical properties of these crystals and this symmetry characteristic. The second-order susceptibility of crystal determines the intensity of generation of the second optical harmonic and is a structure- and symmetry-sensitive property of crystal. For centrosymmetric crystals, the second-order susceptibility should be zero. One might suggest that reduction of symmetry will lead to some dependence of the second-order susceptibility of crystal on the degree of invariance of crystal structure with respect to inversion. In this context, the main goals of our investigation were first-principles calculations of the electronic structure and nonlinear optical properties of crystals of B3 and B20 types, calculation of the pseudoinversion values for these crystal structures, and comparison of the obtained computational data.

Calculations of the electron structure and nonlinear optical properties of crystals were based on the density-functional theory and employed three approximations for exchange–correlation potential, while the degrees of pseudoinversion of these structures were calculated using program package Pseudosymmetry [2]. The results obtained for some crystals are in agreement with the well-known experimental and computational data. For example Fig. shows η—$|\chi_{123}|$ diagrams for *B*3 type crystals by the results of calculations using the LDA potential, together with a histogram of the distribution of these crystals with respect to the degree of pseudoinversion, and a map of the values of a polynomial approximating the empirical function of the density of points on the η—$|\chi_{123}|$ plane.

It is demonstrated that the degree of pseudosymmetry as a quantitative characteristic of crystal structures can be useful for establishing correlations between the structural features of crystals and their physical properties. The results of this work can be useful for researchers engaged in the development of materials with preset properties.

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[2] N.V. Somov, E.V. Chuprunov, Crystallogr. Rep 59 (2014) 37

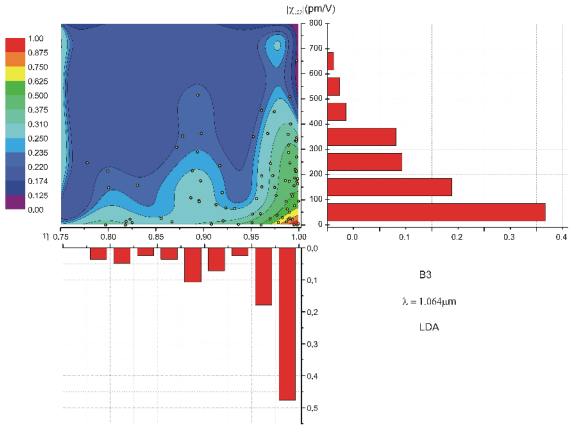

Figure 1. Diagrams η—$|\chi_{123}|$ for *B*3 type crystals calculated in the framework of LDA and histograms of distributions with respect to η (horizontal axis) and $|\chi_{123}|$ (vertical axis)

Keywords: pseudosymmetry, nonlinear optical properties, density functional theory