ON BONDS POLARITY IN A REFRACTORY DIELECTRIC

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Usually, refractory dielectrics are the compounds with chemical bonds of ionic-covalent or covalent-ionic types. Therefore, polarity of binding is an important characteristic affecting their electronic structure (e.g., see the case of boron nitride [1]), and through it – the material's properties as well.

However, dependences of the measurable physical parameters of compounds on the effective charges of constituent atoms are so complex that, they are virtually undetectable experimentally. As for the theoretical effective atomic charges, their values, as shown e.g. by the analysis of data available on boron nitrides, are characterized by a significant scatter making them almost unreliable. The reason for this lies in the impossibility of unambiguous division of the electron density between atoms of elements constituting the compound [2, 3].

Such a situation pushes the search for a semi-empirical solution. In this paper, we derived the relation allowing calculation of effective atomic charges in a binary compound based on empirical structural, dielectric and elastic parameters of the material.

Let the crystalline unit cell of the dielectric compound contains N pairs of atoms of two different elements with effective charges of $\pm qe$, and the deformations induced by the lattice polarization in the applied external electric field are elastic. Then, the effective charge number q is calculated from the formula:

$$q = \frac{S}{eN}\sqrt{\varepsilon_0\left(1-\frac{1}{\varepsilon}\right)Y}\,, \qquad (1)$$

where S is the sectional area of the unit cell transverse to the direction of the applied external electric field, while ε and Y, respectively, are the Young's modulus and the static dielectric constant in the same direction.

According to the proposed formula (1), we have evaluated the positive and negative effective charges of boron atoms B and nitrogen atoms N, respectively, which should be attributed to three different crystalline modifications of boron nitride BN: hexagonal h-BN, cubic c-BN, and wurtzite-like w-BN. The results are shown in the Table 1.

Table 1

Effective atomic charge numbers in boron nitride crystals

Crystal	$\parallel a$-axis	$\parallel c$-axis
h-BN	0.35	0.09
c-BN	0.49	
w-BN	0.76	0.50

These values are physically reasonable. Also quite natural are the qualitative conclusions that follow from them: (1) the bonds polarity within the layers of the h-BN structure is much stronger than between adjacent hexagonal layers; (2) bonding is stronger polarized in denser modifications c-BN and w-BN, which are characterized by the higher coordination numbers as well; (3) the bonds polarities in c-BN and along c-axis in w-BN are almost indistinguishable; and (4) the bonds polarity in w-BN is anisotropic.

Since these effective charges provide with reliable evaluation, they can be used in the refinement of earlier calculations of the density of electronic states and the molar binding energy of boron nitrides (see e.g. [4 – 8]).

Similar estimates of polarity can be carried out for other binary compounds as well.

1.C. Prasad, J. D. Dubey. Phys. Status Solidi B, 125 (1984) 629.
2. A. Garcia, M. L. Cohen. Phys. Rev. B 47 (1993) 4215.
3. A. Garcia, M. L. Cohen. Phys. Rev. B 47 (1993) 4221.
4. L. Chkhartishvili, D. Lezhava, O. Tsagareishvili. J. Solid State Chem. 154 (2000) 148.
5. L. S. Chkhartishvili. Phys. Solid State 46 (2004) 2126.
6. L. Chkhartishvili. J. Solid State Chem. 177 (2004) 395.
7. L. Chkhartishvili. Mater. Sci. Ind. J. 2 (2006) 18.
8. L. S. Chkhartishvili. Phys. Solid State 48 (2006) 846.