SOME CRYSTALS EFFECTIVE CHARGES DETERMINATION ON THE BASIS OF RELATIVISTIC PARTICLES BEAMS CHANNELING

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INTRODUCTION

According to the idea first put forward in [1] it is proposed a new method of effective charges atoms determination in noncovalent crystals on the basis of relativistic particles channeling in charged crystallographic planes and axis. They include, to some extent, almost all possible types of crystals which physical-chemical properties are directly connected with a magnitude and crystals atoms effective charges distribution.

First of all, it is necessary to investigate a physical essence of a conception "effective charge", which first appeared in quantum chemistry to evaluate covalent and ionic connections. One use this conception in ionic crystals to define the polarization degree of connections between atoms.

Unlike pure covalent monoatom crystals (Mendeleyev table of elements) there are not neutral atoms in all other crystals in bunches of crystal grids but ions (positively or negatively charged). These ions charges depend on the charges of elements nuclei and their valence. For example, for ionic crystals these magnitudes will be as maximum as possible. Besides electron density in the regions between neighboring atoms nuclei is very small. It means that ions have concrete dimensions and effective charges magnitude coincide with the charges localized in spheres with radii of corresponding ions.

The situation becomes more complicated when we move on to ionic-covalent crystals. In this case electron density in the regions between atoms does not reduce to small meanings as a result of valent electrons redistribution. Atoms don`t loose their individualities in crystal in respect to their own nuclei characteristics and inside electrons. But valent electrons participate in chemical relations of these atoms and there is no synonimity concerning their belonging to one or other atom. It seems at first sight that in this case we can`t use the conception of "effective charge", but further we will show how to use this conception from the point of view of relativity approach just in this case.

Let there are n neighbouring A-type atoms in the vicinity of B-type atom. Let also every relation between A and B atoms exist at the expense of covalent electrons, but with some polarization in the direction of B atoms. This is such a polarization that n relations cause a resulting negative charge on B atom, besides there is an equivalent positive charge on every of A-type atoms. Thus, we may consider that summary relativity of an atom valent electrons existence in the vicinity of B atoms multiplied by these valent electrons charge magnitude is just an effective negative charge of B-type atoms. Such an explanation of effective charge is based on a following criterion of an electron belonging to a given atom: an electron belongs to a given atom or ion to such an extent to which its wave function is a wave function of a free atom or ion. Thus, for example, writing down a wave function for AB relation as $\Psi_{AB} = \xi\psi_A + \eta\psi_B$, an effective charge is defined as: $Q_{eff} = \alpha \cdot Q$, where $\alpha = ||\xi|^2 - |\eta|^2|$ is ionicity of the connection, and Q is a charge in a case of a pure ionic relation (positive, for example, at $|\xi| = 0$, $|\eta|^2 = 1$ and negative at $|\xi| = 1$, $|\eta|^2 = 0$). Further we'll come across a following problem: how to find effective charges?

One of the first methods of effective charges determination has been proposed by R.I.Barinsky [2]. This X-ray –spectral method investigated a thin structure of X-ray spectra of absorption and bands bias in emission spectra. Effective charges magnitudes calculated by this method often were several times different from the ones got by other methods.

To find effective charges we also use indirect optical methods [3,4]. Besides, it is not easy to determine effective charges by the help of these methods
On the contrary, our universal direct method gives an opportunity to find out three characterictics of the effective charge (magnitude, sign and space distribution) simultaneously, with great precision and for any crystal structure.

Let's proceed to detail consideration of the given method physical essence. Unlike indirect optical and above-mentioned direct methods of crystal electron structure investigation this method proposes quite a new approach. It is based on theoretical calculations first done in [5, 6]. The method of crystal atoms effective charges determination is a reverse problem in charged particles channeling theory in ion and ion-covalent crystals. It is proposed to solve the problem by analyzing the spectra of quasy-characteristic reflection (SQR) of relativistic electrons, which is channeled either along the charged crystallographic planes or in the direction of charged crystallographic axes. In [5,6] it was shown that channeling electrons interaction potentials were sharply dependent on the magnitudes of the charged planes surplus charges or axes. For example, it occures a situation of potential pits complete inversion in hydrogen atoms charged plates for a hydride lithium crystal.

Thus, electrons channeling in such a regime is optimal from the point of view of effective charges characteristics definition on the basis of spectra SQR analysis. Besides, we can use a channeling regime as well in electroneutral crysyallographic planes or axes of the investigated object. In this case one can also also derive information but only concerning the effective electrons space distribution. It is important because we have an opportunity to define this effective charge characteristic independently of two other ones. Hence to approve the information it's necessary to investigate throughly a concrete crystal: first, at the expense of relativistic electrons channeling realization in different crystallographic planes or axes, second, due to the choice of channeling particles various energies and third, thanks to optimization of SQR registration regimes.

The proposed method may be used both for binary crystals of A_mB_n–type (m,n are natural numbers from 1 to 8) and more complicated combinations. Let's consider in detail relativistic electrons channeling along charged plates in crystals of A_1B_7, A_2B_6, and A_3B_5 types calculating crystals with the most structures: chloride natrium and zinc blende (we choice charged (111) planes).

Analytic calculation of electron potentials interaction with charged crystallographicplates of ion and ion-covalent crystals

One-particle interaction potentials for positive and negative charged ions are made using screen coulomb potentials, which are utilized in the case of neutral atoms. The requirements of asymptotic in a zero and on infinity

$$\lim_{r\to 0}\phi_{\pm}(r)=\frac{Z_{1,2}e}{r},\quad \lim_{r\to\infty}\phi_{\pm}(r)=\pm\frac{\alpha Q}{r},$$

may be shown as:

$$\phi_{\pm}(r)=(eZ_{1,2}\mp\alpha Q)\left(\frac{1}{r}+\frac{1}{b_{1,2}}\right)\cdot\exp\left(-\frac{r}{b_{1,2}}\right)\pm\frac{\alpha Q}{r}. \quad (1)$$

Here $Z_{1,2}$ are nuclei charges of the ions A^+ and B^- correspondingly, $b_{1,2}\approx a_0 Z_{1,2}^{-1/3}$ are atoms A and B screen radii accordingly, a_0 is Bohr radius.

Let's now fulfil averaging of potentials (1) by crystallographic plates. Besides first items averaging (named as $\phi_{0\pm}(x)$) characterizing potentials of electroneutral skeletons of corresponding ions will be filfilling a standard procedure [7]. Thus, from (1) we get

$$\Phi_{1,2}(x)=\frac{2\pi}{S}\cdot(eZ_{1,2}\mp\alpha Q)\cdot(2b_{1,2}+|x|)\cdot\exp\left(-\frac{|x|}{b_{1,2}}\right) \quad (2)$$

Further we make an averaging of potentials (2) by crystal atoms thermal oscillations.

$$\langle\Phi_{1,2}(x)\rangle_{u_{1,2}}=\frac{\pi}{S}(eZ_{1,2}\mp\alpha Q)\exp\left(-\frac{u_{1,2}^2}{2b_{1,2}^2}\right)\left\{\exp\left(-\frac{x}{b_{1,2}}\right)\cdot\right.$$

$$\left[\left(2b_{1,2}+x-\frac{u_{1,2}^2}{b_{1,2}}\right)\cdot erfc(\tau_{1,2}^{(-)}(x))+u_{1,2}\sqrt{\frac{2}{\pi}}\cdot\exp[-\tau_{1,2}^{(-)2}(x)]\right]+$$

$$\left.+\exp\left(\frac{x}{b_{1,2}}\right)\cdot\left[\left(2b_{1,2}-x-\frac{u_{1,2}^2}{b_{1,2}}\right)\cdot erfc(\tau_{1,2}^{(+)})+\sqrt{\frac{2}{\pi}}\exp[-\tau_{1,2}^{(+)2}(x)]\right]\right\},$$

$$\tau_{1,2}^{(\mp)}(x)=\frac{1}{\sqrt{2}}\cdot\left(\frac{u_{1,2}}{b_{1,2}}\mp\frac{x}{u_{1,2}}\right) \quad (3)$$

Here $u_{1,2}$ are thermal oscillations amplitudes of A^+ and B^- ions correspondingly.

Let's proceed now to averaging by crystallographic planes of other potentials items (1), fulfilling two stages of this procedure. First consider averaging along [110]-axes (separately for positively and negatively charged)

$$U_{\pm}(\rho)=\mp\frac{2\alpha Q}{d}\ln\rho, \quad (4)$$

where $d=a/\sqrt{2}$ is a distance between atoms in these axes, a – is a constant of a crystal grid. In fig.1 these axes in crystallographic planes (110) are presented as black and white circles (it is shown as an example on the structure of zinc blende).

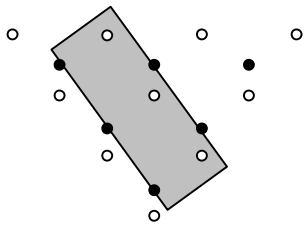

Fig.1.Two-dimensional net [110]-axes in(110) ofcrystals planes of zinc blende type.

The second stage is a crystal expansion in electroneutral region. One of these regions in the direction (111) of planes (this case will be more popular due to these planes non-equidity) is shown schematically in fig.1. Taking into consideration that a contribution from one negatively charged(111) plane is ξ and from the other is 1-ξcorrespondingly we write down a potential of one electroneutral layer after potentials simultaneous averaging (4):

$$W(x)=-\frac{2\pi\alpha Q}{S}\left[|x|-\xi\cdot\left|x-\frac{a}{4\sqrt{3}}\right|-(1-\xi)\cdot\left|x+\frac{a\sqrt{3}}{4}\right|\right], \quad (5)$$

the parameter ξ where we find from a boundary condition $W(a/4\sqrt{3})=0$, i.e. $\xi=3/4$. The boundary condition $W(-a\sqrt{3}/4)=0$ at this is satisfied automatically.

Calculating the potential (5) we choose the coordinate system in such a way that a plane yz coincicles with positively charged plane (111) and axis x is directed towards a nearby negatively charged one (111). As a result we get from (3), (5) a potential of electron interaction V(x,α) number of charged (111) planes for the

crystals having a zinc blende structure. Similar calculations may be made for crystals with a chloride natrium structure, taking into account that charged (111) planes in this case are equidistant ($\xi = 0{,}5$). To illustrate the calculations (fig.2a,b) we have built the potentials $Vn(x) \equiv V(x,\alpha_n)$ for three varions meanigs of effective charge (at n = 1 $\alpha_1 = 0$ is a pure covalent combination, at n = 2 $\alpha_2 = 0{,}5$-ion-covalent combination and at n = 3 $\alpha_3 = 1$ – hypothetical pure ion combination where all eight valent electrons are localized nearby ion residual B^{n+}): in fig.2a for one of the crystals with zinc blende structure (of the crystal AlP) and in fig.2b accordingly for one of the crystals with chloride natrium structure a (of the crystal NaF).

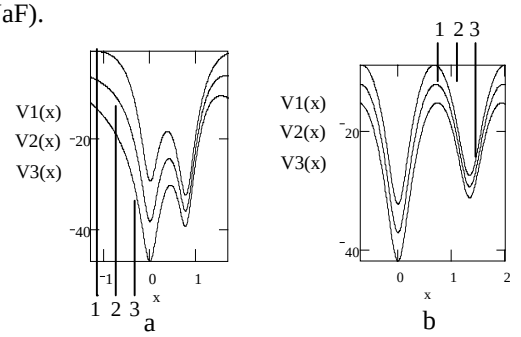

Fig.2a,b: The structures of electron potentials of interaction in charged (111) planes (a) for the crystal AlP- zinc blende structure and (b) for NaF– chloride natrium structure calculated various meanings of the effective charge (the coordinate x is measured in angrestremes and potentials Vn(x) in electron-volts accordingly).

The theoretical calculations analysis and the method brief description

As it is seen from fig.2a,b the potential structures of relativistic electrons interaction with a charged (111) planes system are sharply dependent on a magnitude α which characterizes an effective charge absolute meaning. Magnitude Q characterises an effective charge sign. This sign was known from the very beginning for the examined cases, since relations AB were polarized in B-type atom direction.

Next stage is a calculation of a spectrum of transverse energetic levels channeling $E_{n\perp}$ in potentials $V(x,\alpha)$. Combining the method of isospectral potentials (see, for example,[8]), where it is shown a possibility of approximation of real electrons potentials interaction with the method of perturbation stationary theory the spectrum may be calculated with a great precision.

Further on it is necessary to compare a calculated spectrum of transverse energies with this one got on experimental data basis by frequency spectra SQR.

Mathematics algorithm of effective charges in crystals parameters method, block-scheme of which is shown in fig.3, was created on the basis of detail theoretical calculations.exit1

As it is seen from fig.3 this block-scheme consists of three main modules. Electron potentials of interaction with crystalographic planes and crystalographic axes are

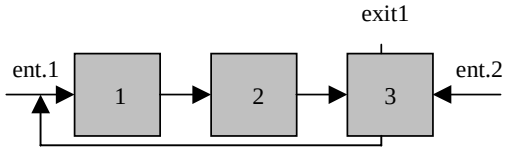

Fig.3. Block-scheme of mathematics algorithm of effective chargesparameters determination.

calculated in module1. Parameters of thesis planes axes are got on entrance 1. They are of two types. First type comprises crystal constant characteristics. For example, nuclei charges of crystal atoms Debye temperature, crystal grids parameters and so on. Second type includes the parameters undergoing changes during algorithm processing on the basis of experimental data, which get on the entrance 2 of module 3. These are just the effective charges characteristics: effective charges absolute meanings, these charges signs and wave functions parameters of investigated ions A^+ and B^-.

Further planar and axial electron potentials are going from module1 to module 2 where there are spectra of transverse energetic levels and the ones of channeling electrons SQR as a result of Schrödinger equation solution (or Klein-Gordon equation). The information of these spectra is coming in module 3 where we compare the spectra of transverse energetic levels calculated in a module 2 and SQR spectra with similar ones got from experimental data. Final results after whole set of cycles are got on the exit 1.

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