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Theoretical Calculation of Electrical and Optical Properties of BaZrO3

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***Abstract*—**In this project electrical and optical properties of BaZrO3 have been accomplished through the full-potential linear augmented plane wave (FP-LAPW) by applying Wein2k software. In this study band structure, density of state, gap energy, refractive index and optical conduction have been studied. The results of calculations show that BaZrO3 is an insulator with an indirect gap in which 3.2 ev and studied refractive index equal 2.07. These results are in accordance with the ones obtained in experimental researches.

***Keywords*—**Density Functional Theory (DFT), Full Potential Linearized Augmented Plane Wave (Fp-LAPW), Generalized Gradient Approximation (GGA), Linearized Augmented Plane Wave (LAPW), Local Density Approximation (LDA)

I. Introduction

THE phase of ABO3 proskyte crystals has been studied broadly for having vital importance and value in transition physics. They are considered as the most important ferroelectric material. [1,2,5] The complete structure of proskyte is very simple and have a complete cubic symmetry in which atoms positions are as follows: A atom is located in the cube angles, B atom is located in the center, oxygen atom is located around B atom in the centers of sides of the cube. In fact, BaZrO3 is located in the spatial group of pm3m. BaZrO3 crystal is a cubic proskyte and has one phase. This crystal has several applications in industry especially in electro-optics , full capacity computer memory cells and refractory fusion because of having high melting temperature and being ferroelectric [7,6]. This paper studies electrical structure of BaZrO3 applying local density approximation (LDA) and generalized gradient approximation (GGA) and with the method of full potential lineared augmented plane wave (FP-LAPW). Also this paper uses density functional theory for studying electrical properties of BaZrO3. Optical properties of BaZrO3 crystal are studied by the use of Kramers-Kronig analysis and interband transition, moreover, refractive coefficient and optical conductance are interpreted for this crystal in next sections.

II. Methods and Materials

Primary calculations were conducted through applying full potential-lineared augmented plane wave (FP-LAPW) depended on density functional theory and implemented in WIEN2K Soft ware, and Kohn-Sham equations were solved applying Full potential-lineared augmented plane wave (FP-LAPW) self-consistently. [2,3,9] Here amount of convergence parameters that specify number of fundamental functions equals: $RMT \times KMAX = 7$ in which $KMAX$ is the plane wave matrix and RMT is the radiant of Muffin-Tin cube, amount of which for "barium" atom equals 3.5 au for" zirconium" atom equals 2.07 au and for oxygen atom equals 1.83au. Shape of exchange-correlation function was indentified through local density approximation (LDA) [5,6] and number of k in Brillouin area was considered as 400. Separation energy is -6 Ry. Optical properties were studied and analyzed through dielectric function. Dielectric function was applied for description of the crystal reflection to electromagnetic field. The real and magic parts of dielectric function have been displayed in the following equations. [9]

$$\mathrm{Re}\ \varepsilon(\omega) = 1 + \frac{2}{\pi} p \int_0^{\infty} \frac{\omega' \varepsilon_2(\omega')}{\omega'^2 - \omega^2} d\omega'$$

$$\mathrm{Im}\ \varepsilon(\omega) = \frac{e^2 \hbar^2}{\pi m^2 \omega^2} \sum_{\nu,C} \int_{BZ} \left| \langle u_{ck} | e \nabla | u_{vk} \rangle \right|^2 \delta\left[E_{ck} - E_{vk} - \omega\right] d^3 k \quad (1)$$

In which K shows number of points in Brillouin area and is the integral limitation on the first Brillouin area. Element of $\langle u_{ck} | e \nabla | u_{vk} \rangle$ is the identifier of dipole matrix elements for direct transitions between conduction and valence bands states; and $[E_{ck} - E_{vk} - \omega]$ is the identifier of energy exalted from valence band to conduction band , and $\vec{e}$ is the polarization vector of electrical field. Quantity of refractive 'n' has been calculated from real and magic dielectric functions.[5]

$$n(\omega) = \sqrt{\frac{\varepsilon_1(\omega)}{2} + \frac{\sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)}}{2}} \quad (2)$$

In zero frequency the refractive coefficient equation becomes as follows: $n = \sqrt{\varepsilon(0)}$ which is called static refractive coefficient.

III. Results

Electrical properties including band structure, density of state and density of electron cloud have been calculated. Band

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structure for cubic phase has been shown in Fig. 1 for BaZrO3 crystal.

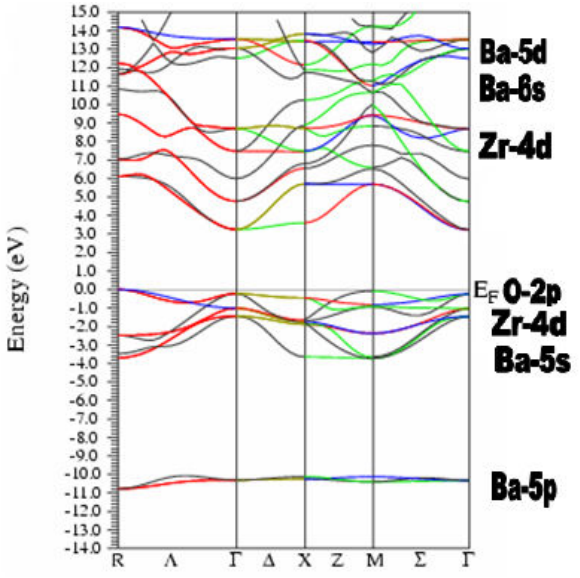


Fig. 1 Energy band structure of BaZrO3 in cubic phase in GGA96

In Fig. 1, scale of energy is based on electron volt (ev) and is considered based on Fermi surface. Fermi surface is a place in which energy is zero. Valence bands are located under Fermi surface and conduction bands are located above Fermi surface. Considering Fig. 1 it is observed that this crystal has an indirect energy band gap in Γ– M and its amount is about 3.2 ev that shows BaZrO3 is an insulator. This band gap is observed between maximum amount of valence band in M point and minimum amount of conduction band in Γ point. In fact there are 8 valence bands under Fermi energy and several conduction bands that are full or empty above Fermi energy. Most valence bands are located in the limit of zero to -4 ev that are related to contribution of orbitals O-2p and Zr-4p.In fact, S and P states of Zirconium atom and S state of barium atom influence partially on these bands, and their existence is observable. There is the lowest band structure that is completely full in the limit of energy -10 ev to -15 ev and is related to orbital 5p of barium atom.. In the limit of energies above Fermi energy that is conduction band there are unoccupied states including unoccupied states of 4d of zirconium atom and states of 6s and 5d of barium atom.

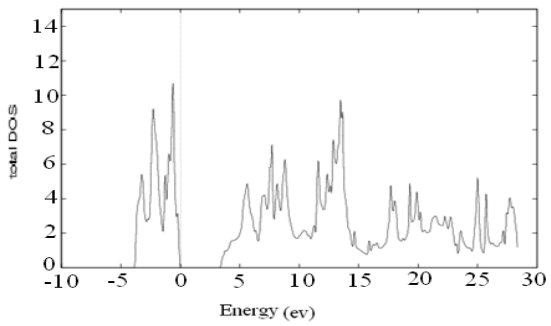


Fig. 2 Total Calculated DOS for BaZrO3

Density of total states spectrum of BaZrO3 has been drawn in the limit of energy -5ev to 25 ev. Valence bands under Fermi level have been separated from conduction band above Fermi band by an energy gap of about 3.2 ev.

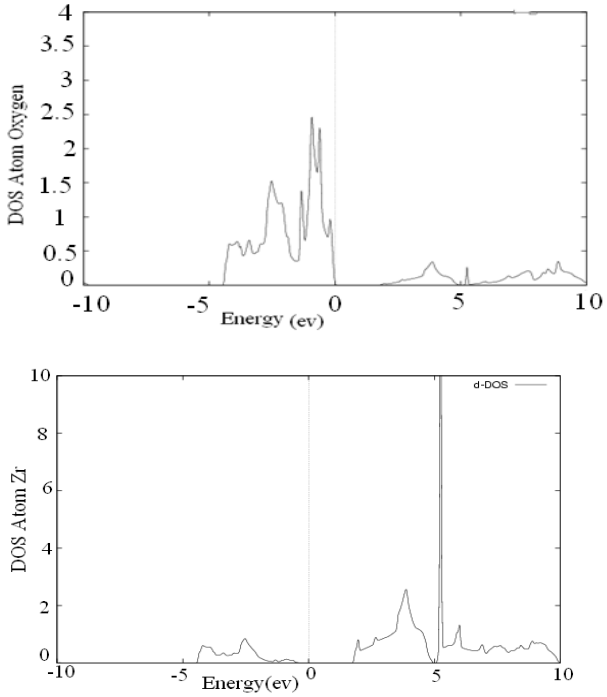
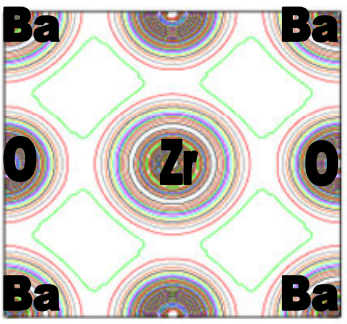
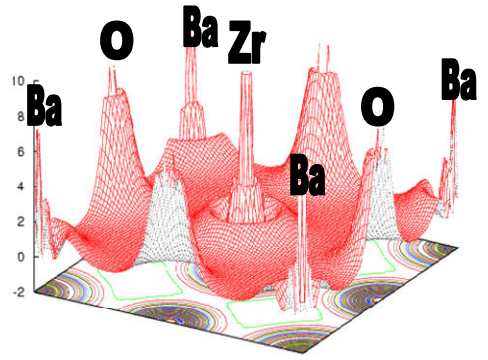


Fig. 3 Density of partial states of orbitals p of oxygen atom and d of zirconium atom

Valence band has been overshadowed by orbitals p of oxygen atom and 4d of zirconium in the limit of energy between zero to -5 ev that has been shown in Fig. 3. In fact, existence of orbitals 4d Zirconium shows influence of a covalence joint for this material. A lot of small and large picks are observed in the energy limit of zero to 25 ev, that are related to conduction bands and are under the influence of orbitals 4d of zirconium atom and 5d of barium atom .Actually the specified energy gap is between occupied states of 2p of oxygen atom and states of 4d of zirconium atom. Density of electronic cloud of cubic BaZrO3 has been shown in real space of (1 1 0) sheet in two and three dimensions in Fig. 4.



(a)



(b)

Fig. 4 Density of electronic cloud in sheet (1 1 0) (A):two dimensional display (B) : three dimensional display

If we observe charge distribution around barium atom in Fig. 4, we find out that composition of BaZrO3 has an ionic bond. This bond is somehow weak since bond between zirconium and oxygen atoms has a covalence nature. In fact, density of electronic charge in plate (1 1 0) clearly states that bond between zirconium and oxygen atoms is a strong covalence bond, and there is a remarkable amount of electric charge in this bond ,while bond between barium and oxygen is completely ionic. Optical properties of this crystal have been calculated by refractive coefficient and optical conductance that is shown in Figs. 5 and 6.

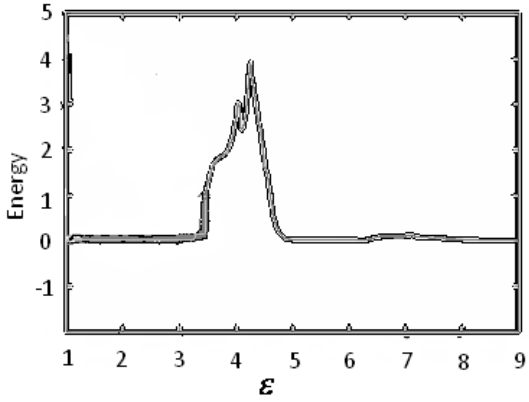
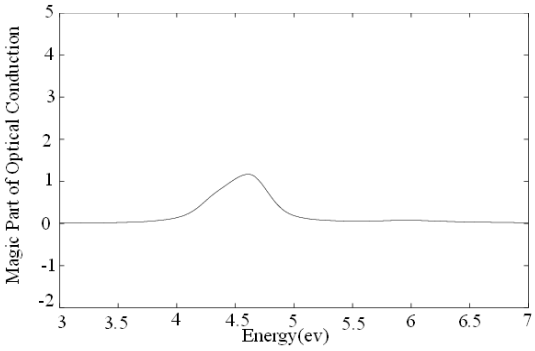


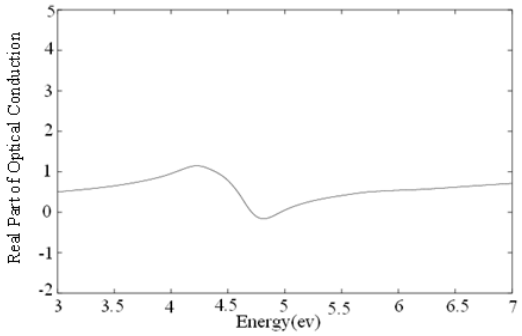
Fig.. 5 dielectric function $\varepsilon(0)$ is calculated as 4.3. If we calculate its square root it equals 2.07 that shows refractive coefficient of BaZrO3 in zero frequency.

$$n = \sqrt{\varepsilon(0)} = \sqrt{4.3} = 2.07 \quad (3)$$

Experimental amount of calculated refractive coefficient equals 2.13 [5] that shows the calculated amount has a good consistency with the experimental amount.



(a)



(b)

Fig. 6 Optical conductance changes (A) real part (B) magic part in the side of X per inner energy

In Fig. 6 optical conductance has started from energy about 3.2 ev and optical conductance increases with increase of photons. Optical conductance reaches to its maximum amount in the limit of energy between 4 ev to 4.5 ev. In fact, the reason for start of optical conductance is energy of about 3.2 ev energy gap, i.e. in the limit of energies lower than 3.2 ev descending photon energies are lower than gap energy. Therefore, the excited electrons don't have enough energy to pass through energy gap and reach the conduction band. Here interband transition is zero and consequently optical conductance becomes zero. The reason of optical conductance increase in energy limit between 4 ev to 4.5 ev is transition of orbitals 2p of oxygen atom to 4d of zirconium atom in conduction band.

IV. Conclusion

Results show an indirect energy band gap of 2.3 ev in Γ– M in the Brillouin area, and also the static refractive coefficient of this crystal equals 2.07 that has a good consistency to the experimental amount.

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