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Research Article

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Investigation of the Optical Properties of Lanthanum Oxide, Using Density Functional Theory and LSDA and WC Approximations

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ABSTRACT

In this study, optical properties of lanthanum oxide crystals including dielectric constant, refractive extinction index, reflection dissipation function, and optical conductivity. Calculations were performed using the full potential linearized plane wave (FP-LAPW) method within the framework of density functional theory and applying WIN2K software and LSDA and WC functions. Complex dielectric function is calculated by LSDA and WC approximations. Results' comparisons indicate significant differences between optical functions and electronic properties.

Keywords: *Optical Properties, Lanthanum Oxide, Density Functional Theory, LSDA, WC, WIEN2K*

INTRODUCTION

Lanthanum oxide is used in long-stand camera lenses, microscopes, telescopes, rifle scopes, and binoculars to enhance the resolution. Lanthanum fluoride is used in optical fibers to speed up data transfer.

Lanthanum oxide has band gap of about 5.8 V [1]. The minimum energy network is with a very high dielectric constant at $\in = 2$ [2]. Lanthanum oxide is widely used in industry as well as research laboratories. Lanthanum oxide is solid, odorless, white, and insoluble in water, but it is soluble in dilute acids; depending on different crystal structure combination, PH value can be obtained [3]. Lanthanum oxide possesses P-type semiconductor properties that its resistance decreases with increase in temperature [4]. Its average temperature at room is 10 kilometers per centimeter [5].

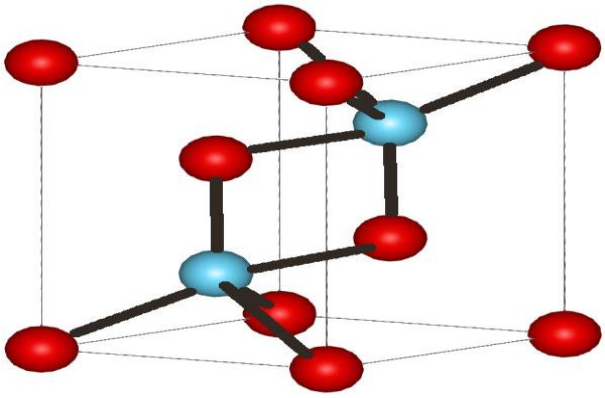

Figure 1: Lanthanum oxide contracting cell

1. Description of calculations

Calculation of the properties of the crystal structure of lanthanum oxide composition in the hexagonal phase was done by FP-LAPW method within the framework of density functional theory using WIEN2k code [6, 7]. In these calculations, the two PBE and WC functions were used; they were applied in many studies to obtain network constant in solids [8]. In calculations, the convergence parameter value of $K_{max} * R_{MT} = -6$ is considered. R_{MT} is the smallest Muffin-Tin radius, and K_{max} is the cut-off energy for plane wave in the first Brillouin zone of 20,000 points for structural properties and 20,000 points for optical properties. Muffin-Tin radius values for oxygen and lanthanum oxide atoms are 1.96 and 2.28, respectively.

1.1. Dielectric function

To observe the material response to electromagnetic waves (light), the dielectric function of the material is examined. Dielectric function has two intra-band and inter-band shares; intra-band share is used for metals. Inter-band transitions are divided into two types of direct and indirect transitions. Dielectric function is a complex function shown as $\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$. Having $\varepsilon_2(\omega)$ changes, $\varepsilon_1(\omega)$ changes can be obtained based on Kramers-Kronig transformation. $\varepsilon_1(\omega)$ roots have physical concept. In fact, in the area which $\varepsilon_1(\omega)$ is negative, the waves are not released, and the processes of absorption and dissipation take place. $\varepsilon_1(\omega)$ roots are obtained for energies at real direction, 4.82 and 6.38, and at imaginary direction, 6.67 and 6.46 eV for LSDA and WC functions. The real and imaginary parts of dielectric function for lanthanum oxide are shown in Figures 2 and 3; the energy shift is 0.3 eV.

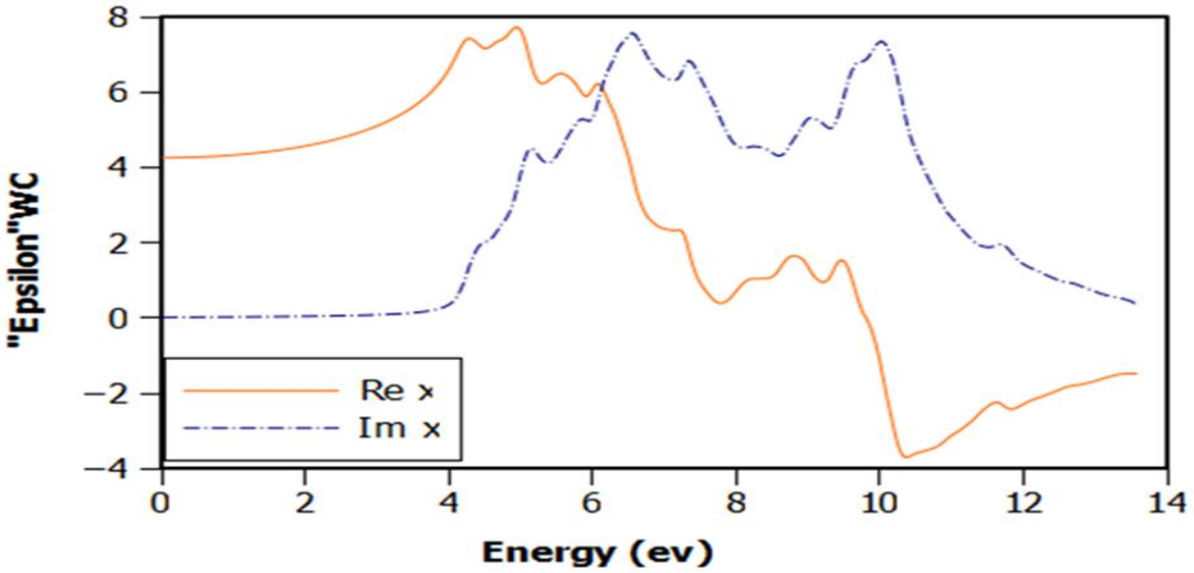

Figure 2: The real and imaginary parts of WC dielectric function at X directions

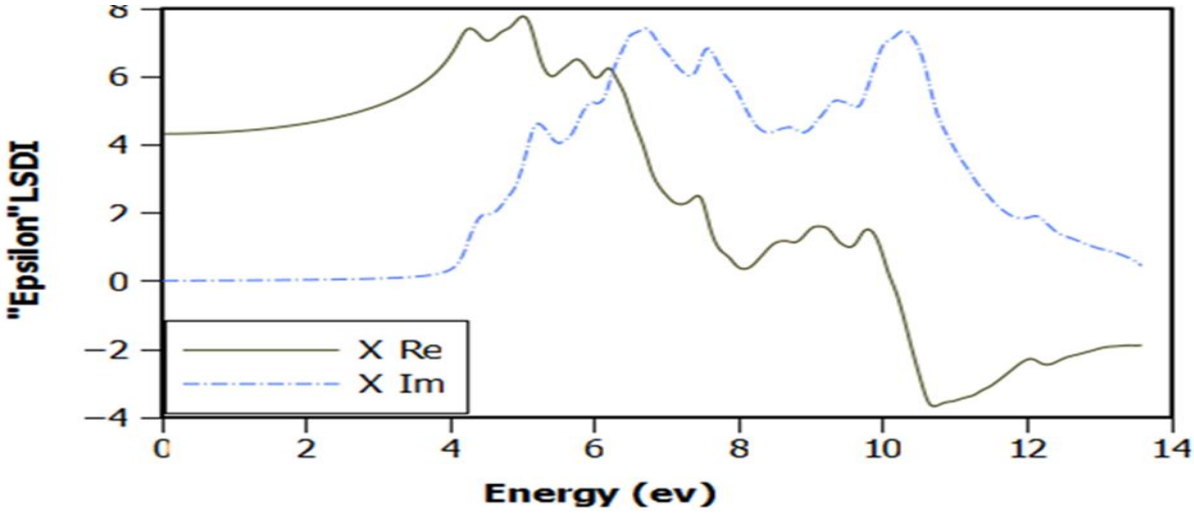

Figure 3: The real and imaginary parts of LSDA dielectric function at X directions

1.1. Electronic dissipation function

Electron energy dissipation spectroscopy is a powerful method to analyze occupied states above the Fermi level or partial breakdown. This spectrum includes mass stimulation of valence electrons (plasmons) at occupied states in the conduction band. Electron energy dissipation in this structure starts from about 0.075 corresponding to the band gap. The most prominent peak in the electron energy dissipation function is known as plasmon peak which represents the collective excitation of the electronic charge density in the crystal. In lanthanum oxide in X direction, only one peak is observed corresponding to the volume plasmons. The maximum energy dissipation of crystal is obtained at Z and X directions of 11.53 and 12.65 eV energies for WC function, respectively. The crystal energy is obtained at Z and X directions of 8.82 and 8.53 eV energies for LSDA function, respectively. Lanthanum oxide energy dissipation curve is shown in Figure 4.

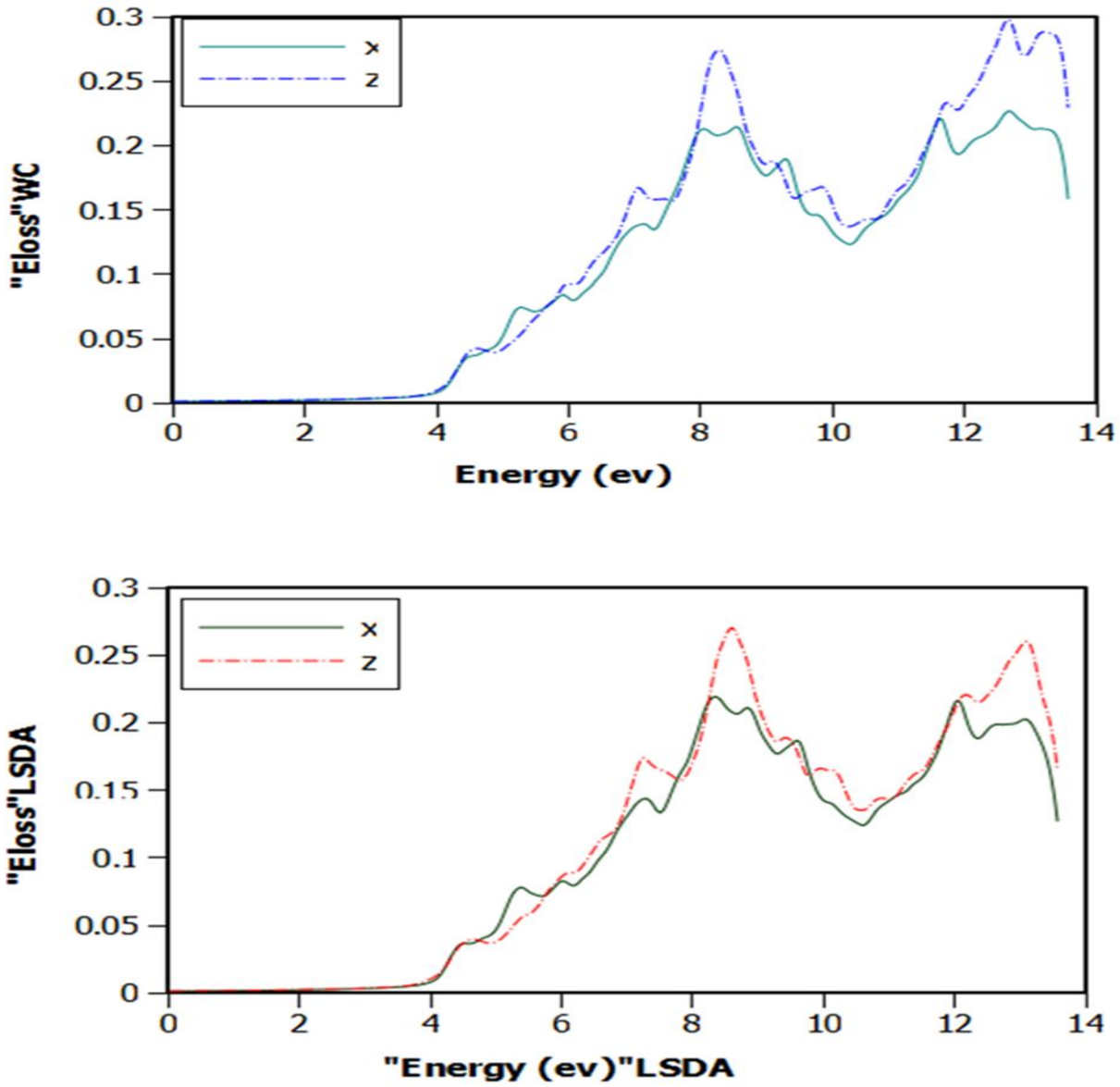

Figure 4: Energy dissipation function for real and imaginary parts of Z, X, WC, and LSDA

Based on free electron model, plasmon energy is obtained by $E_p = \hbar\omega_p = \sqrt{\frac{ne^2}{m_0 \varepsilon_0}}$ relation. Where *n* is the density of free electrons in the cell volume; *m* is the electron mass, and *e* is the electric charge unit.

2.3. Conductivity coefficient

Frequency-dependent intra-band optical conductivity relation, σ (ω), with the imaginary part of dielectric function is as follows:

$$\sigma(\omega) = \left(\frac{\omega}{4\pi}\right)\varepsilon_2(\omega) \quad (1)$$

Conductivity of lanthanum oxide is shown in Figure 5. The maximum peak in Figure 5 in real direction for 9.76 and 9.50 energies, and in imaginary direction, for 10.26 and 6311 eV energies are obtained for LSDA and WC functions.

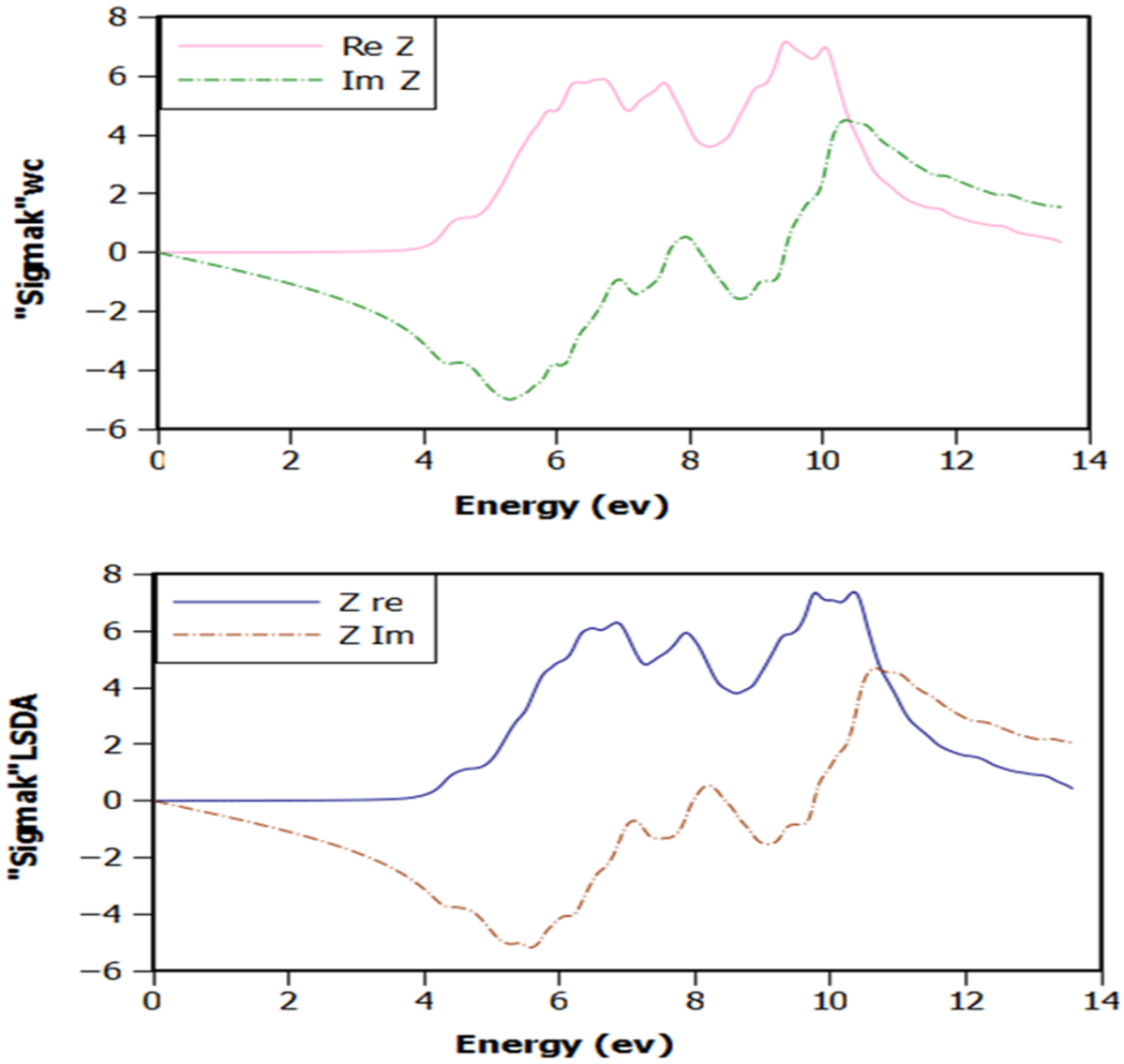

Figure 5: The conductivity coefficient for real and imaginary parts of Z, WC, and LSDA

Conclusion

The curves of all optical properties obtained by the calculations of hexagonal structure of lanthanum oxide crystal in both X and Z directions at upper and lower energies are well correlated. Experimental results on the lanthanum oxide crystal were not found to be compared with the results obtained from WIEN2K software.

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