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Investigation of optical properties of SiO₂ using DFT method

Samin birashk and Haleh Kangarlou

Department of Physics, Urmia Branch, Islamic Azad University, Urmia, Iran

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ABSTRACT

In this research optical properties such as dielectric function, absorption coefficient, energy loss function and reflectivity coefficient of SiO₂ crystal have been studied. The calculations have been performed using the Full-Potential-Linearised Augmented Plane Waves (FP-LAPW) method within the framework density functional theory (DFT) by WIEN2K package. Optical properties are calculated by (LSDA) approximations and (GGA) approximation with WC functional. The results revealed that optical properties are anisotropic along x and z directions.

Keywords:

Optical Properties, SiO₂, DFT

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INTRODUCTION

Quartz is a chemical compound made of two parts, one part Silicon and the other part is Oxygen (SiO₂) (Eugene, Papier, 2000), Which in pure form or in the form of silicate minerals forms about 60 percent of the Earth's solid crust (Grunthaner, P.J. *et al.*, 1987). From the molecular perspective, silica crystal beads are crystalline and there is no electronic connection in its networks. Quartz is able to pass the ultraviolet rays through itself. It has piezoelectric properties, and produces electrical load in presense of mechanical pressure. Beta quartz is resistant in the temperatures of 573 °C up to 870 °C. This type of quartz is found in the form of band-gap crystals in Quartz porphyry and graffiti granite (Bates, R.L. and J.A. Jackson, 1980). High-temperature quartz is found in the form of crystallized prismatic crystals in the 622-rate hexagonal systems. SiO₂ cells have been illustrated in figure 1.

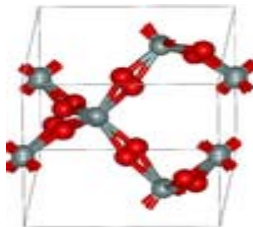


Fig. 1: SiO₂ cells.

Calculation method:

Beta-quartz silica crystal enjoys the space group $P6_2 22$ $\alpha=\beta=90$ and $\gamma=120$ in the hexagonal phase. The calculations were conducted using the WIEN2K package developed by Blaha and Schwarz (Blaha, P. *et al.*, 2000) This program employs linearized augmented plane wave (LAPW) (Singh, D.J., 1994) in the framework of the density functional theory (DFT) (Hohenberg, P. and W. Kohn, 1964) used. Also, LSDA and GGA approximations with the three functionals of PBE, PBE sol and WC (Perdew, John P. *et al.*, 1987), (Perdew, j.p. *et al.*, 2009) used. WC is a new functional based on PBE functional in which the interchangeable functional part has undergone so much change, compared to PBE functional, that gradient expansion of the exchange energy has been applied up to four times. The muffin-tin radius of the compound stood at 1.8 a.u. and 1.1 a.u. for silicon and oxygen respectively. To separate capacity states from core states, we selected 6D Rydberg energy. We also selected the range of energy conversion from 0.0001. To achieve such a conversion, we put Rkmax at 7. There were 12 points in the first Brillouin zone, forming a 4*4*4 lattice.

Results:

To minimize beta-quartz, a number of structures with the parameters of a and c lattices located 0.02 angstroms from the empirical minimum point were modified so as to change constant c value for each constant

a value. This process was repeatedly applied to the other constant values of a as well, obtaining the lowest volume of energy as energy minimum and its corresponding structure as optimum structure. Details of the optimization process applied to the lattice constant of silica beta-quartz have been presented in table 1.

Table 1: Optimization of fixed network using different functional.

Lattice Constant c	Lattice Constant a=b	
5.621	5.153	Functional (PBE)
5.616	5.143	Functional (LSDA)
5.608	5.136	Functional (WC)
5.47	5.01	Experimental (Allan,D. and M. Teter,1987)

As seen in table 1, the best correspondence between empirical and theoretical results belongs to WC functional. Figure 2 illustrates the results of energy optimization in relation with the volume.

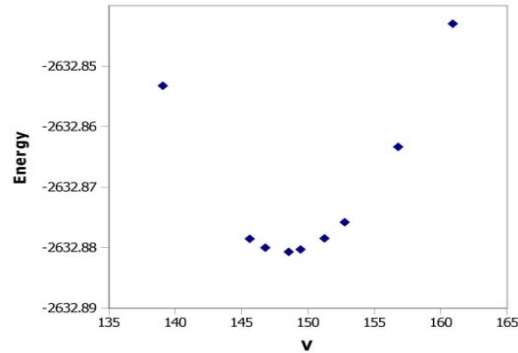


Fig. 2: Energy optimization in relation with the volume.

Discussions:

Electron energy loss function:

Electron energy loss spectroscopy is a powerful way for analyzing populated states above the Fermi level or conducting partial separation. This spectrum involves the mass-stimulation of valence electrons (plasmons) into the populated states of the conduction band. The most distinctive peak in the electron energy loss function, known as the "Plasmon peak", is indicative of the mass-stimulation of the electron charge density in the crystal. The highest energy loss of the crystal is 5.70 electron-volts along X direction (a vector) and 6 electron-volts along Z direction (vector c). SiO₂ energy loss graph has been presented in figure 3.

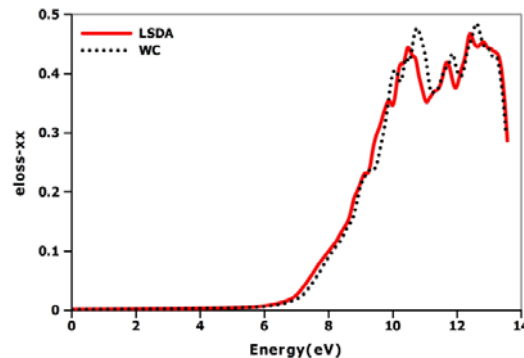


Fig. 3: Beta-quartz energy loss function along X direction.

Based on the free electron model, the Plasmon energy is obtained through the following relation:

$$E_p = \omega_p = \sqrt{ne^2/m_0\epsilon_0} \quad (1)$$

Where, n is free electron density in cell size, m_0 is electron mass and e is electric charge unit.

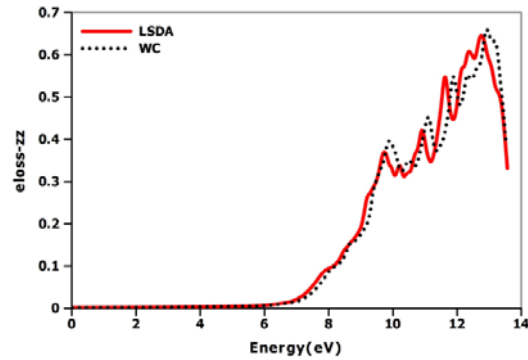


Fig. 4: Beta-quartz energy loss function along Z direction.

Reflection coefficient:

Reflection coefficient is calculated when a propagated wave is not continuous. It determines the intensity or range of a reflected wave in relation with an incident wave. Reflection coefficient is closely related to transfer coefficient. As seen in figure 5, the reflectance spectrum enjoys propagation for energies exceeding the energy gap.

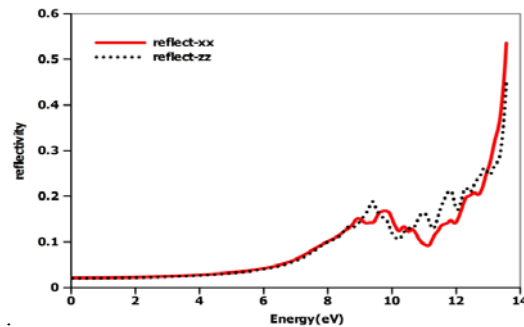


Fig. 5: Beta-quartz reflection coefficient along X and Z directions.

Dielectric function:

To observe material's responses to electromagnetic waves (light), the dielectric function of the material is calculated. The dielectric function has two inter-band and intra-band components. The intra-band component is applied to metals. The dielectric function is a mixed function shown as

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega) \quad (2)$$

$\varepsilon_1(\omega)$ changes could be obtained based on Kramers-Kronig transformation when $\varepsilon_2(\omega)$ are available.

$\varepsilon_1(\omega)$ roots have physical concepts and in fact are the requirement for volume plasmons in the material, while the existence of energy loss is the requirement for the existence of these roots. Also, waves are not propagated and processes of absorption and loss do not take place when $\varepsilon_1(\omega)$ is negative.

The real part of SiO₂ dielectric function along X and Z directions, namely vectors *a* and *c* of the hexagonal structure, have been presented for LSDA and WC functionals in figures 6 and 7, while the imaginary part of the function has been illustrated in figures 8 and 9.

Absorption coefficient:

Absorption coefficient is indicative of drop and loss in sound intensity when sound passes through a certain place. Absorption coefficient data contribute to calculating refractive index. Based on calculations on SiO₂ to determine its absorption coefficient with the help of LSDA and WC functionals as well as a comparison between the results of this calculation process and those obtained through empirical methods, the results achieved through the use of WC functional closely correspond with results obtained through empirical methods. Figure 10 illustrates a combination of the results of theoretical and empirical methods used to calculate absorption coefficient.

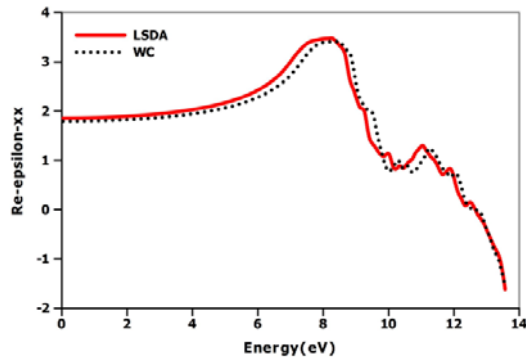


Fig. 6: The real part of SiO2 dielectric function along X direction.

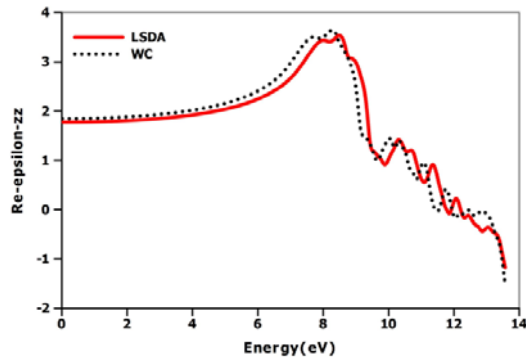


Fig. 7: The real part of SiO2 dielectric function along Z direction.

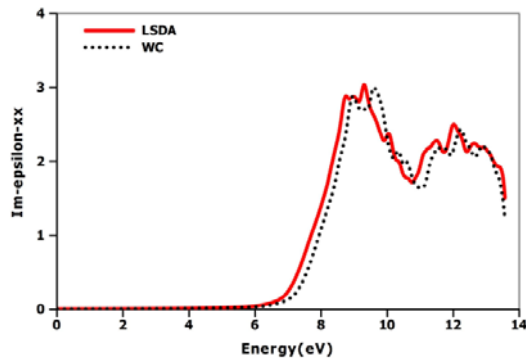


Fig. 8: The imaginary part of SiO2 dielectric function along X direction.

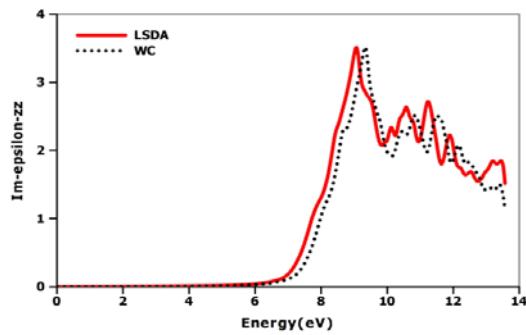


Fig. 9: The imaginary part of SiO2 dielectric function along Z direction.

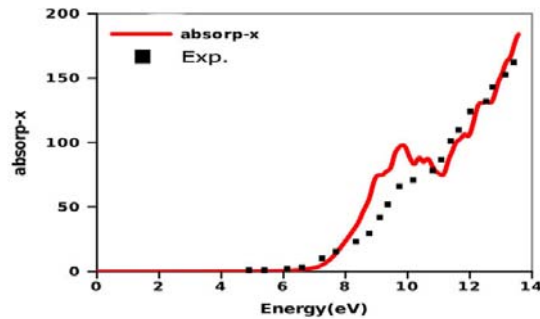


Fig. 10: Comparison of empirical and theoretical results related to calculating absorption coefficient along X direction

Conclusion:

Since SiO₂ beta-quartz is used in optical fiber and optical sensor industries, the current study examined the optical properties of SiO₂ with LSDA and WC functionals through the use of Wein2k software program and compared the results with available empirical results. The comparison showed that there was a good correspondence between the results of this study and empirical results. We calculated the dielectric function along X and Z directions and compared the results related to the real and imaginary parts of the functionals, finding out that there is little difference between the results obtained through the use of LSDA and WC functionals. As for the absorption coefficient, there was a good consistence between the results obtained through theoretical and empirical methods. The results indicated that SiO₂ shows different optical properties depending on the direction of descending waves, something that is of great importance for non-cubic structures.

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