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Investigation of optical nanosensors using quartz optical properties

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Abstract

In this paper optical properties such as dielectric function, absorption coefficient ، energy loss function and reflectivity coefficient of SiO2 crystal have been studied. The calculation have been performed using the Full-Potential-Linearrised Argumented Plane Waves (FP-LAPW) method within the framework density functional theory (DFT) by WIEN2K package.

Optical properties is calculated by (GGA) approximation with PBE functional .The results revealed that optical properties are anisotropic along x and z directions.

Keywords:, SiO2, DFT, PBE , WIEN2k

Introduction

Quartz, a chemical compound composed of one component of silicon and two components of oxygen (SiO2) [1], is found in silicate minerals as a pure element or compounded with other elements and makes up about 60 percent of earth crust [2]. Silica grains are molecularly crystallized in lattices lacking electron connections. Quartz is capable of transmitting ultra-velvet rays, enjoys piezoelectric properties, and produces electrical charge under mechanical pressure. SiO2 is resistant against temperatures ranging between 573 °C and 870°C. This type of quartz is found in the form of band-gap crystals in Quartz porphyry and graffiti granite [3]. High-temperature quartz is found in the form of crystallized prismatic crystals in the 622-rate hexagonal systems [4]. SiO2 cells have been illustrated in figure 1.

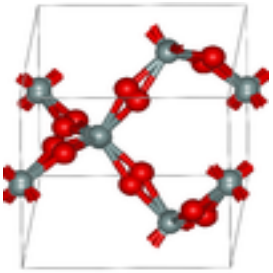

Figure 1- SiO2 cells

1- Calculation method

Beta-quartz silica crystal enjoys the space group $P6_222$ β=α=90 and γ=120 in the hexagonal phase. The calculations were conducted using the WIEN2K package developed by Blaha and Schwarz [5]. This program employs linearized augmented planewave (LAPW) [6] in the framework of the density functional theory (DFT) [7]. Also, LSDA and GGA approximations [8]

with the three functionals of PBE, PBEsol and WC [9, 10, and 11] were used during the calculation process. 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.

1.1.Calculation 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- lattice constant optimization using various functionals

Lattice constant c	Lattice constant c=b	
5.621	5.153	Functional (PBE Beta)
5.616	4.93	Functional (PBE Alfa)
5.608	5.136	Functional (WC)
5.47	5.01	Empirically [12]

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.

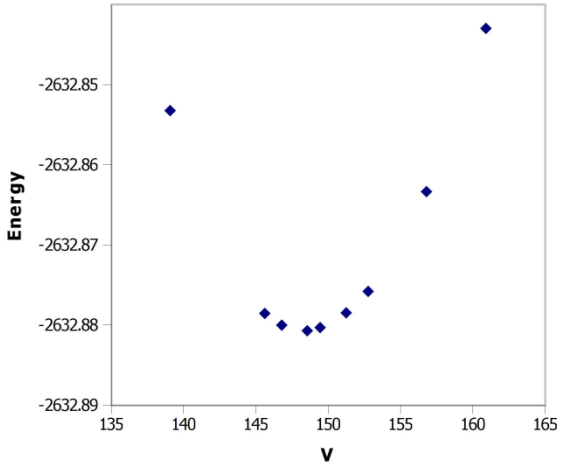

Figure 2- energy optimization in relation with the volume

1.2. 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.

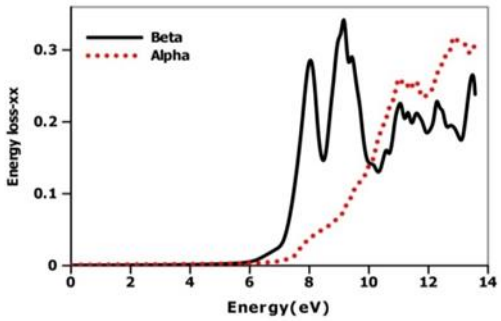

Figure 3- Beta-quartz and Alfa-quartz energy loss function along X direction

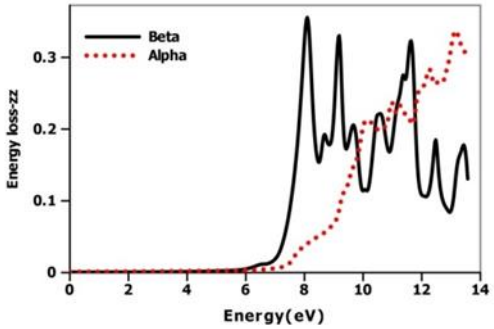

Figure 4- beta-quartz and Alfa-quartz energy loss function along Z direction

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

$$(1)\ E_{\mathrm{p}} = \omega_{\mathrm{p}} = \frac{\sqrt{ne^2}}{m_o \varepsilon_o}$$

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

1.3.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.

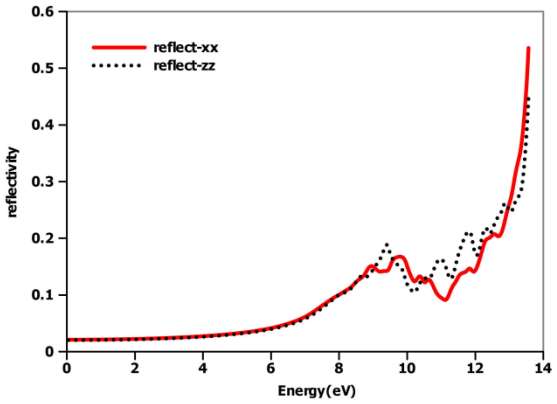

Figure 5- Alfa-quartz reflection coefficient along X and Z directions

1.4.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 PBE functionals in figures 6 and 7, while the imaginary part of the function has been illustrated in figures 8 and 9 .

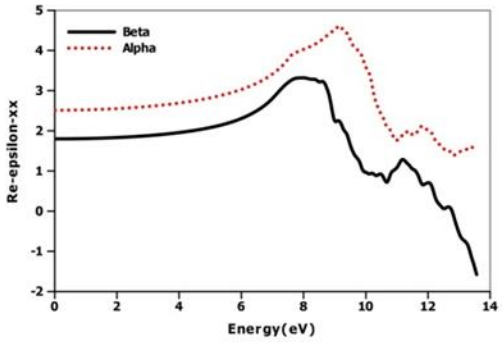

Figure 6- the real part of SiO2 dielectric function along X direction

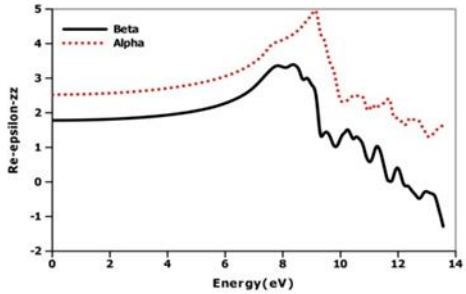

Figure 7- the real part of SiO2 dielectric function along Z direction

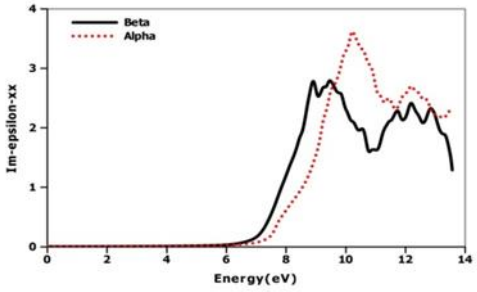

Figure 8- the imaginary part of SiO2 dielectric function along X direction

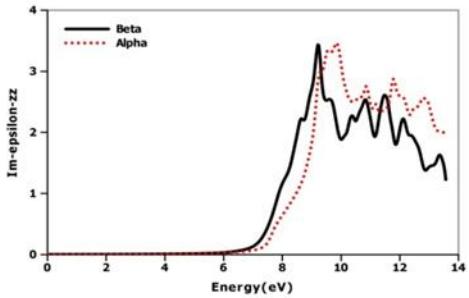

Figure 9- the imaginary part of SiO2 dielectric function along Z direction

A comparison between PBE functionals shows that there is a lot of difference between the results of these functionals.

1.5.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 functinals 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.

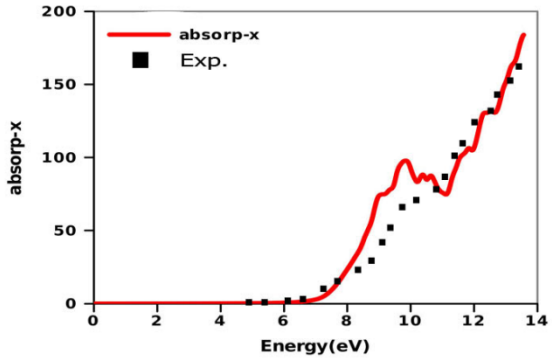

Figure 10- comparison of empirical and theoretical results related to calculating absorption coefficient along X direction

Conclusion

Since SiO2 beta-quartz is used in optical fiber and optical sensor industries, the current study examined the optical properties of SiO2 with PBE 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 a lot of difference between the results obtained through the use of beta-quartz and Alfa-quartz 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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