Ab initio Modeling of Elastic and Optical Properties of Sb and Bi Sesquioxides

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Abstract. First-principle calculations performed the structural, mechanical, electronic, and optical properties of Sb\(_2\)O\(_3\) and Bi\(_2\)O\(_3\) compounds in monoclinic (claudetite and \(\alpha\)-Bi\(_2\)O\(_3\)) and orthorhombic (valentinite) structures. Local density approximation has been used for modeling exchange-correlation effects. The lattice parameters, bulk modulus, and the first derivate of bulk modulus (to fit to the Murnaghan’s equation of state) of considered compounds have been calculated. The second-order elastic constants have been calculated, and the other related quantities have also been estimated in the present work. The electronic bands structures and the partial densities of states corresponding to the band structures are presented and analyzed. The real and imaginary parts of dielectric functions and energy-loss function are calculated. Our structural estimation and some other results are in agreement with the available experimental and theoretical data.

1. Introduction

Sb\(_2\)O\(_3\) and Bi\(_2\)O\(_3\), the members of compounds with the general formula \(A^V_2B^VI\) (A=Bi, Sb, As and \(B=S, Se, Te\)), are important semiconductors with wide band gaps intensified recent years \cite{1}, due to their attractive physical properties. Sb\(_2\)O\(_3\) includes three crystalline structures: cubic \(\alpha\)-phase (senarmontite), orthorhombic \(\beta\)-phase (valentinite), and a very recently found new phase (\(\gamma\)-phase). As\(_2\)O\(_3\) also include two crystalline structures: cubic arsenolite and monoclinic claudetite. Bi\(_2\)O\(_3\) include six crystalline structures: monoclinic \(\alpha\)-phase, tetragonal \(\beta\)-phase, cubic \(\gamma\)-phase, cubic \(\delta\)-phase, or orthorhombic \(\epsilon\)-phase, and triclinic \(\omega\)-phase \cite{2-5}. Sb\(_2\)O\(_3\) is used extensively in industry as a flame retardant in polymer, coatings, and textiles while Bi\(_2\)O\(_3\) is used in the field of gas sensors, fuel cells, optical coatings or ceramic glass manufacturing \cite{1, 5}.

The positions corresponding to these compounds have been obtained from experimental and theoretical data \cite{2, 6-8}. In the past, some detailed works \cite{1, 2, 5, 9-13} have been carried out on the theoretical or experimental works of Sb\(_2\)O\(_3\) and Bi\(_2\)O\(_3\) compounds. Matsumoto et al. \cite{2} systematically investigated the relationships between the electronic structures, energetic and atomic arrangements of three sesquioxides (As\(_2\)O\(_3\), Sb\(_2\)O\(_3\), and Bi\(_2\)O\(_3\)) using first-principles lattice-dynamics calculations. Pereira et al. \cite{5} investigated experimentally and theoretically under high pressure the Sb\(_2\)O\(_3\) in cubic phase (senarmontite) by means of X-ray diffraction (XRD) and the density-functional theory (DFT). Condurache-Bota et al. \cite{1} studied the structural characteristics of Sb\(_2\)O\(_3\) and Bi\(_2\)O\(_3\) by means of X-ray diffraction. Fruth et al. \cite{9} analyzed the structural changes of \(\alpha\)- Bi\(_2\)O\(_3\) by means of powder X-ray diffraction.
diffraction, SEM/EDX analysis and infrared spectroscopy. Chouinard et al. [10] observed the structural transition of α-Bi$_2$O$_3$ under hydrostatic pressure using different experimental techniques. Pereira et al. [11, 12] investigated the structural and vibrational properties using the density functional theory of α-Bi$_2$O$_3$ under pressure. Li et al. [13] investigated the atomic-scale interfacial structure and the electronic-scale interface properties between α- Bi$_2$O$_3$ and β- Bi$_2$O$_3$ homo-junction using the density functional theory within the generalized gradient approximation.

In this work, we have especially focused on the electronic, mechanical and optical properties of Sb$_2$O$_3$ and Bi$_2$O$_3$ compounds by using ab initio total energy calculations. To our knowledge, the elastic constants, Young’s modulus, shear modulus, Poisson’s ratio, sound velocities, Debye temperature (outside the Debye temperature of α-Bi$_2$O$_3$), and optical properties have not been reported in detail for Sb$_2$O$_3$ and Bi$_2$O$_3$ so far.

2. Method of calculation
Our calculations have been performed using the density functional formalism and local density approximation (LDA) [14] through the Ceperley and Alder functional [15] as parameterized by Perdew and Zunger [16] for the exchange-correlation energy in the SIESTA code [17, 18]. This code calculates the total energies and atomic forces using a linear combination of atomic orbitals as the basis set. The basis set is based on the finite range pseudoatomic orbitals (PAOs) of the Sankey Niklewsky type [19], generalized to include multiple-zeta decays.

The interactions between electrons and core ions are simulated with separable Troullier-Martins [20] norm-conserving pseudopotentials. We have generated atomic pseudopotentials separately for atoms, Sb, Bi and O by using the 5s$^2$5p$^3$, 6s$^2$6p$^3$ and 2s$^2$2p$^1$ configurations, respectively. The cut-off radii for present atomic pseudopotentials are taken as s: 3.82 au, p: 2.71 au, 2.92 au for the d and f channels of Bi, 2.35 for the s, p and d channels of Sb, 1.47 au for the s, p, d and f channels of O.

SIesta calculates the self-consistent potential on a grid in real space. The fineness of this grid is determined in terms of an energy cut-off $E_c$ in analogy to the energy cut-off when the basis set involves plane waves. Here by using a double-zeta plus polarization (DZP) orbitals basis and the cut-off energies between 100 and 500 $Ry$ with various basis sets, we found an optimal value of around 350 $Ry$ for Sb$_2$O$_3$ and Bi$_2$O$_3$ in claudetite, α-Bi$_2$O$_3$ and valentinite structures. For the final computations, 100 k-points for Sb$_2$O$_3$ and Bi$_2$O$_3$ were enough to obtain the converged total energies ΔE to about 1meV/atoms.

3. Results and discussion
3.1 Structural properties
For Sb$_2$O$_3$ and Bi$_2$O$_3$, structures that are monoclinic (claudetite and α-Bi$_2$O$_3$) and orthorhombic (valentinite) are considered. The equilibrium lattice parameters, the bulk modulus, and its pressure derivative were calculated by means of Murnaghan’s equation of states (eos) [21], and the results are shown in Table 1 along with the experimental and theoretical values. The lattice constants are found to be a= 4.90 Å, b= 12.61 Å, c=5.39 Å in valentinite structure and a= 10.13 Å, b= 5.07 Å, c=15.11 Å in claudetite structure for Sb$_2$O$_3$ and a= 11.71 Å, b= 5.70 Å, c=5.65 Å in valentinite structure and a= 5.88 Å, b= 8.22 Å, c=7.48 Å in α-Bi$_2$O$_3$ structure for Bi$_2$O$_3$. The lattice parameters obtained are in good agreement with the experimental and theoretical values [2, 4, 7, 11, 13 and 22]. In all our calculations, we have used the computed lattice constants. In the present case, the calculated bulk moduli are 140.93 GPa (valentinite) and 123.56 GPa (claudetite) for Sb$_2$O$_3$ and 133.54 GPa (valentinite) and 113.74 GPa (α-Bi$_2$O$_3$) for Bi$_2$O$_3$. The bulk modulus of the solid as fundamental physical properties provides valuable information, including the average bond strengths of the atoms for the given crystals [23]. In the present case, the largest value of bulk modulus is obtained for Sb$_2$O$_3$ in valentinite structure, and it implies that this structure is the least compressible one among the others. The obtained bulk modulus for α-Bi$_2$O$_3$ is in good agreement with the experimental value, but is larger (%20.78) than the theoretical value [11].
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Table 1. The calculated equilibrium lattice parameters (a, b, and c), bulk modulus (B), and the pressure derivative of bulk modulus (B') together with the theoretical and experimental values for Sb₂O₃ and Bi₂O₃ compounds in monoclinic (claudetite and α-Bi₂O₃) and orthorhombic (valentinite) structures

| Compound       | Reference               | Structure  | a (Å) | b (Å) | c (Å) | B (GPa) | B'      |
|----------------|-------------------------|------------|-------|-------|-------|---------|---------|
| Sb₂O₃          | Present Experimental[4] | valentinite| 4.90  | 12.61 | 5.39  | 140.93  | 4.72    |
|                | Theory (GGA-VASP) [2]   |            | 4.91  | 12.46 | 5.41  | 123.56  | 4.57    |
|                |                         |            | 5.20  | 12.56 | 5.52  |         |         |
| Sb₂O₃          | Present Experimental[4] | claudetite | 10.13 | 5.07  | 11.51 | 133.54  | 4.54    |
|                | Theory (GGA-VASP)[2]   |            | 9.73  | 4.87  | 14.51 |         |         |
| Bi₂O₃          | Present Experimental[11]| valentinite| 11.71 | 5.70  | 5.65  | 113.74  | 4.55    |
|                | Theory (GGA-VASP)[7]   |            | 11.81 | 5.74  | 5.69  |         |         |
| Bi₂O₃          | Present Experimental[11]| α-phase    | 5.88  | 8.22  | 7.48  | 107.07  | 1.6GGA  |
|                | Theory (GGA-VASP)[7]   |            | 5.85  | 8.17  | 7.51  | 90.1GGA | 4.8GGA  |
|                | Theory (GGA-CASPEP)[13]|          | 5.84  | 8.16  | 7.50  |         |         |

3.2. Elastic Properties

The mechanical behavior of materials reflects the resistance or the deformation of the material against the applied load or force. The stiffness, strength, hardness and ductility comprise the basic parameters used in the design. The elastic constants of the material establish a relationship between the mechanical and dynamic behavior of solids, and gives information about the stability and mechanical hardness of the materials. The magnitude of the elastic constants are a measure of resistance (so, of bond strength between atoms) against separation from each other of the neighboring atoms [24-26].

SIESTA for elastic constants makes calculations using the "volume-conserving" technique [27]. The elastic constants for Sb₂O₃ and Bi₂O₃ in the valentinite, claudetite, and α-Bi₂O₃ structures are given in Table 2. Unfortunately, there are no theoretical results for comparing the present work.

Table 2. The calculated elastic constants (in GPa) for Sb₂O₃ and Bi₂O₃ compounds

| Compound       | Structure | C₁₁   | C₁₂   | C₁₃   | C₁₅   | C₂₂   | C₂₃   | C₂₅   | C₃₃   | C₅₅   | C₅₆   | C₆₆   |
|----------------|-----------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| Sb₂O₃          | claudetite| 202.1 | 56.2  | 94.1  | 10.6  | 236.3 | 111.6 | 29.6  | 240.1 | 15.7  | 49.5  | 18.7  |
|                | valentinite| 234.2 | 102.2 | 103.2 | -228.8| 98.7  | -153.0| -69.5 | -55.1 | 72.3  | 52.9  | 45.9  |
| Bi₂O₃          | α-phase   | 222.1 | 80.6  | 83.2  | -2.1  | 198.2 | 55.2  | 29.1  | 249.3 | 31.9  | 59.2  | 16.7  |
|                | valentinite| 215.3 | 99.6  | 88.2  | -203.5| 73.2  | -251.9| -77.7 | -97.9 | 83.9  |       |       |

The elastic constants C₁₁, C₂₂, and C₃₃ measure the α-, b-, and c-direction resistance to linear compression, respectively. The C₅₅ for valentinite structure is lower than the C₁₁ and C₂₂ while the C₁₁ for claudetite structure of Sb₂O₃ is lower than the C₂₂ and C₃₃. The calculated C₂₂ for both structure of Bi₂O₃ is lower than the C₁₁ and C₃₃. Thus, Sb₂O₃ compound is more compressible along c-axis for valentinite structure and a-axis for claudetite structure while Bi₂Se₃ compound is more compressible along the b-axis for both structures. The large C₆₆ shows a strong resistance against the monoclinic shear distortion in (100) plane. The C₅₆ relates to the shear resistance in the direction <110>. In the Sb₂O₃ and Bi₂O₃ compounds, C₄₆ and C₆₆ in valentinite and α-Bi₂O₃ structures of Bi₂O₃ compounds have the highest value.
Table 3. The calculated isotropic bulk modulus (B, in GPa), shear modulus (G, in GPa), Young’s modulus (E, in GPa), Poisson’s ratio, sound velocities (v_l, v_t, v_m, in m/s) and Debye temperature for Sb_2O_3 and Bi_2O_3 compounds.

| Compound | Reference | Structure       | B (GPa) | G (GPa) | E (GPa) | v_l (m/s) | v_t (m/s) | v_m (m/s) | θ_D (K) |
|----------|-----------|-----------------|---------|---------|---------|-----------|-----------|-----------|---------|
| Sb_2O_3  | Present   | claudetite      | 129.3   | 59.1    | 153.8   | 0.302     | 5970      | 3181      | 3554    | 414.9   |
|          | Present   | valentinite     | 132.7   | 59.3    | 154.8   | 0.305     | 5882      | 3113      | 3479    | 412.7   |
| Bi_2O_3  | Present   | α-phase         | 118.9   | 72.2    | 180.1   | 0.248     | 4679      | 2709      | 3007    | 357.2   |
|          | Exp. [42] |                 |         |         |         |           |           |           |         |         |
|          | Present   | valentinite     | 132.2   | 77.7    | 194.9   | 0.254     | 4983      | 2860      | 3177    | 373.2   |

The polycrystalline elastic moduli are calculated from Voigt and Reuss approximation methods [28-34] using elastic constants. We use the Hill average [34] to calculate Young’s modulus (E) and Poisson’s ratio (ν) using the refs. [35, 36]. The calculated bulk modulus, isotropic shear modulus, Young’s modulus and Poisson’s ratio are given in Table 3. The bulk modulus is a measure of resistance against the volume change under an applied pressure. The size of bulk modulus shows the hardness of solid. The calculated bulk moduli of Sb_2O_3(Bi_2O_3)-valentinite and Sb_2O_3-claudetite (α- Bi_2O_3) structures are 132.7 (132.2) GPa and 129.3 (118.9) GPa. In general, the calculated bulk modulus for either phase is Sb_2O_3 > Bi_2O_3. Therefore, Sb_2O_3 for either phase is harder than Bi_2O_3. The shear modulus is a measure of resistance to reversible deformations upon shear stress [37]. The calculated shear modulus for Bi_2O_3 is higher than Sb_2O_3 compound (see Table 3). Young’s modulus is a measure of the ratio of stress and strain. The material is stiffer if the value of Young’s modulus is high. The Young’s modulus (194.9 GPa for valentinite and 180.1 for α-Bi_2O_3) of Bi_2O_3 compound is relatively stiffer than Sb_2O_3 (154.8 GPa for valentinite and 153.8 GPa for claudetite). The value of the Poisson’s ratio is small (ν =0.1) for covalent materials, whereas for ionic materials a typical value of ν is 0.25 [38]. The calculated Poisson’s ratios of Sb_2O_3(Bi_2O_3)-valentinite and Sb_2O_3-claudetite (α-Bi_2O_3) structures are approx. 0.305 (0.254) and 0.302 (0.248). Therefore, the ionic contribution to inter atomic bonding for these compounds is dominant.

The Debye temperature and sound velocity that separates [39-41] the low and high temperature region of solids are calculated for Sb_2O_3 and Bi_2O_3 compounds by use of the elastic constants. The calculated values of the longitudinal, transverse, and average sound velocities are shown in Table 3 along with the Debye temperature. For materials, usually, the higher Debye temperature, the larger microhardness. The calculated Debye temperature for Sb_2O_3 in both structures is higher than Bi_2O_3. The Debye temperature obtained is greater than experimental value (see Table 3).

### 3.3. Electronic properties

The electronic band structures of Sb_2O_3 and Bi_2O_3 single crystals in monoclinic (claudetite and α-Bi_2O_3) and orthorhombic (valentinite) structures have been calculated along high symmetry directions in the first Brillouin zone (BZ).

![Energy band structures for Sb_2O_3 in a) valentinite and b) claudetite structures](image-url)
The energy band structures calculated using LDA for Sb$_2$O$_3$ and Bi$_2$O$_3$ are shown in Fig. 1 and Fig. 2. As can be seen in Fig. 1a, the Sb$_2$O$_3$ compound in valentinite structure has a direct band gap (at the Γ point) semiconductor with the value 1.97 eV. The band gap is 0.23 eV smaller than that obtained by theory [2]. The band gap of Sb$_2$O$_3$ compound in claudetite structure (see Fig. 1b) has the different character with that of valentinite structure, that is, it is an indirect band gap semiconductor. The top of the valance band positioned at the Y point of BZ, the bottom of the conduction band is located of BZ. The indirect band gap values of claudetite structure are 2.24eV. The band gap is 0.27 eV smaller than that obtained by theory [2]. The calculated band structures of Bi$_2$O$_3$ are given in Fig. 2. As can be seen from the figure, valentinite and α-Bi$_2$O$_3$ structures have the same character, that is, it have an indirect band gap semiconductor with the value 1.54 eV and 2.14 eV, respectively. For valentinite structure, the top of the valance band and the bottom of the conduction band are located at the S point and X point of BZ, respectively. The band gap is 0.2 eV smaller than that obtained by theory [2]. Similarly, the top of the valance band for α-Bi$_2$O$_3$ structures positioned at the nearly B point between B and A point of BZ, the bottom of the conduction band is located at the Γ point of BZ. The band gap is 0.15 eV, 0.66 eV and 0.57 eV smaller than that obtained by theory [2, 13] and experiments, respectively [43]. The total and partial densities of states of Sb$_2$O$_3$ and Bi$_2$O$_3$ compounds were calculated too. The lowest valence bands (approx. -20 and -17 eV) are dominated by O 2s states. While the highest occupied valance bands are essentially dominated by O 2p states. The middle valance bands (approx. -12 and -7eV) are dominated by Sb 5s and Bi 6s states. The lowest unoccupied conduction bands just above Fermi energy level is dominated by Sb 5p and Bi 6p. The band structures of Sb$_2$O$_3$ and Bi$_2$O$_3$ single crystals are compared, band structures of these crystals are highly resemble one another. Thus, on formation of the band structures of Sb$_2$O$_3$ and Bi$_2$O$_3$ the 2s 2p orbitals of O atoms are more dominant than 5s5p and 6s6p orbitals of Sb and Bi atoms.

3.4. Optical properties

The linear optical properties obtained from the complex dielectric function [44, 45, 24] of Sb$_2$O$_3$ and Bi$_2$O$_3$ are investigated. The imaginary parts of the frequency-dependent linear dielectric function were calculated. The real part of the linear dielectric function can be obtained by the Kramers-Kronigrelations [45] using the imaginary component. We first calculated the real and imaginary parts of the x- and z-components of the frequency-dependent linear diellectric function. The $\varepsilon_{xx}^1$ behaves mainly as a classical oscillator. It vanishes (from positive to negative) at approx. 7.34 (6.77) eV and 11.75 (11.35) eV, whereas the other function $\varepsilon_{zz}^1$ is equal to zero at approx. 6.20 (6.23) eV and 12.58 (11.92) eV for Sb$_2$O$_3$ in valentinite (claudetite) structure. For Bi$_2$O$_3$, the $\varepsilon_{xx}^1$ is equal to zero at approx. 6.66 eV, 11.37 eV, 13.11 eV, 13.33 eV, 16.89 eV, and 18.04 eV in valentinite structure and at approx. 6.47 eV, 10.74 eV, 14.53 eV, and 18.66 eV in α-Bi$_2$O$_3$ structure, whereas the other function $\varepsilon_{zz}^1$ is equal to zero at approx. 6.93 eV, 11.76 eV, 16.87 eV, 16.98 eV, 17.57 eV, and 18.58 eV in valentinite structure and at approx. 6.83 eV, 10.80 eV, 14.36 eV, and 19.08 eV in α-Bi$_2$O$_3$ structure. The peaks of the $\varepsilon_{xx}^2$ and $\varepsilon_{zz}^2$ correspond to the optical transitions from the valence band to the conduction band and are in agreement with the previous results. The maximum peak values of $\varepsilon_{xx}^2$ and $\varepsilon_{zz}^2$ for Sb$_2$O$_3$ in

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**Figure 2.** Energy band structures for Bi$_2$O$_3$ in a) valentinite and b) α-Bi$_2$O$_3$ structures

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valentinite (claudetite) structures are around 5.03 (3.84) eV and 3.95 (4.27) eV, respectively, whereas the maximum values of $\varepsilon_1$ and $\varepsilon_2$ for Bi$_2$O$_3$ in valentinite (α-Bi$_2$O$_3$) structures are around 4.52 (4.16) eV and 4.68 (4.41) eV, respectively. The corresponding energy-loss functions, $L(\omega)$, were also calculated. The function $L(\omega)$ describes the energy loss of fast electrons traversing the material. The sharp maxima in the energy-loss function are associated with the existence of plasma oscillations [46]. The curves $L(\omega)$ have a maximum near 11.78 (11.43) eV and 12.74 (12.03) eV for Sb$_2$O$_3$ in valentinite (claudetite) structures, respectively and 20.41 (19.32) eV and 20.90 (19.57) eV for Bi$_2$O$_3$ in valentinite (α-Bi$_2$O$_3$) structures, respectively.

4. Conclusion
In this study, the structural, mechanical, electronic, and optical properties of Sb$_2$O$_3$ and Bi$_2$O$_3$ compounds in valentinite, claudetite, and α-Bi$_2$O$_3$ structures are investigated by using the local density approximation. The calculated lattice parameters are in agreement with experimental and theoretical values. The elastic constants obtained show that Sb$_2$O$_3$ compound is more compressible along the c-axis for the valentinite structure and the a-axis for the claudetite structure while Bi$_2$Se$_3$ compound is more compressible along the b-axis for both structures. From the calculated bulk modulus using elastic constants, it can be said that Sb$_2$O$_3$ for either phase is harder than Bi$_2$O$_3$. The calculated Poisson’s ratio of Sb$_2$O$_3$(Bi$_2$O$_3$)-valentinite and Sb$_2$O$_3$-claudetite (α-Bi$_2$O$_3$) structures is approx. 0.305 (0.254) and 0.302 (0.248). Therefore, the ionic contribution to inter atomic bonding for these compounds is dominant. The Debye temperature and sound velocities have been calculated, and the calculated Debye temperature for Sb$_2$O$_3$ in both structures is higher than Bi$_2$O$_3$. The obtained electronic band structures show that Sb$_2$O$_3$ and Bi$_2$O$_3$ compounds are semiconductor in nature. Lastly, we have examined photon-energy dependent dielectric functions and the energy-loss function along the x- and z-axes.

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