The First-Principle Study on The Holmium Oxonitridosilicate ($Ho_3Si_5N_9O$) Compound: Mechanical and Electronic Properties

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ABSTRACT

We have used to ab-initio methods for determining the structural, electronic, and elastic properties for the $Ho_3Si_5N_9O$ compound in the orthorhombic Pbcm structure (Space Group No:57, Z=4). The DFT-PBE and PP-PAW approaches are used for predictions which implemented in the VASP package. We have computed the basic physical parameters such as lattice constants, bulk modulus, elastic constants. The calculations reveal that $Ho_3Si_5N_9O$ is mechanically stable and that an indirect band gap semiconductor compound.

1. INTRODUCTION

The class of oxonitridosilicates, which can be seen as the intersection between oxosilicates and nitridosilicates, show similar structural motives to both classes [1]. These compounds gained significant relevance in materials science because of their remarkable chemical and thermal stability [2]. They also have been considered as a host lattices for rare-earth-doped phosphors in light-emitting diode (LED) applications [2]. The compounds $Dy_3[Si_5N_9O]$, $Ho_3[Si_5N_9O]$, $Er_3[Si_5N_9O]$, and $Yb_3[Si_5N_9O]$ were synthesized by Wilhelm as the first isotypic series of the oxonitridosilicates [1]. With this motivation, the systematic density functional theory (DFT) investigation of structural, electronic, and mechanical properties of $Ho_3[Si_5N_9O]$ compound was done for the first time. The organization of this study is as follows: The method of calculation is given in Section 2, the results and overall conclusions are presented and discussed in Section 3.

2. METHOD

All calculations have been carried by using the VASP code [3-4] based on the density functional theory (DFT). The electron–ion interaction was considered in the form of the projector-augmented-wave (PAW) method with plane wave up to an energy of 500 eV [5], an adequate value for studying the physical properties. Perdew–Burke–Ernzerhof (PBE) type functional [6] within the generalized gradient approximation (GGA) has been used for the exchange and correlation terms in the electron–electron interaction. 6x2x3 Monkhorstand Pack [7] grid of k-points has been used. The stress-strain method, implemented in the VASP code, was used to predict the second order elastic constants [8].

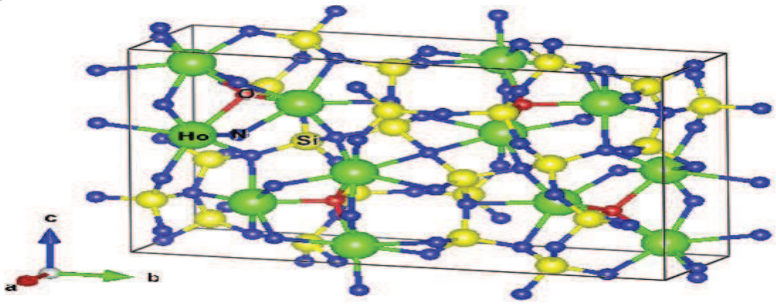

Figure 1. The of the crystal structure of $Ho_3Si_5N_9O$ compound.

3. RESULTS AND DISCUSSION

3.1. Structural properties

$Ho_3Si_5N_9O$ compound is considered in the orthorhombic Pbcm structure (Space Group No:57, Z=4) [1]. The structural view of the titled compound is given in Fig. 1. The experimental structural parameters were used as an

input for structural energy minimization. The calculated lattice parameters, ground state energy E_0 and volume are listed in Table 1. Our results for $Ho_3Si_5N_9O$ agree well with experimental reports.

Table 1. The calculated lattice parameters (a, b, c in Å), ground state energy (E_0 in eV/fu), and volume (V_0 in Å^3/fu) with available experimental values.

a	*b*	*c*	*E0*	*V0*	*Ref.*
4.996	16.204	10.689	-148.46	216.40	Present
4.97	16.13	10.63		213.43	Exp. [1]

3.2. Electronic properties

We were calculated the electronic band structure of $Ho_3Si_5N_9O$ compound and given in Fig. 2. It is seen that $Ho_3Si_5N_9O$ is an indirect band gap with the value of 2.671 eV, and its valence band maximum and the conduction band minimum occur at the X and Γ point, respectively.

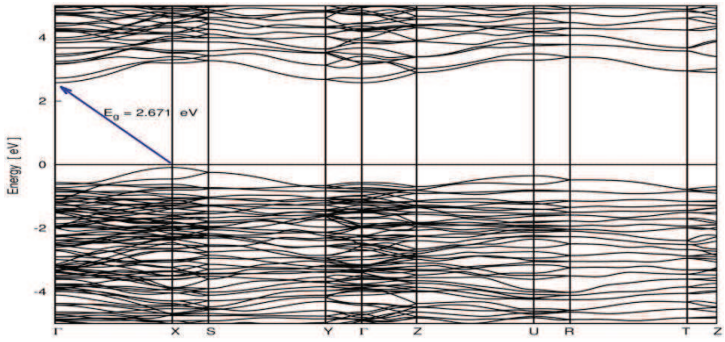

Figure 2. The calculated band structure of $Ho_3Si_5N_9O$ compound.

3.3. Mechanical properties

The elastic constants of solids provide a link between the mechanical and dynamical behaviors of crystals and give important information concerning the nature of forces operating in solids [9]. In particular, they provide information on the stability and stiffness of materials [10]. We have used the "stress-strain" relations [8] to compute the elastic constants, and the findings are given in Table 2.

Table 2. The calculated elastic constants (C_{ij} in GPa unit).

C11	*C12*	*C13*	*C22*	*C23*	*C33*	*C44*	*C55*	*C66*
305.9	85.0	96.6	348.5	111.8	322.3	108.4	110.1	104.6

The traditional mechanical stability conditions in orthorhombic crystals on the elastic constants are known as [11, 12];

- $C_{11} > 0$, $C_{22} > 0$, $C_{44} > 0$, $C_{33} > 0$, $C_{55} > 0$, $C_{66} > 0$
- $C_{11} + C_{22} > 2C_{12}$
- $C_{22} + C_{33} > 2C_{23}$
- $C_{11} + C_{33} > 2C_{13}$
- $C_{11} + C_{22}C_{33} + 2C_{12} + 2C_{23} + 2C_{13} > 0$

Our results for elastic constants are given in Table 2 satisfy these stability conditions. The mechanical properties, such as bulk modulus (B), Young's modulus (E), shear modulus (G), Poisson's ratio (v) and shear anisotropy factor (A) which are functions of the elastic constants, are calculated by using the Voigt–Reuss–Hill approximation [13], and are listed in Table 3.

Table 3. Calculated bulk modulus (B in GPa), isotropic shear modulus (G in GPa), Young's modulus (E in GPa), Poisson's ratio (v), B/G ratio, Shear anisotropic factors (A_1, A_2, and A_3), the percentage of anisotropy in the compression and shear (A_B, A_G in %),

B	G	E	v	B/G	A_1	A_2	A_3	A_B	A_G
173.3	110.0	272.3	0.24	1.57	1.01	0.97	0.86	0.24	0.17

According to criterion, a material is brittle (ductility) if the B/G ratio is less (high) than 1.75. The calculated value of the B/G (1.57) is less than 1.75 for the titled compound; hence, the compound will behave in a brittle manner.

The typical value of Poisson's ratio is about ν = 0.1 for covalent materials and 0.25 for ionic materials. In the present case the value of ν is 0.24 for $Ho_3Si_5N_9O$. Thus, the ionic contributions to the atomic bonding are dominant for $Ho_3Si_5N_9O$.

For a completely isotropic material, the factor *A* takes the value of 1. When the value of *A* is smaller or greater than unity, it is a measure of the degree of elastic anisotropy. The results show that the compound has little shear anisotropy.

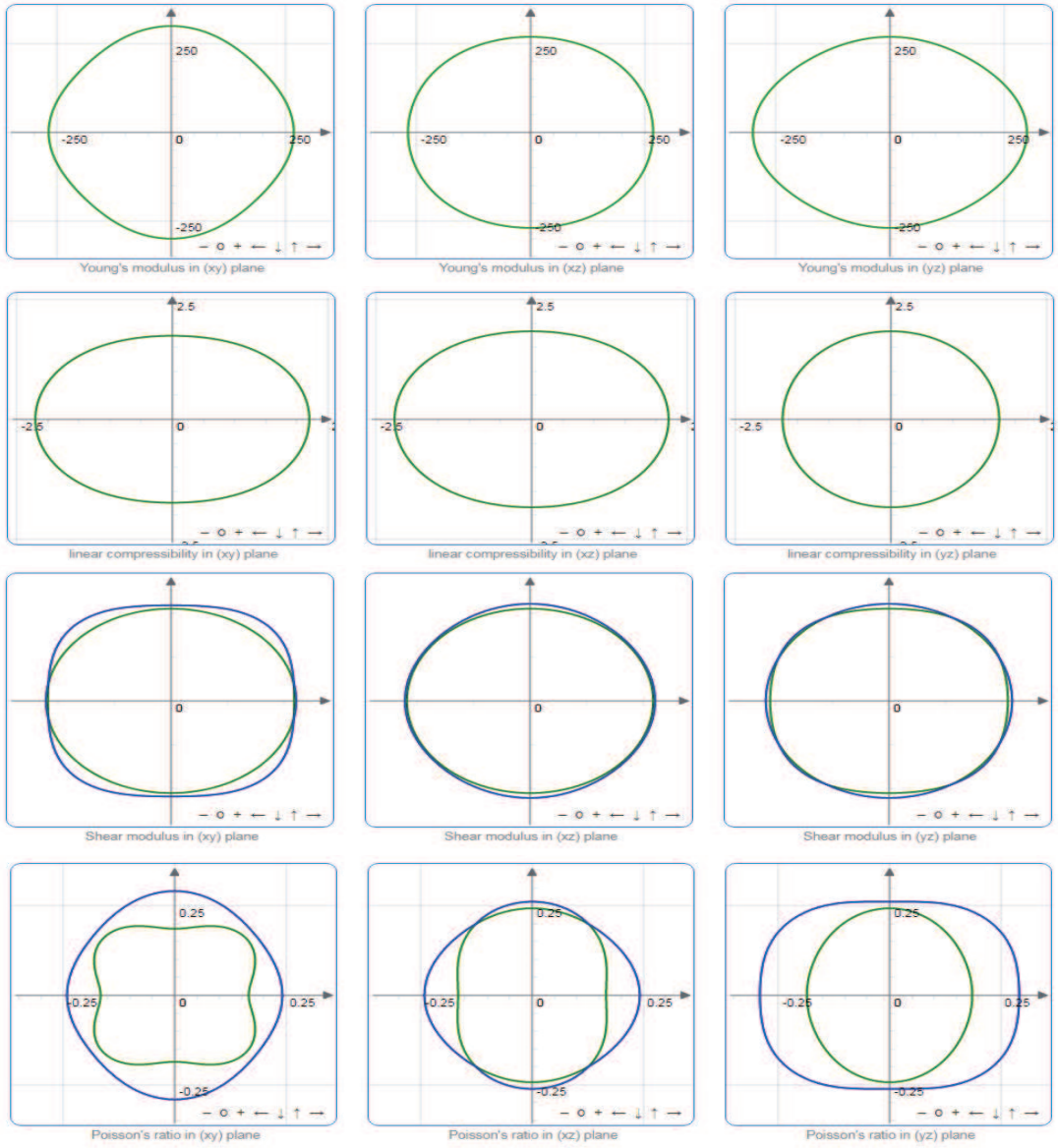

Figure 2. The calculated directional dependence of the mechanical properties; Young's modulus, linear compressibility, Shear Modulus, and Poisson's ratio for the $Ho_3Si_5N_9O$ compound.

We also visualize and calculate the directional dependence of the Young's modulus, linear compressibility, Shear modulus, and Poisson ratio by using ELATE code [14, 15]. In the plots of these physical properties, the degree of anisotropy is indicated by the deviation from the spherical shape. These parameters along the crystallographic directions (in 2D) have been given in Figure 2 for $Ho_3Si_5N_9O$ compound.

According to Fig. 2, Young's modulus in *xy*- and *yz*-planes exhibiting to be more isotropic than *xz*-plane. Shear modulus in *yz*-plane is nearly isotropic where *xy* and *xz*-planes show little anisotropy. The same trend was observed in Shear modulus. But for the Poission's Ratio, the maximum values for the yz-plane show more anisotropy along together.

4. CONCLUSION

In summary, we have performed the first principles total energy calculation for $Ho_3Si_5N_9O$ using the plane-wave pseudopotential approach to the density-functional theory within the generalized gradient approximation. The calculated lattice parameters are consistent with the literature values. We have revealed that the band structure of this compound is semiconductor in nature. The B/G ratio is 1.57 and the brittle character is dominant. $Ho_3Si_5N_9O$ has a little elastic anisotropic character. We hope that our other predicted results will be serving as a reliable reference for the future experimental and theoretical studies.

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