Journal of Materials Science and Engineering B 4 (12) (2014) 392-395
doi: 10.17265/2161-6221/2014.12.010

A Benchmark for Some Physical Properties of Zinc-Blende ZnS

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Received: November 18, 2014 / Accepted: December 04, 2014 / Published: December 25, 2014.

Abstract: Somephysical properties of zinc-blende polytype of ZnS were investigated via geometry optimization calculations. After employing a shell model interatomic potential to our computations, some physical parameters such as typical cubic elastic constants, young modulus, shear modulus, bulk modulus, poisson ratio, elastic wave velocities, static and high frequency dielectric constants, and static refractive index zinc-blende ZnS were deduced. Later, previous theoretical results and our current results with each other as well as with former experimental findings were evaluated. Present results exhibit a fair consistency with experiments and better than those of several recent density functional theory results for the considered parameters of related material.

Key words: Zinc-blende, ZnS, bulk modulus, elastic constants.

1. Introduction

From the II-VI semiconductor family, the member ZnS has attracted much scientific attention because of its outstanding physical properties, i.e., the wide energy band gap, high refraction index, and high transmittance in the visible range. ZnS is also one of the ideal candidate for the fabrication of optical, electronic, and optoelectronic devices [1-3].

Under ambient pressure, there are two types of structures for ZnS, i.e., the high temperature phase hexagonal wurtzite (WZ) structure and the low temperature phase cubic zinc-blende (ZB) structure [4].

The precise knowledge of the material is critical for device fabrications. Further, to design proper semiconductor devices, basic investigations on the fundamental physical properties, such as elastic and electronic properties are still needed. In particular, elastic properties of a solid are crucial because they relate to various fundamental solid-state phenomena. It is possible to obtain useful information about the bonding characteristic between adjacent atomic planes, as well as the anisotropic character of the bonding and structural stability from elastic constants. However, as clearly underlined in Ref. [4], although there are many experimental [5-7] and density functional theoretical [8-10] works linking with the elastic behavior of ZnS, there are still distinct discrepancies between theory and experiments. Therefore, the focus of this work is to clarify the some physical parameters of ZB ZnS in the framework of geometry optimization. We focused on the typical cubic elastic constants, young, shear and, bulk modulus, poisson ratio, elastic wave velocities, static and high frequency dielectric constants and static refractive index of ZB ZnS in a comparative and complementary way to contribute to the literature for further calculations and experiments.

In the next section, we will give a brief outline of computational details for geometry optimization applied during research. We will also impart a benchmark between our results, the experiments, and theoretical findings in the results and discussion section.

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2. Computational Procedure

During the presentsearch, we performed all calculations with General Utility Lattice Program (GULP) code 4.0 [11, 12]. This molecular dynamics simulation code allows wide-range property calculations for 3D periodic solids, 2D surfaces, and gas phase clustersby employing two-body, three-body, four-body, six-body, and many-body (EAM) potentials [13, 14] depending on the demands of research. Thus, we employed an appropriate type interatomic potential [15] for ZB ZnS with a lattice constant a_0 = 5.4093 Å.

Most of the calculations in GULP code consist of the optimization of a trial structure to the local energy minimum, under givenconditions of pressure and temperature. Further, severaltypes of standard minimization techniques are available in GULP. The two conventional techniques are to optimize the related structures at constant pressure, in which all internal and cell variables are included or at constant volume, where the unit cell remains frozen [16]. So, we applied a constant pressure optimization for the ZB ZnS. The geometry of cells was optimized by the Newton-Raphson method based on the Hessian matrix calculated from the second derivatives and Hessian matrix was recursively updated during optimization using the BFGS [17-20] algorithm. After setting the preconditions for ZB ZnS, we adopted our runs at zero Kelvin (0 K) temperature and under 0 GPa.

3. Results and Discussion

Figs.1-3 represent the comparison of typical cubic elastic constants of ZB ZnS with experiments [21], density functional theory (DFT) data from a recent study [22] and our present findings. As well explained in Refs. [13, 14, 23], cubic crystal structures have three typical elastic constants namely C_{11}, C_{12} and C_{44} which describe the hardness of a given material and needed for specifying the stability of the material.

Physically, C_{11} defines the longitudinal elastic behavior, whereas C_{12} and C_{44} portray the off-diagonal and shear elastic characteristic of cubic crystals related to shearing, respectively. It is very evident from Fig. 1 that presently calculated C_{11} is better than those of local density approximation (LDA) [22], full-potential linear augmented plane-wave method plus local orbital (FP-APW + lo) [9], full potentiallinear muffintin orbital (FP-LMTO) [8], project or augmented wave pseudo potential (PAW) [24] data. For the elastic constant C_{12} in Fig. 2, our results are better than LDA and FP-APW + lo findings and closer to PAW data with a little under estimation from the experimental measurements. In Fig. 3, LDA, FP-APW + lo, FP-LMTO and PAW data show a sharp over estimation for the experimental value of elasticconstant C_{44} whereas our result slightly underestimates. Fig. 4 displays comparison for the bulk modulus (B) of ZB ZnS. The bulk modulus B is the only elastic constant of matter that reveals much information about the bonding strength. In addition, it

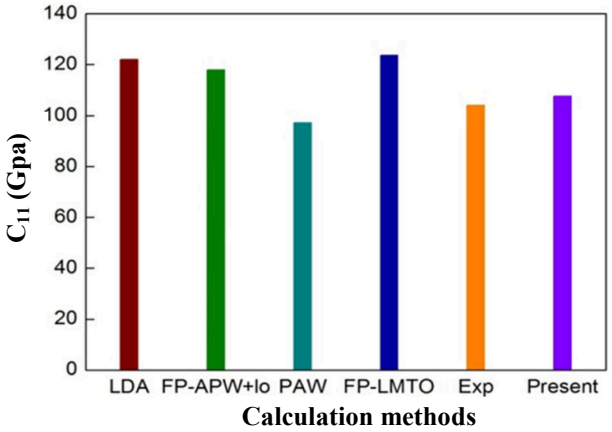

Fig. 1 Comparing C_{11} elastic constant for ZB ZnS.

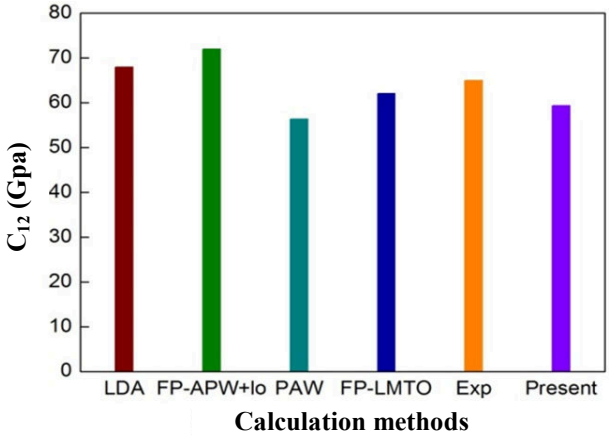

Fig. 2 Comparing C_{12} elastic constant for ZB ZnS.

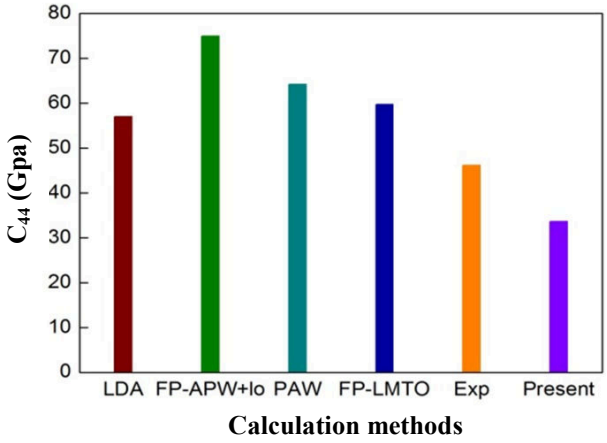

Fig. 3 Comparing C_{44} elastic constant for ZB ZnS.

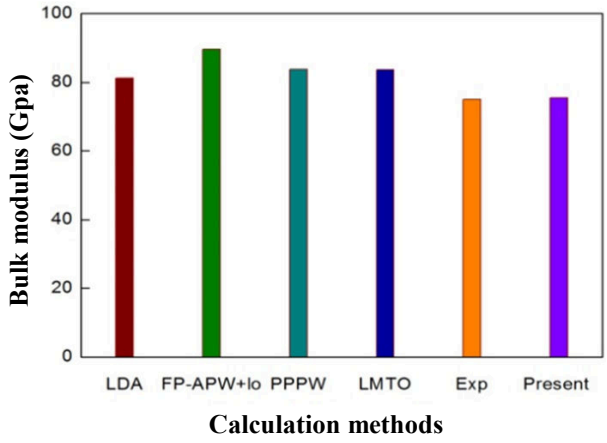

Fig. 4 Comparing bulk modulus (B) of ZBZnS.

Table 1 Comparing some mechanical and optical data of ZB ZnS.

Parameter	Exp. [26]	Present
E (GPa)	75.0	65.4
G (GPa)	29.5	29.4
v	0.27	0.35
V_S (km/s)	3.3	2.7
V_L (km/s)	5.5	5.3
ε_0	8.9 [25]	6.4
ε_∞	5.1 [25]	4.7
n_s	≈ 2.4	2.5

is a measure of the matter's resistance to external deformation and occurs in many formulas describing diverse mechanical-physical characteristics. PPPW stands for pseudo-potential plane-wave DFT potential employed in Ref. [25]. As obvious from Fig. 4, present result better fits the experimental value of bulk modulus when compared with the overestimating former DFT data.

From a morephysical perspective, and Figs. 1-4, it is easy to see the existence of traditional Born mechanical (dynamical) stability conditions (P = 0 GPa);

$C_{11} > 0, C_{44} > 0$, $C_{11} - C_{12} > 0$, $C_{11} + C_{12} > 0$, and C_{12} $B < C_{12}$ for ZB ZnS.

Table 1 summarizes the other results of considered parameters where these parameters are well explained in Ref. [13]. As seen in Table 1, our present results exhibit reasonable agreement when compared with the previous experimental data of shear modulus (G), young modulus (E), poissonratio (v), elastic wave velocities (V_S and V_L), static (ε_0) and high frequency (ε_∞) dielectric constants and static refractive index (n_s).

4. Conclusions

In summary, we report some physical properties of ZB ZnS via geometry optimization calculations with a proper interatomic potential. Our computational results showa satisfactory agreement with the experimental dataoftypical cubic elastic constants, young modulus, shear modulus, bulk modulus, poisson ratio, elastic wave velocities, static and high frequency dielectric constants, and static refractive index of ZB ZnS. The present results are also better than earlier DFT results because of the chosen interatomic potential which is highly reliable. Our further research linking with the high pressure elastic behavior for ZB ZnS is still under way.

Finally, the results of our research will not only contribute to related literature of ZB ZnS material, but also inspire the further theoretical predictions to obtain good quality outcomes that are closer to experimental data.

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