The Mechanical Properties of ZrSbTe and HfSbTe Compounds

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ABSTRACT

By means of first principles calculations, we have studied the structural and mechanical properties of the ZrSbTe and HfSbTe compounds. The elastic constants of these compounds are calculated, then bulk modulus, shear modulus, Young's modulus, Possion's ratio and Debye temperature of polycrystalline aggregates have been derived and relevant mechanical properties are discussed. We have found that these compounds have mechanically stable.

1. INTRODUCTION

Thermoelectric materials have acquired increased attention by researchers around the globe owing to the unique capability of such materials to convert heat directly into electricity [1, 2]. As known, these materials have been considered for many important applications from clean energy to photon sensing devices. An important criterion of a suitable thermoelectric is that it should be a semiconductor with a narrow band gap [2, 3].

The best materials for thermoelectric devices at or below room temperature are alloys of bismuth, antimony, and tellurium [4]. Therefore, the ternary antimonides and tellurium have been investigated for their potential use as thermoelectric materials [5–7]. Recently, Soheilnia et al. [8] have synthesized two new antimonide-tellurides which ZrSbTe and HfSbTe compounds. They have reported that these compounds are metallic conductors with a small Seebeck coefficient.

The present work is devoted to the mechanical properties of the ZrSbTe and HfSbTe compounds, using the density functional theory (DFT). Specifically, we address their bulk modulus, shear modulus, Young's modulus, Possion's ratio, Debye temperature. But until now, to our best knowledge, no systematic research has been reported these properties of ZrSbTe and HfSbTe compounds.

2. COMPUTATIONAL METHODS

Our calculations are performed within the framework of the density functional theory (DFT) using the projector augmented wave (PAW) method [9] as implemented in the Vienna ab initio Simulation Package (VASP) [10]. The exchange and correlation are treated within the generalized gradient approximation using the parametrization obtained by Perdew, Ernzerhof and Burke (GGA-PBE) [11]. We used a kinetic energy cutoff of 500 eV for plane-wave expansion of the PAWs. Brillouin-zone sampling has done in the Monkhorst-Pack [12] scheme with a k-point mesh of 8 × 6 × 4 for all compounds.

3. RESULTS AND DISCUSSION

ZrSbTe and HfSbTe crystallize in the orthorhombic structure (space group *Immm*, *NbPS*-type, *Z=4*). We have fully relaxed the cell volume and the ionic positions of atoms in reciprocal coordinates which are

supported by VASP code [9, 10] for these compounds, we have used these relaxed parameters. The calculated lattice parameters are presented in Table 1. It is seen that the present lattice parameters for ZrSbTe and HfSbTe compounds are in good agreement with the experimental values [8].

Table 1. Calculated equilibrium lattice parameters (*a*, b, and *c* in Å) along with the available experimental

Materials	***a***	***b***	***c***	**Refs.**
ZrSbTe	3.916	5.822	13.668	Present
	3.911	5.805	13.463	Exp. [8]
HfSbTe	3.909	5.804	13.517	Present
	3.867	5.7511	13.442	Exp. [8]

The present elastic constants are obtained from the strain-stress relationship [13], and the findings are given in Table 2. For a stable orthorhombic structure, its nine independent elastic constants should satisfy the well-known Born stability criteria [14] $C_{11}>0$, $C_{22}>0$, $C_{33}>0$, $C_{44}>0$, $C_{55}>0$, $C_{66}>0$, $[C_{11}+C_{22}+C_{33}+2(C_{12}+C_{13}+C_{23})]>0$, $(C_{11}+C_{22}-2C_{12})>0$, $(C_{11}+C_{33}-2C_{13})>0$, and $(C_{22}+C_{33}-2C_{23})>0$. Clearly, the calculated elastic constants satisfy the Born stability criteria for considered structures, suggesting that these compounds are mechanically stable.

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

Materials	C_{11}	C_{12}	C_{13}	C_{22}	C_{23}	C_{33}	C_{44}	C_{55}	C_{66}	**Refs.**
ZrSbTe	127.2	25.0	72.7	203.6	33.1	133.4	50.6	85.3	46.1	Present
HfSbTe	134.4	26.5	77.1	206.3	35.1	141.6	51.4	88.3	46.1	Present

Clearly, the calculated elastic constants satisfy the Born stability criteria, suggesting that these compounds are mechanically stable. Unfortunately, there are no theoretical or experimental results for these compounds for comparing with the present work. Then, our results can serve as a prediction for future investigations. After obtaining elastic constants, the polycrystalline bulk modulus (*B*), shear modulus (*G*) are calculated from the Voigt-Reuss-Hill (VRH) approximations [15]. The Young's modulus (E) and Poisson's ratio (*v*) are calculated through $E = 9BG/(3B + G)$ and $v= (3B - 2G)/2(3B+G)$. Exploring the mechanical properties, our results have been summarized in Table 3.

Table 3. The calculated isotropic bulk modulus (*B* in GPa), shear modulus (*G* in GPa), Young's modulus (*E* in GPa), Poisson's ratio (*v*) and Debye Temperature (Θ_D in K)

Materials	***B***	***G***	***E***	***v***	***B/G***	Θ_D	**Refs.**
ZrSbTe	80.3	54.2	132.7	0.22	1.48	304.1	Present
HfSbTe	84.1	55.7	136.8	0.22	1.50	274.4	Present

The bulk modulus measures the resistance of a solid to volume change against external forces. The obtained bulk modulus is lower than 100 GPa, and therefore these compounds should be classified as high compressibility material. According to Pugh formulation [16], a material is brittle (ductility) if the *B/G* ratio is less (high) than 1.75. The value of the *B/G* is lower than 1.75 for these compounds; hence, these compounds will behave in a brittle manner

Young's modulus is defined as the ratio of stress and strain, and is used to provide a measure of the stiffness of the solid. When the value of E is large, the material is stiff. On this context, due to the higher value of Young's modulus (136.8 GPa) for HfSbTe is relatively stiffer the other compounds.

The value of the Poisson's ratio is indicative of the degree of directionality of the covalent bonds. The value of the Poisson's ratio is about 0.1 for covalent materials, whereas for ionic materials a typical value of *v* is 0.25 [17]. The calculated Poisson's ratios are about 0.20 for these compounds. Therefore, both compounds are ionic materials.

The Debye temperature is known as an important fundamental parameter closely related to many physical properties such as specific heat and melting temperature. We have calculated the Debye temperature by using the common relation given in Refs. [18-20]. According to Table 3, among the compounds ZrSbTe has the highest Debye Temperature (304.1 K).

4. CONCLUSION

The first-principles calculations have been performed to investigate the structural and mechanical properties of ZrSbTe and HfSbTe compounds. The calculated elastic constants showed that these compounds are mechanically stable in considered structure. The polycrystalline elastic parameters have been further calculated within the scheme of Voigt–Reuss–Hill (VRH) approximation. These compounds possess brittle in nature with respect to the *B/G*.

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