



# First-principles study of mechanical, thermodynamic, transport and superconducting properties of Sr<sub>3</sub>SnO



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## ABSTRACT

We have performed a comprehensive set of first-principles calculations to study mechanical, thermal, transport and superconducting properties of Sr<sub>3</sub>SnO, an antiperovskite Dirac-metal oxide. Sr<sub>3</sub>SnO cubic crystal is found to be elastically stable, anisotropic and brittle in nature. The Debye temperature and bulk modulus are found to decrease with increasing temperature but increase with increasing pressure. However, the specific heats are found to increase due to the increase of temperature. The Gaspari and Gyorffy formalism within the rigid muffin tin approximation is used to calculate the electron phonon coupling constant and hence transition temperature ( $T_c$ ). The density of states is dominated by Sr-4d and Sn-5p electrons near the Fermi level and the mixing of Sr-4d and Sn-5p causes the topological superconductivity in Sr<sub>3</sub>SnO. The calculated  $T_c$  (8.38 K) is reasonably close to the experimental value (~5 K). © 2017 Elsevier B.V. All rights reserved.

## 1. Introduction

In antiperovskite oxide crystal structure, the occupancy of cations and anions are reversed, i.e., the position of metal and oxygen ions are reversed. Thus the ions of metal have negative valence states [1]. Antiperovskite oxide crystals show some interesting and important properties such as superconductivity, negative thermal expansion, piezomagnetic effects, etc. as lattice, spin and charge interact strongly in such structure [2–5]. Since electron-phonon coupling is the most prominent interaction to cause superconductivity, it is reasonable for antiperovskite oxide to exhibit superconducting properties. The superconducting phenomena of a crystalline material is directly related to its structural, electronic, thermal and magnetic properties. Widera and Schafer first reported that Sr<sub>3</sub>SnO exhibits cubic antiperovskite structure [6]. Oudah et al. have recently showed that Sr<sub>3</sub>SnO exhibits superconductivity with transition temperature around 5 K [7]. The Sr-Sr distance is 3.548 Å which is very near to SrO, with 3.650 Å [8] but is shorter than pure Sr, with 4.296 Å [9]. The Sr<sub>3</sub>SnO crystal has the charge balanced formula (Sr<sup>2+</sup>)<sub>3</sub>(Sn<sup>4-</sup>)(O<sup>2-</sup>) [7]. In Sr<sub>3</sub>SnO, there are Dirac points in its electronic structure that originates from the inversion of bands

possessing different parities. Recently, it is reported that a class of crystalline insulator exists within the antiperovskite oxides, Sr<sub>3</sub>SnO. However, the Sr<sub>3</sub>SnO crystal stands on the border of topological phase as it is expected [10]. The nontrivial topology exists with type-II Dirac points protected by the reflection symmetry. The electron-phonon (E-P) coupling constant can be calculated by using the parameters available in the density of states calculation [11]. The rigid muffin tin approximation (RMTA) is the mostly used method to calculate McMillan-Hopfield parameter [12–14]. However, the calculated values obtained by RMTA are reasonably deviated from the experimental value [13–15].

In this paper, we analyze mechanical, thermal, transport and superconducting properties of Sr<sub>3</sub>SnO crystal. We determine elastic constants and moduli of elasticity and hence judge the mechanical stability of the crystal by born criteria. We calculate Debye temperature ( $\theta_D$ ) and Grüneisen parameter ( $\gamma$ ). Moreover, we calculate Coulomb Pseudo potential ( $\mu^*$ ) and electron-phonon coupling constant for Sr<sub>3</sub>SnO using RMTA. The required parameters that enter into RMTA was generated by WIEN2k. Using the average Debye temperature,  $\mu^*$  and E-P coupling constant, we calculate superconducting transition temperature  $T_c$ .

## 2. Computational details

First-principles calculations presented in this paper have been

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performed using the Cambridge Serial Total Energy Package (CASTEP) [16,17]. CASTEP employs the plane wave pseudopotential approach based on density functional theory (DFT) [18]. The electronic exchange–correlation energy is treated under the generalized gradient approximation (GGA) in the scheme of Perdew–Burke–Ernzerhof (PBE) [19,20]. We determined ground state energy, structural properties and mechanical properties at zero temperature. The interactions between electrons and ions of the crystal structure were investigated by using ultra-soft Vanderbilt-Pseudopotentials [21]. The cutoff energy about 500 eV of a plane wave was implemented by generating  $15 \times 15 \times 15$  k-point grids in accordance with Monkhorst-Pack [22]. Geometry optimization was obtained by applying cutoff energy  $5 \times 10^{-6}$  eV/atom to find total energy, 0.01 eV/Å, to find the maximum force, 0.02 GPa, and the maximum displacement.

The total density of states (DOS) at Fermi level  $N(E_F)$ , projected density of states (PDOS)  $N_l(E_F)$  and other required parameters to calculate Hopfield parameter ( $\eta$ ) were calculated by using PBE scheme within GGA with the full potential linearized augmented plane wave (LAPW) in WIEN2k [23,24]. A well-converged basis set was used to calculate DOS and PDOS. The parameter  $R_{mt}K_{max}$ , where  $R_{mt}$  is the smallest muffin-tin radius (in atomic units) and  $K_{max}$  is the plane wave cutoff, controls the size of the basis. It was set to a high value of 7.0. The values of  $R_{mt}$  for the atomic spheres were 2.35 (Sr), 2.50 (Sn) and 2.35 (O) for  $Sr_3SnO$ . We used a mesh of 120 k-points for calculating the electronic structures.

Temperature and pressure dependent thermodynamic properties were employed by using quasi-harmonic Debye model in GIBBS program [25]. The calculations of transport properties such as electrical conductivity and Pauli magnetic susceptibility were performed in BoltzTraP [26]. BoltzTraP program is used to calculate semi-classical transport coefficient.

### 3. Results and discussion

#### 3.1. Mechanical properties

The antiperovskite cubic  $Sr_3SnO$  belong to  $Pm\bar{3}m$  (221) with lattice parameter  $a = 5.165$  Å that deviates slightly from experimental value [7]. Elastic constants obtained from Hook's law are the most important parameters that are related with other physical quantities such as bulk modulus, shear modulus, Young's modulus and Poisson's ratio. The necessary and sufficient conditions for elastic stability of cubic  $Sr_3SnO$  can be written as [27].

$$C_{11} - C_{12} > 0; \quad C_{11} + 2C_{12} > 0; \quad C_{44} > 0$$

Thus first two conditions means that  $C_{11} > 0$ . The calculated elastic constants ( $C_{11} = 85.9$ ,  $C_{12} = 18.6$  and  $C_{44} = 38.4$  GPa) satisfy these conditions. Thus, antiperovskite superconducting  $Sr_3SnO$  is elastically stable. The bulk modulus ( $B$ ), shear modulus ( $G$ ), Young's modulus ( $Y$ ), and Poisson's ratio ( $\sigma_p$ ) are 41.0, 36.5, 79.2 GPa, and 0.16 respectively. We see that the bulk modulus is comparatively small ( $< 100$  GPa), thus  $Sr_3SnO$  can be regarded as medium hard material. Since  $C_{12} - C_{44} < 0$ , i.e. Cauchy's pressure [28], and  $G/B = 0.408 < 1.75$  [29], thus  $Sr_3SnO$  is brittle in nature. Anisotropic properties of a cubic crystal can be found by using the expression [30]  $A = \frac{C_{44}}{C_{11} - C_{12}} = 1.143$ , which indicates that  $Sr_3SnO$  is highly anisotropic material.

#### 3.2. Thermodynamic properties

Thermodynamic properties of a superconductor are very important because they are directly related to superconductivity. We calculated thermodynamic parameters such as bulk modulus,

Debye temperature, specific heats and Grüneisen parameter at different temperature and pressure. We also calculated equilibrium Debye temperature at  $T = 0$  K and  $P = 0$  GPa by the following equation [31].

$$\theta_D = \frac{h}{k_B} \left( \frac{3N}{4\pi V} \right)^{1/3} \left[ \frac{1}{3} \left( \frac{2}{v_t^3} + \frac{1}{v_l^3} \right) \right]^{-1/3}$$

where  $v_t$  and  $v_l$  stand for transverse and longitudinal wave velocity respectively and can be derived from  $v_t = \left( \frac{3B+4G}{3\rho} \right)^{1/2}$ ,  $v_l = \left( \frac{G}{\rho} \right)^{1/2}$ .

The Debye temperature  $\theta_D = 276.1$  K is obtained by plugging the values of  $B$ ,  $G$ ,  $\rho$  into the desired equations. The variations of Debye temperature, specific heats and Grüneisen parameter at different temperature and pressure are illustrated in Fig. 1.

We see that the Debye temperature at  $T = 0$  K and  $P = 0$  GPa is 271.2 K (obtained by GIBBS program) which deviates from the calculated value by using Debye model. The Debye temperature decreases with increasing temperature but Grüneisen parameter increases with increasing temperature. However, this is completely opposite case when we increase pressure as shown in Fig. 2. Thus, phonon contribution vanishes for high temperature but becomes much effective for high pressure, as expected.

Thus Grüneisen parameter is proportional to temperature with some constants dependent on material properties and Debye temperature is inversely proportional to temperature. Since increasing temperature increases the vibration of atoms in the crystal, thus decrease the average phonon velocity and therefore, decreases Debye temperature. The variations of bulk modulus and specific heat at constant pressure and volume respectively are plotted in Fig. 2. We see that the bulk modulus decreases with increasing temperature but increases due to the increase of pressure. The specific heats decrease with increasing pressure. However, specific heats increase with increasing temperature. Thus, we observe that the specific heats inversely varied with bulk modulus. Since there is no experimental values to verify these thermal properties of this crystal, we could not compared our obtained results.

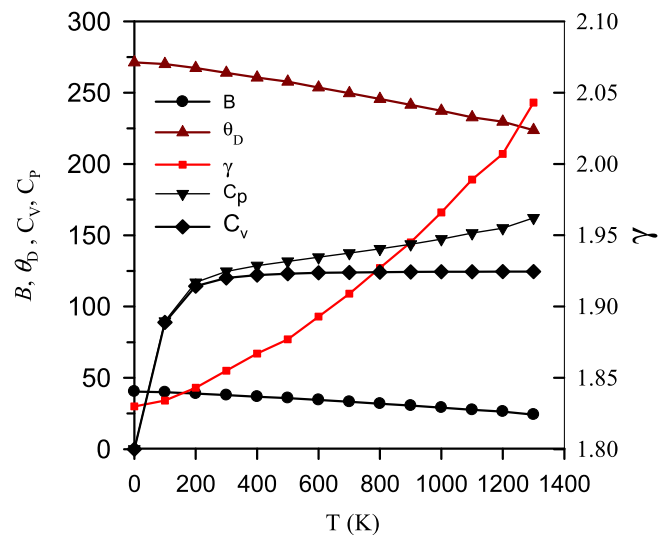


Fig. 1. Variations of different thermodynamic parameters, Debye temperature  $\theta_D$  in K, Grüneisen parameter  $\gamma$ , specific heat at constant volume  $C_V$  in J/mol.K, specific heat at constant pressure  $C_P$  in J/mol K, as well as bulk modulus ( $B$ ) in GPa, with temperature  $T$  (K).

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