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First Principle Simulation Mechanical Properties of PbS, PbSe, CdTe and PbTe by Molecular Dynamics

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Abstract

We report first principle simulation mechanical properties of PbS, PbSe, CdTe and PbTe semiconductors with the rocksalt structure at temperature range 300–700 K by molecular dynamics (MD). The MD simulation has been applied the temperature pressure and volume influence interatomic interaction by Lenard-Jone formula and atoms vacancy. The equations of atoms motion were used time integration by Verlet's algorithm and the interation of long range Coulomb by Ewald's summation. The potential parameter was based on Busing-Ida function contribution thermodynamics equilibrium which ignored phase transition with the cluster atoms site 4×4×4 on 512 atoms (256 cations and 256 anions). The mechanical properties of stress, strain, compressibility, Young's modulus, shear modulus and bulk modulus dependence on temperature were analyzed.

1. Introduction

PbS, PbSe, CdTe and PbTe systems are promising thermoelectric materials for conversion of waste-heat into electricity [1-3]. The PbS, PbSe, CdTe and PbTe compounds are show NaCl structure, the pressure dependence of the energy gap of these compounds in the NaCl structure [4]. The temperature and pressure are under the thermodynamic properties which are difficult for experimental studies. The high pressure phase of PbSe is indicated that reaching optimal thermoelectric behaviour [2]. The mean values of Young's modulus, shear modulus and Poisson's ratio are 53.1 GPa, 21.4 GPa and 0.245, respectively measuring by Resonant Ultrasound Spectroscopy (RUS) [6]. The mechanical properties such

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as stress, strain, compressibility, Young's modulus, shear modulus and bulk modulus is very important in order to better understanding the thermoelectric materials [7, 8]. The elastic moduli are required for stress and strain calculations [9] and moreover, the elastic moduli can be used to monitor the level of microcrack damage that may accumulate during processing, fabrication or use of thermoelectric materials [10]. However, the temperature has effected of mechanical properties, a few report and unclealy in the literature.

In this study, we obtained the mechanical properties of PbS, PbSe, CdTe and PbTe such as stress, strain, compressibility, Young's modulus, shear modulus and bulk modulus dependence on temperature calculating by MD simulation and might be useful for thermoelectric materials study.

2. Computational Details

The MD simulation for mechanical properties of PbS, PbSe, CdTe and PbTe are used 512 ions (256 anions and 256 cations on MXDORTO program [11], the unit cell was arranged 4×4×4 in cubic structure. The calculation is controlled at both constant pressure and volume equilibrium, the quantum effect is based in system [12]. The parameters of PbS, PbSe, CdTe and PbTe simulation is determined by trial and error numbers of Pb^{2+}, Cd^{2+}, S^{2-}, Se^{2-} and Te^{2-} fit with lattice parameter experiment literature. The calculated atom velocities with integrate Newton equation of motion by Verlet's algorithm [13] and run time per step at 2.0×10^{-15} s, the interaction of long range coulomb with Ewald's summation [14]. The equilibrium has run on 1×10^{4} step, although the step numbers was small, the system was achieved equilibrium as observed them from the changed temperature (±1%), pressure (± 9%), density (±0.2%), internal energy (±0.03%). The calculated is used temperature range from 300 K to 700 K and pressure control range at 0.001, 0.75, 1.5 GPa. The interatomic interaction of N atoms had related follow by $\vec{F}_i = -\vec{\nabla} U\left(r_1, r_2, ..., r_N\right)$, where the potential function for N atoms is $\vec{\nabla} U\left(r_1, r_2, ..., r_N\right)$. We used 2-bodies $U_{ij}\left(r_{ij}\right)$ is potential function of pair atoms i and j, the potential parameters is using with Busing-Ida potential function [15] in 2-bodies of materials ions interaction from Eq. (1)

$$U_{ij}(r_{ij}) = \frac{z_i z_j e^2}{r_{ij}} + f_0(b_i + b_j)\exp\left(\frac{a_i + a_j - r_{ij}}{b_i + b_j}\right) - \frac{c_i c_j}{r_{ij}^6} + D_{ij}\left\{\exp[-2\beta_{ij}(r_{ij} - r_{ij}^*)] - 2\exp[-\beta_{ij}(r_{ij} - r_{ij}^*)]\right\} \quad (1)$$

where Z_i and Z_j are the effective partial electronic charges of ion i and j, r_{ij} is the atom distance; r_{ij}^* is the bond length of anion-cation pair, $f_0 = 4.186$; D_{ij} and β_{ij} are the depth and shape of this potential.

The potential function is corresponds to the covalent bond, which the first term is coulomb interaction, represent the second term is the short range repulsive potential, a_i and a_j are the radii, b_i and b_j are hardness of ions i and j respectively, the third term represent by the Van Der Waals interaction which arise from dipole moment diffuse potential and the Morse type potential [16] represent in the last term. We are calculating the mechanical properties by the following Eq. (2)

$$a(T) = \frac{a(0)}{a(T)}, \ \beta = \frac{3}{a(P_0)}\left(\frac{\partial a(P)}{\partial P}\right)_T, \ \beta = -\frac{1}{V}\frac{\partial V}{\partial p}\bigg|_T, \ K_T = \frac{1}{\beta}, \ \tau = \frac{F}{A_0}, \ \varepsilon = \frac{\Delta l}{l}, \ E = \frac{\tau}{\varepsilon}, \ G = \frac{2(K - \lambda)}{2} \ (2)$$

where $a(T)$ is the lattice parameter at $T(\text{K})$, T_0 is room temperature, $a(P)$ is the lattice parameter at pressure $P(\text{Pa})$, and P_0 is atmospheric pressure, β is isothermal compressibility, V is volume, K_T is isothermal bulk modulus, τ is stress, F is action force, A_0 is based area, l is length of cluster, Δl is length of differential, ε is strain, E is Young's modulus, G is Shear modulus and λ is Lame's parameter.

3. Results and Discussion

The compressibility values are calculated by lattice parameter at pressure 0.0001, 0.75 and 1.5 GPa. The inverse of compressibility is the isothermal bulk modulus, it's interested for mechanical properties study under at high temperature. The lattice parameter of PbS, PbSe, PbTe and CdTe are very good agreement with experimental data. Temperature dependence on lattice parameters and stress of are shown in Fig.1. The bulk modulus with temperature was compared to the result of J. E. Ni et al. (exp.) and F. Ren et al. [6, 17]. The mean values of bulk modulus for PbS, PbSe, CdTe and PbTe were found in between the values of the two finding and decreased with increasing temperature and volume at constant pressure as shown in Fig. 2. Young's modulus was decreased with increasing temperature an in good agreement with experimental data as shown in Fig. 3.
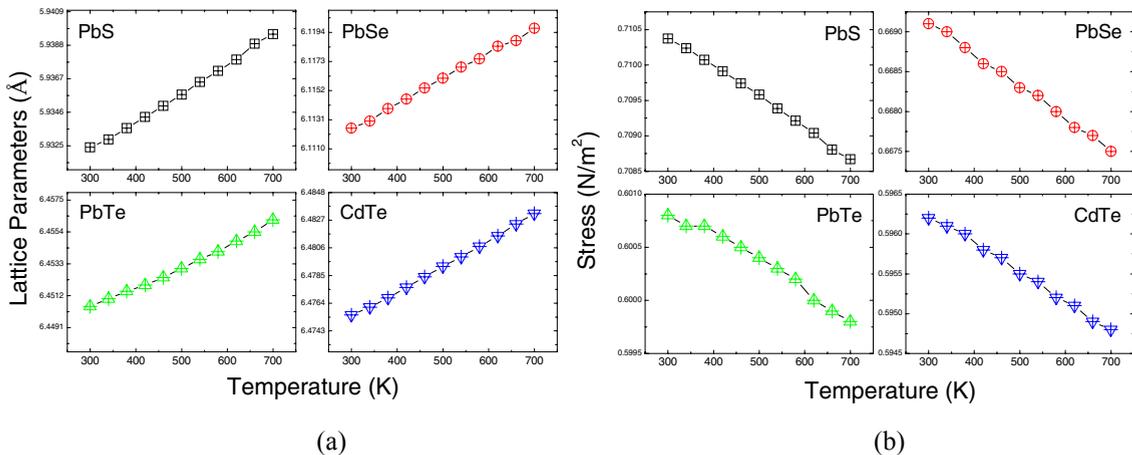

(a)   (b)

Fig. 1. Temperature dependence on (a) lattice parameters and (b) stress of PbS, PbSe, PbTe and CdTe

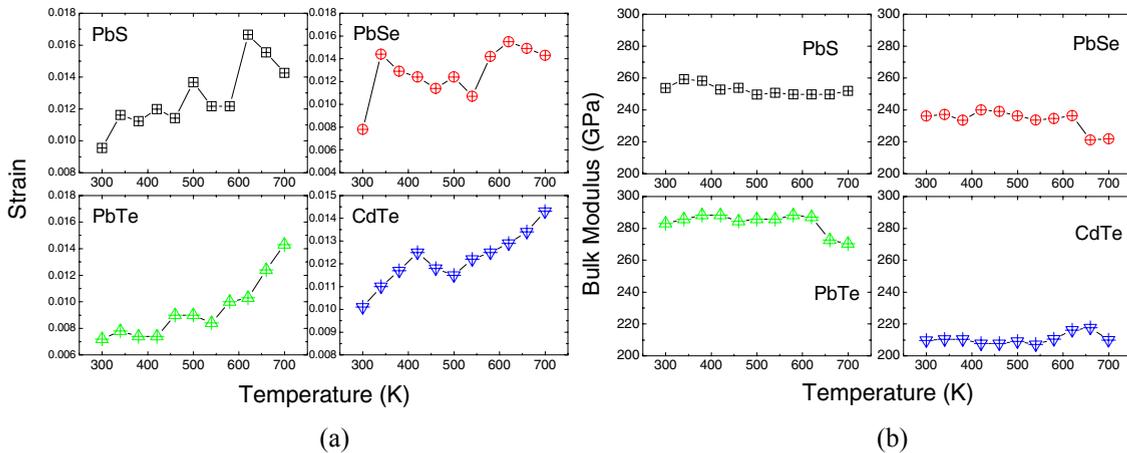(a)   (b)

Fig. 2. Temperature dependence on strain and bulk modulus of PbS, PbSe, PbTe and CdTe
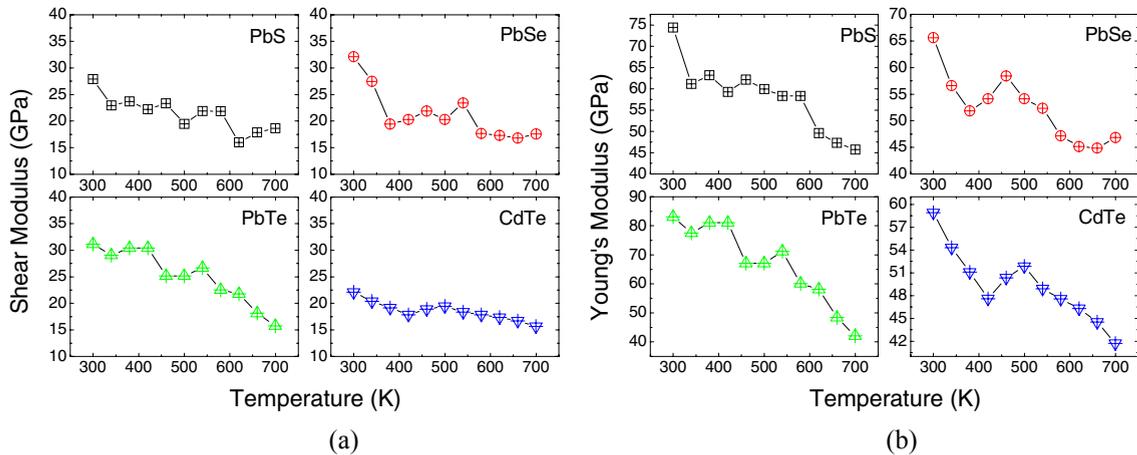
Fig. 3. Temperature dependence on shear and Young's modulus of PbS, PbSe, PbTe and CdTe

4. Conclusions

The mechanical properties are composed of stress, strain, compressibility, Young's modulus, shear modulus and bulk modulus for PbS, PbSe, CdTe and PbTe thermoelectric materials were successfully calculated by molecular dynamic simulation. The first principle simulation mechanical properties used of parameters such as temperature in range 300–700 K, rocksalt structure, the cluster atoms site of 4×4×4 on 512 atoms and fitted experimental data and literature data. It was found that the simulation results were in good agreement with experimental data.

Acknowledgements

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