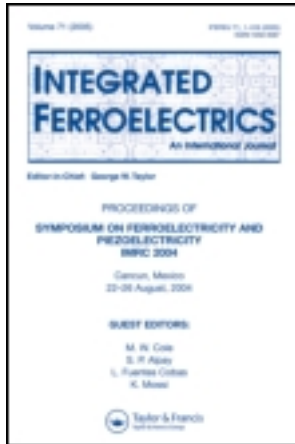


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# Thermal Properties of Bi Doped PbTe Simulated by Molecular Dynamics

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*The parameters of thermoelectric performance for thermal conductivity are investigated and need to more and more small value. In this work an analytical simulation model is affected of Bi doped PbTe compound on thermal properties simulated by classical molecular dynamics (MD). The MD simulation has been applied with temperature pressure and volume influence interatomic interaction by Lenard-Jone formula and atoms vacancy. The potential parameter is based on Busing-Ida function contribution thermodynamics equilibrium which ignored phase transition with the cluster atoms site  $4 \times 4 \times 4$  on 512 atoms (256 cations and 256 anions). The lattice parameter, compressibility, linear thermal expansion coefficient and heat capacity are calculated. The result for thermal conductivity of PbTe is decreased by doping Bi and strong agreement with experimental data.*

**Keywords** PbTe; thermal conductivity; classical molecular dynamics

## 1. Introduction

The classical molecular dynamics method is widely used calculation for the thermal properties of thermoelectric materials PbTe systems, which are promising thermoelectric materials for conversion of waste heat into electricity [1]. The PbTe compounds show the NaCl structure [2]. The temperature and pressure are under the thermodynamic properties which are difficult for experimental studies. However, there are a few reports the effect to the temperature on thermal properties of PbTe.

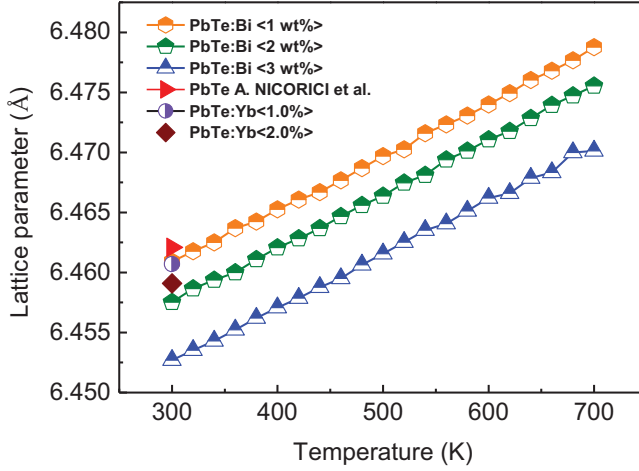
In this study, we obtained the thermal properties of PbTe, such as lattice parameter, compressibility, linear thermal expansion coefficient, heat capacity and thermal conductivity dependence on temperature calculated by MD simulation and will be useful for thermoelectric materials study.

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**Figure 1.** Simulated temperature dependence on lattice parameters of Bi doped PbTe. (1 wt%, 2 wt%, and 3 wt%).

## 2. Computational Details

The MD simulations for thermal properties of PbTe are employed 512 ions (256 anions and 256 cations) on MXDORTO program [3]. The unit cell was arranged  $4 \times 4 \times 4$  in cubic structure. The calculation is controlled at both constant pressure and volume equilibrium. The quantum effect is based on the system [4]. The temperature was calculated ranging from 300 K to 700 K and pressure control range at 0.001, 0.7501, 1.5001 GPa.

We employed the semi-empirical two-body potential function which was proposed by Busing-Ida [5] for cations and anions interactions 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  $f_0$  equals 4.186,  $z_i$  and  $z_j$  is the effective partial electronic charges on the  $i$ th and  $j$ th ions,  $r$  represents the interatomic distance,  $a$ ,  $b$  and  $c$  which are the characteristic parameters depending on the ion species, and  $D_{ij}$  and  $\beta_{ij}$  describe the depth and shape of this potential, respectively.

The thermo physical properties composed of the compressibility  $\beta$ , the linear thermal expansion coefficient  $\alpha_{lin}$ , the heat capacity at constant volume  $C_V$ , the heat capacity of lattice dilatational term  $C_d$ , the heat capacity at constant pressure  $C_P$ , and the thermal conductivity  $\kappa$ .

$$\beta = \frac{3}{a(P_0)} \left( \frac{\partial a(P)}{\partial P} \right)_T, \quad \alpha_{lin} = \frac{1}{a(T_0)} \left( \frac{a(T) - a(T_0)}{T - T_0} \right)_P \quad (2)$$

where  $a(P)$  is lattice parameter at pressure  $P$  (Pa) and  $P_0$  is atmospheric pressure,  $a(T)$  is the lattice parameter at  $T$  (K) and  $T_0$  is room temperature.

$$C_V = \left( \frac{\partial E(T)}{\partial T} \right)_V, \quad C_d = \frac{(3\alpha_{lin})^2 V_m(T)}{\beta} T, \quad C_P = C_V + C_d \quad (3)$$

where  $E(T)$  is the internal energy at  $T$  (K) and  $V$  is the molar volume.

We calculated the thermal conductivity ( $\kappa$ ) using the Green-Kubo relation [6].

$$\kappa = \frac{V}{3k_B T^2} \int_0^\infty \langle S(t) \cdot S(0) \rangle dt \quad (4)$$

where  $V$  is the volume,  $S$  is the heat flux,  $T$  is the absolute temperature, and  $k_B$  is the Boltzmann constant. The heat flux is given by

$$S = \frac{1}{V} \left[ \sum_j e_j v_j - \frac{1}{2} \sum_j \sum_{j=i} r_{ij} (f_{ij} \cdot v_j) \right]. \quad (5)$$

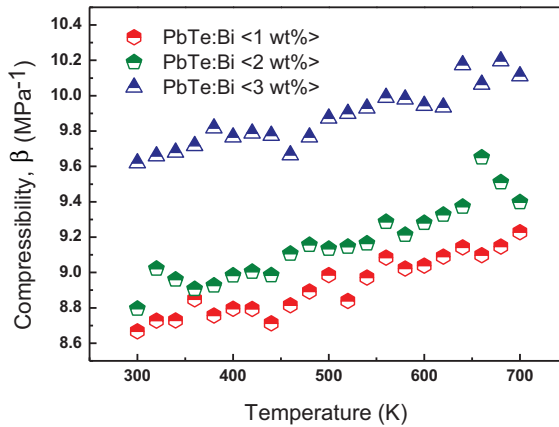
where  $v_j$  is the velocity of atom  $j$  and  $r_{ij}$  and  $f_{ij}$  are the interatomic distance and force between atoms  $i$  and  $j$ , respectively. The instantaneous excess energy of atom  $j$ ,  $e_j$  is given by

$$e_j = \left\{ \frac{1}{2} m_j v_j^2 + \frac{1}{2} \sum_{i=j} u(r_{ij}) \right\} - e_{av} \quad (6)$$

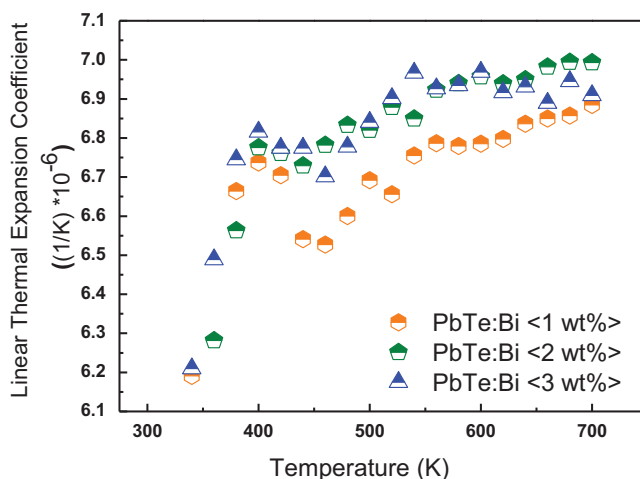
where  $m_j$  is the mass of atom  $j$ ,  $u$  is the interatomic potential between atom  $i$  and  $j$ , and  $e_{av}$  is the average energy of the system.

### 3. Results and Discussion

The lattice parameter of PbTe had a very good agreement with the experimental data. Temperature was dependent on lattice parameters and is shown in Fig. 1. The lattice



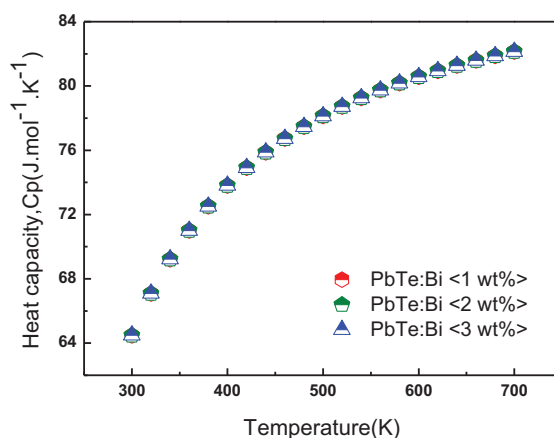
**Figure 2.** Simulated temperature dependence on compressibility of Bi doped PbTe. (1 wt%, 2 wt%, and 3 wt%).



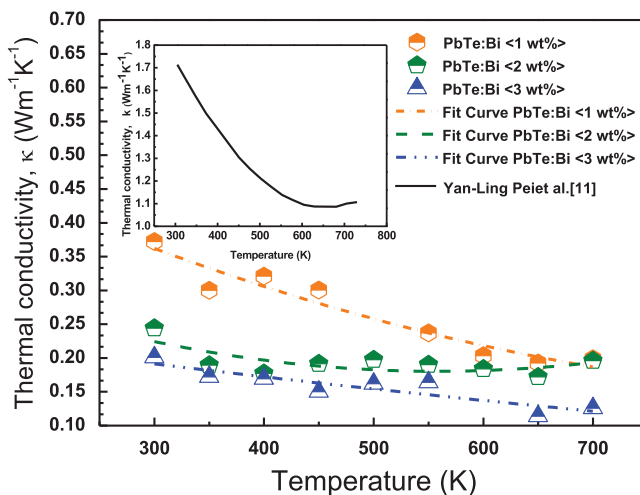
**Figure 3.** Simulated temperature dependence on linear thermal expansion coefficient of Bi doped PbTe. (1 wt%, 2 wt%, and 3 wt%).

parameter with temperature was compared to the result of A. Nicorici *et al.* [7]. The compressibility values are calculated by lattice parameter at pressure 0.0001, 0.7501 and 1.5001 GPa. The inverse of compressibility is of interest for thermal properties study under the temperature range of 300–700 K as shown in Fig. 2. The calculation reported the results together with literature data [8, 9, 10]. The linear thermal expansion coefficient of PbTe was evaluated from the variation which increased with increasing temperature, as shown in Fig. 3. The temperature dependence of Bi doped PbTe is scarcely influenced by adding Bi in the temperature range of 300–700 K as shown in Fig. 4.

The temperature dependence of calculated thermal conductivities indicated that the thermal conductivity of PbTe was able to be evaluated by the MD method. We found that the calculated thermal conductivity decreased with increasing Bi content [12] as shown in



**Figure 4.** Simulated temperature dependence on heat capacity at constant pressure,  $C_p$  of Bi doped PbTe. (1 wt%, 2 wt%, and 3 wt%).



**Figure 5.** Simulated temperature dependence on thermal conductivity of Bi doped PbTe. (1 wt%, 2 wt%, and 3 wt%).

Fig. 5. The present study showed that the MD method was a useful application to determine the thermo physical properties of Bi doped PbTe.

#### 4. Conclusions

The thermal properties composed of lattice parameter, compressibility, linear thermal expansion coefficient heat capacity and thermal conductivity for PbTe thermoelectric materials were successfully calculated by molecular dynamic simulation. The simulation thermal properties used parameters such as temperature in range 300–700 K, rocksalt structure, the cluster atoms site of  $4 \times 4 \times 4$  on 512 atoms fitted the experimental data and literature data. In addition, the simulation results were in good agreement with experimental data.

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