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Predication of Thermal Conductivity of Mg_2X (X = Ge and Sn) by Molecular Dynamics

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Molecular dynamics (MD) simulations of elastic and thermal properties of Mg_2X (X = Ge and Sn) based on anti-fluorite structure (CaF_2) at temperature range 300–700 K were presented. The MD simulation in this study involving the Morse–type potential functions, and the Busing–Ida potential to determine the interatomic interaction among cluster atoms size 4×4×4 unit cells of 768 atoms {512–$Mg^{1.2+}$, 256–$(Ge, Sn)^{2.4-}$}. The potential parameter functions of the cluster atoms were indicated by random numerical method and fit lattice parameter from the experimental data obtained at room temperature. The calculation of lattice parameter, pressure, temperature and energy contributes to evaluation of the elastic properties. The results showed that Mg_2Ge had better elasticity than Mg_2Sn. On the other hand, Mg_2Sn had less thermal conductivity than Mg_2Ge. Since thermal conductivity decreases with increasing temperature, the interesting feature of thermal conductivity is particulary useful to enhance thermoelectric performance of materials.

Keywords Molecular dynamics; Mg_2Sn; Mg_2Ge; thermal properties; elastic properties

1. Introduction

Mg_2X (X = Ge, Sn) compounds based on anti–fluorite (CaF_2) type structure are p–type thermoelectric (TE) materials. In general, good TE properties have large Seebeck coefficient, high electrical conductivity, and low thermal conductivity [1–4]. The composition element of Mg_2Ge and Mg_2Sn are green TE materials [1], and are in the interest of researchers to further study on TE properties. In addition, the height pressure behaviours of Mg_2Ge and Mg_2Sn are isostructure alkali–metal oxide Li_2O [5] and anti–fluorite type which can be assimilated to perfect crystal structure [6]. However, elastic properties, which is composed of low thermal expansion coefficient, high hardness, low compressibility,

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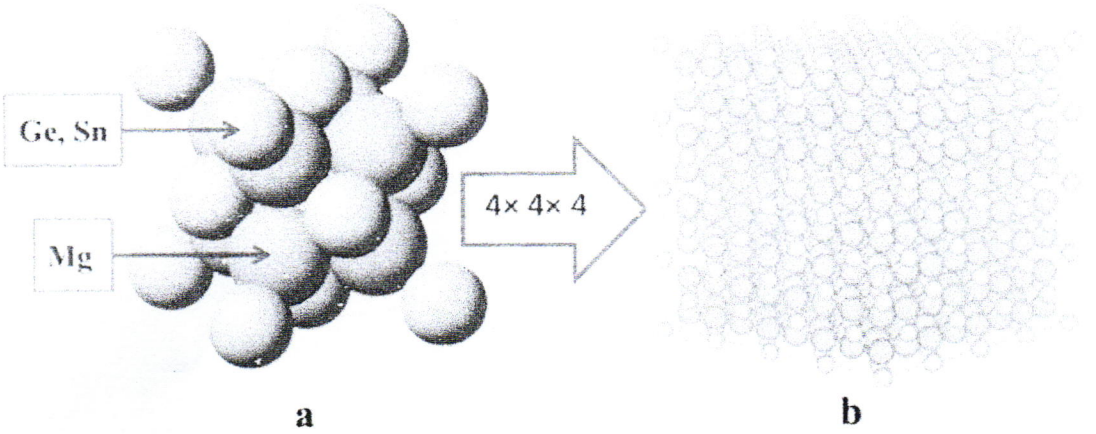

Figure 1. (a) 1 unit cell and (b) 4 × 4 × 4 unit cells of Mg_2Ge and Mg_2Sn for MD calculation.

high bulk modulus, and high elastic modulus (Young's modulus), is also reported [7–12]. Thermal properties is given heat capacity, as defined by Dulong–Petit law at temperature more than 500 K for Mg_2Ge and more than 400 K for Mg_2Sn. Much studies also reveal that thermal conductivity of Mg_2Ge and Mg_2Sn decreased with increasing temperature is a good behavior of TE materials [6, 8, 13–17]. In addition, a study of TE properties can be used computer simulation for determining before experiment. Recently, molecular dynamics was used to explore thermal conductivity of Bi–doped PbTe thermoelectric material and reported its success [18].

In this work, we focus on molecular dynamics study of the elastic properties and thermal properties of Mg_2X (X = Ge, Sn) to predict thermal conductivity.

2. Computational Details

The Mg_2Ge and Mg_2Sn of 768 atoms $\{512–Mg^{1.2+}, 256–(Ge, Sn)^{2.4-}\}$ were calculated through the MD method as shown in Fig. 1. The scaling method, Nose method [19] and Andersen method [20] were used to control pressure and temperature, and employed in calculation process of the lattice parameter, heat capacity and thermal conductivity, as shown in Table 1.

Table 1
Calculation conditions for MD method of Mg_2Ge and Mg_2Sn

Calculation conditions	Lattice parameter	Heat capacity	Thermal conductivity
System	768 atoms (512 cations and 256 anions) Mg = 512, Ge, Sn = 256; CaF_2 crystal structure		
Control			
- Temperature	Scaling	Scaling	Nose [19]
- Pressure	Scaling	No control	Andersen [20]
Number of steps	100,000	100,000	100,000

The MD process calculated the atom positions and volecities from Newton equation of motion through Verlet's algorithm [21], and measured the running time per step at 2.0×10^{-15} s. Ewald's summation [22] evaluated the total internal energy base on MXDORTO program [23], as described by equations below;

$$\vec{F}_i = m_i \frac{\partial^2 \vec{r}_i}{\partial t^2} \; i = 1, ..., \mathrm{N} \tag{1}$$

$$\vec{F}_i = -\frac{\partial U(r_1, ..., r_\mathrm{N})}{\partial \vec{r}_i} \tag{2}$$

$$E_i = U_{ij} + E_{Ki}; \; E_{Ki} = \frac{1}{2} m_i v_i^2 \tag{3}$$

$$U(r) = \sum_{ij} U_{ij}(r) + \sum_{ijk} U_{ijk}(r) + \sum_{ijkl} U_{ijkl}(r) + ... \tag{4}$$

whereas, $\vec{F}$, m, $\vec{r}$, $U(r_1, ..., r_N)$, E_K, v, U, i, j and k were force, mass, position, potential function for N atoms, kinetic energy, volocity, and potential energy and atom of i, j and k, respectively. To determine the potential function $U(r)$ for interatomic interaction, this work employed the Morse–type [24], and the Busing–Ida potentail functions[25];

$$U_{ij}(r_{ij}) = \frac{z_i z_j e^2}{r_{ij}} + f_0(b_i + b_j)\exp\left(\frac{a_i + a_j - r_{ij}}{b_i + b_j}\right) - \frac{c_i c_j}{r_{ij}^6} + D_{ij}\left\{\exp\left[-2\beta_{ij}(r_{ij} - r_{ij}^*)\right] - 2\exp\left[-\beta_{ij}(r_{ij} - r_{ij}^*)\right]\right\} \tag{5}$$

whereas, f_0 is repulsion betaween atom in vacuum = 4.186, z_i and $z_j$are the effective partial electronic charges on the i^{th} and j^{th} ions. r_{ij} is the inter–atomic distance, r_{ij}^* is the bond length of the cation–anion pair in vacuum. a, b and c are the characteristic parameters depending on the ion species. The potential function, D_{ij} and β_{ij}, describes the depth and shape of this potential, respectively. The first term describes the Coulomb interactions and denotes core repulsions for the secound term. The third term is a Morse–type that applied only to cation–anion pairs.

3. Results and Discussion

3.1 Structure Expansion

The structure expansion was described by lattice parameter, linear thermal expansion coefficient (α_{lin}) and mean square displacement (MSD), as shown in Figs. 2, 3 and 4. The lattice parameters were calculated by MD method, and fit to literature data [26–28] at room temperature.

The α_{lin} had similar results as S. Ganeshan [9] and H. Wang [8] studies which was different about 6% for Mg_2Sn and 4% for Mg_2Ge. In this study, the lattice parameters were expanded and atoms in the structure which increased the area of vibraion with increasing temperature. The structure of Mg_2Sn was larger and expanded better than Mg_2Ge. The linear thermal expansion coefficient and mean square displacement could be analyzed by following equations;

$$\alpha_{lin} = \frac{1}{a(\mathrm{T}_0)}\left(\frac{a(\mathrm{T}) - a(\mathrm{T}_0)}{T - T_0}\right)_{P_0} \tag{6}$$

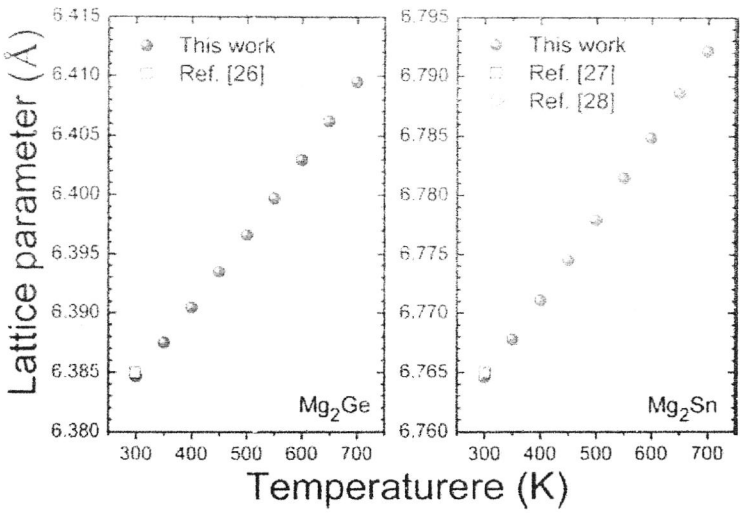

Figure 2. Lattice parameters of Mg_2Ge and Mg_2Sn at various temperatures.

$$\mathrm{MSD} = \left\langle [r(t) - r(0)]^2 \right\rangle = \left\langle r(t)^2 \right\rangle + r(0) - 2r(0) \left\langle r(t) \right\rangle \tag{7}$$

where α_{lin}, a(T), T_0, P_0, $r(t)$ and $r(0)$ were linear thermal expansion coefficient, lattice parameter at temperature T(K), room temperature, atmospheric pressure, displacement at time t and displacement at initial time, respectively.

3.2 Elastic Properties

The elastic properties, comprising compressibility (β), bulk modulus (B), stress (τ), strain (ε) and Young's modulus (E_Y), were analyzed by lattice parameter at 0.0001, 0.75 and 1.5

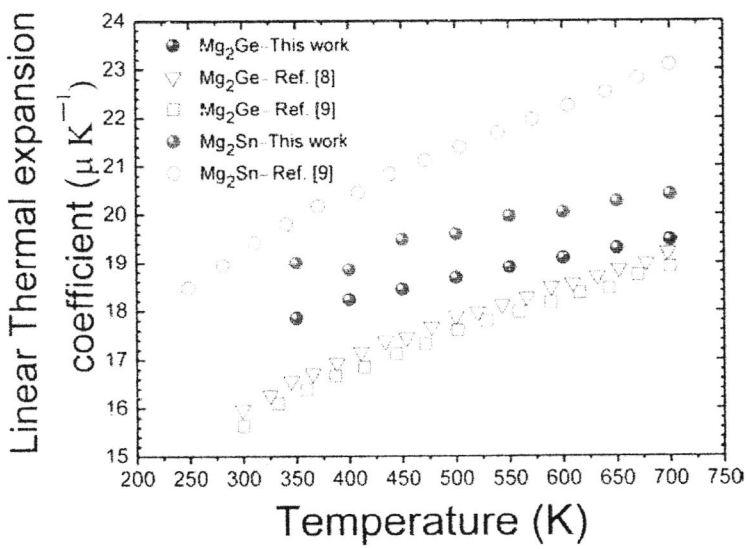

Figure 3. Linear thermal expansion coefficient of Mg_2Ge and Mg_2Sn at various temperatures.

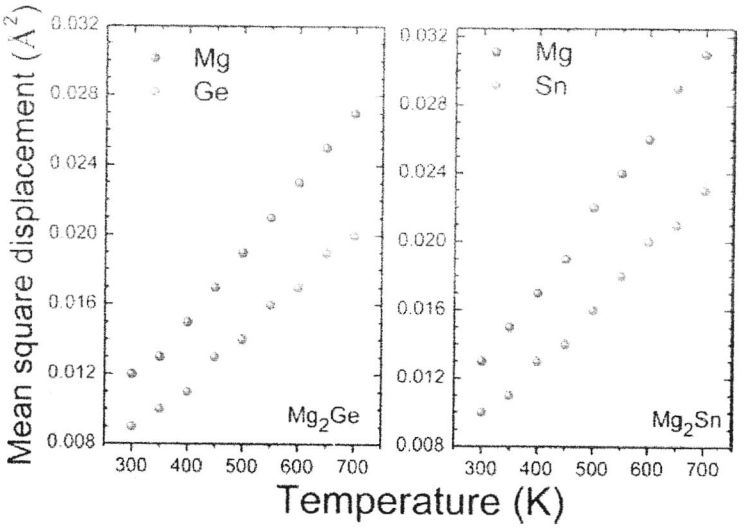

Figure 4. Mean square displacement of $Mg_2Ge$and Mg_2Sn at various temperatures.

GPa and temperature range 300−700 K, as following equations;

$$\beta = \frac{3}{a(\mathrm{P}_0)}\left(\frac{\partial a(\mathrm{P})}{\partial P}\right)_T \tag{8}$$

$$B = \frac{1}{\beta} \tag{9}$$

$$\tau = \frac{F}{A_0} \tag{10}$$

$$\varepsilon = \frac{\Delta l}{l} \tag{11}$$

$$E_\mathrm{Y} = \frac{\tau}{\varepsilon} \tag{12}$$

where β, a(P), B, τ, F, A_9, ε, l and E_Y involved compressibility, lattice parameter at pressure P(Pa), bulk modulus, stress, strain, action force, based area, length of cluster and Young's modulus, respectively.

The linear compressibility (β_{lin}) compared with the volume compressibility (β_{vol}) [7], was resulted from the compressibility, which was analyzed though lattice parameter. In this work, the linear compressibility of Mg_2Ge and Mg_2Sn were different from the reference data about 9% and that of Mg_2Sn intersected with the reference data at temperature 500 K as shown in Fig 5. The bulk modulus (B) was evaluated by inverse of β and good agrees with the results of H. Wang [8] and S. Ganeshan [9] as shown in Fig. 6. From the comprssibility and bulk modulus showed that Mg_2Ge had a resist of pressing better than Mg_2Sn. The stress (τ) and strian (ε) of Mg_2Ge and Mg_2Sn indicated Young's modulus as shown in Fig. 7. The calculation has shown that Mg_2Ge had more stress than Mg_2Sn. On the otherhand the strian of Mg_2Ge was less than Mg_2Sn. The Young's modulus was compared with the results of S. Ganeshan [9], shown in Fig. 8. From the foregoing, the Young's modulus described Mg_2Ge which had better elasticity than Mg_2Sn because bulk modulus and stress were greater but less strain.

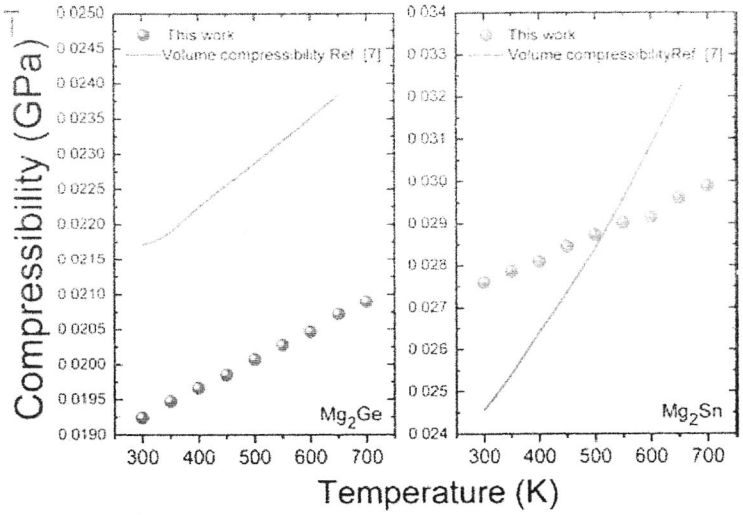

Figure 5. The relationship of temperature to compressibility of Mg_2Ge and Mg_2Sn.

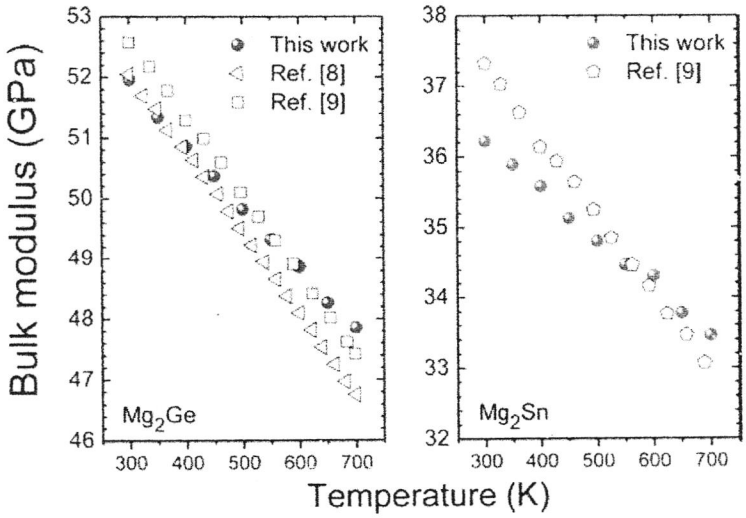

Figure 6. The relationship of temperature to bulk modulus of Mg_2Ge and Mg_2Sn.

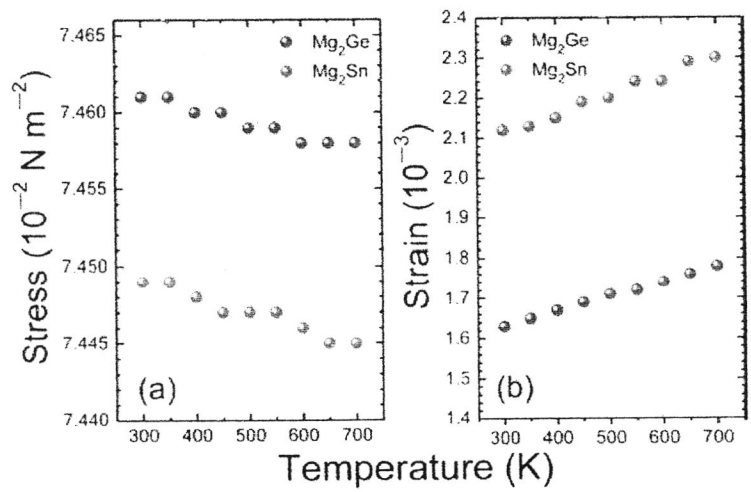

Figure 7. The relationship of temperature to stress and strian of Mg_2Ge and Mg_2Sn.

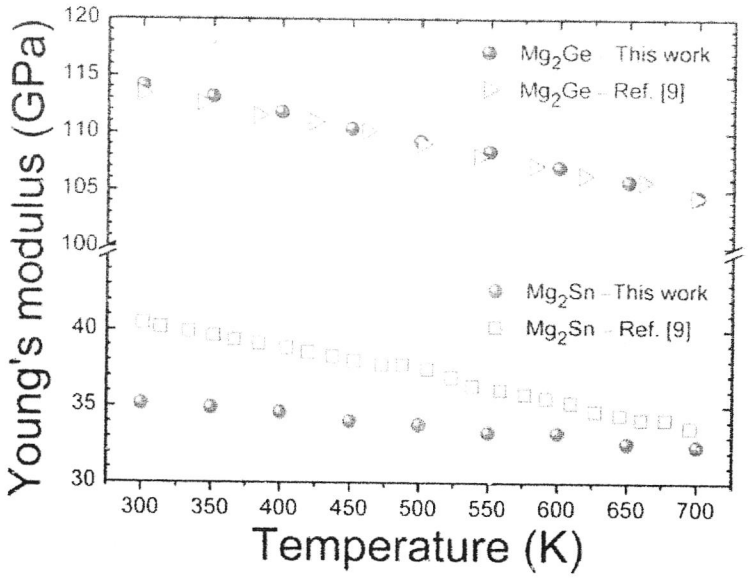

Figure 8. The relationship of temperature to Young's modulus of Mg_2Ge and Mg_2Sn.

3.3 Thermal Properties

The thermal properties were composed of heat capacity and thermal conductivity. The heat capacity of lattice dilatational term (C_d) was evaluated by lattice parameter, α_{lin} and β_{lin}. The heat capacity at constant volume (C_V) was also evaluated by gradient of the total internal energy. In addition, the heat capacity at constant pressure (C_P) was evaluated by sum of C_V and C_d. The internal energy showed that Mg_2Ge had energy less than Mg_2Sn due to the MSD of Mg_2Ge was less than Mg_2Sn. In Fig. 10 the heat capacity was compared with the results of S. Ganeshan [9], H. Wang [8], L. Na-Na [15] and also shows that heat capacity of Mg_2Ge less than Mg_2Sn. The heat capacity of Mg_2Ge agreed with the result data [8, 13] at temperature 300–550 K. ThusC_V was in a constant–rate at 650 K which was agreed with Dulong–Petit law. The $C_V$of Mg_2Sn showed a good agreement with the result data [8], and Dulong–Petit law at temperature 600 K. The relationship of temperature to

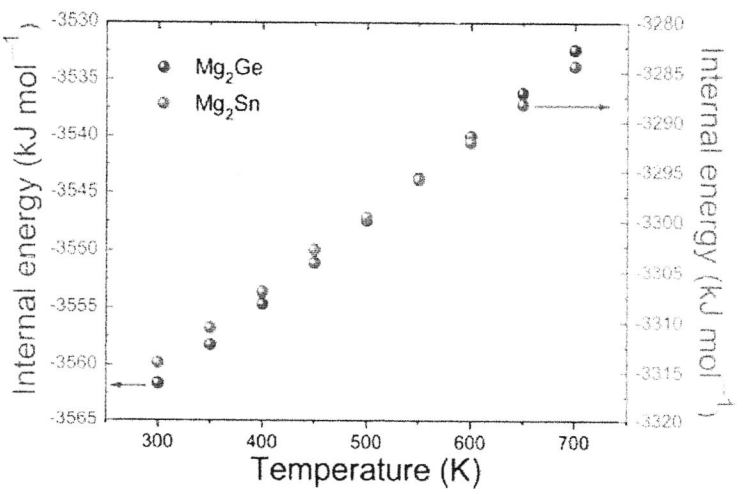

Figure 9. Internal energy of Mg_2Ge and Mg_2Sn at various temperatures.

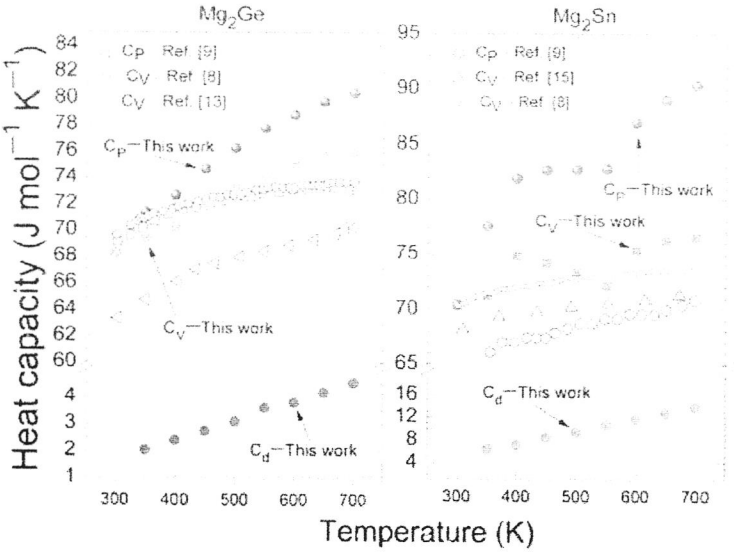

Figure 10. The relationship of temperature to heat capacity of Mg_2Ge and Mg_2Sn.

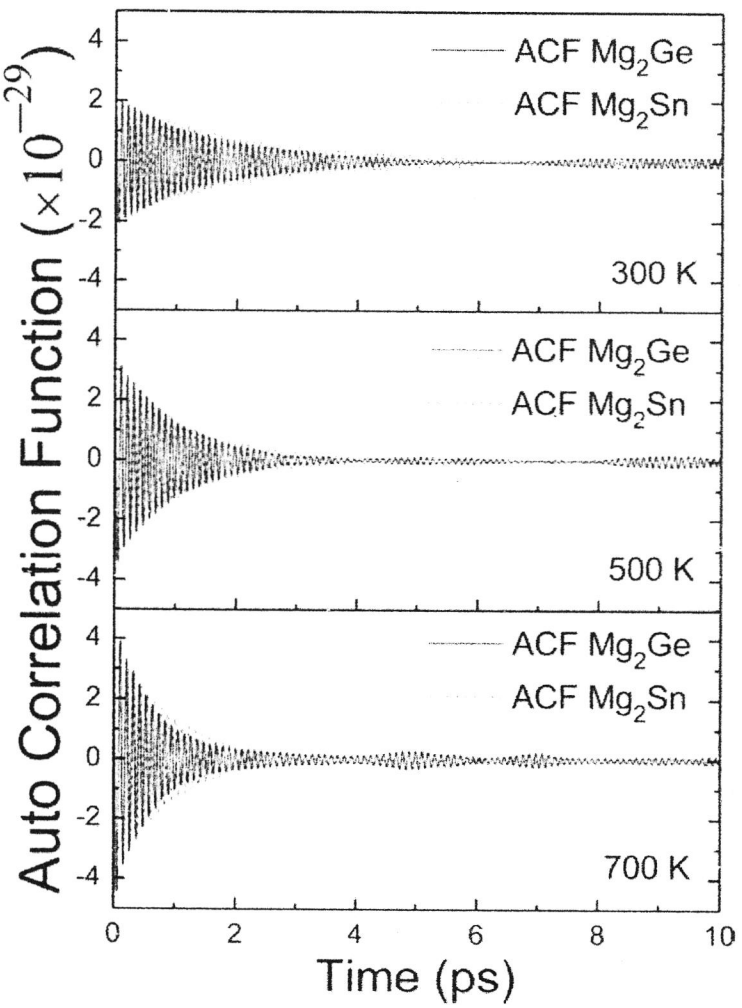

Figure 11. Heat flux auto-correlation function (ACF) of Mg_2Ge and Mg_2Sn at 300 K, 500 K and 700 K versus time.

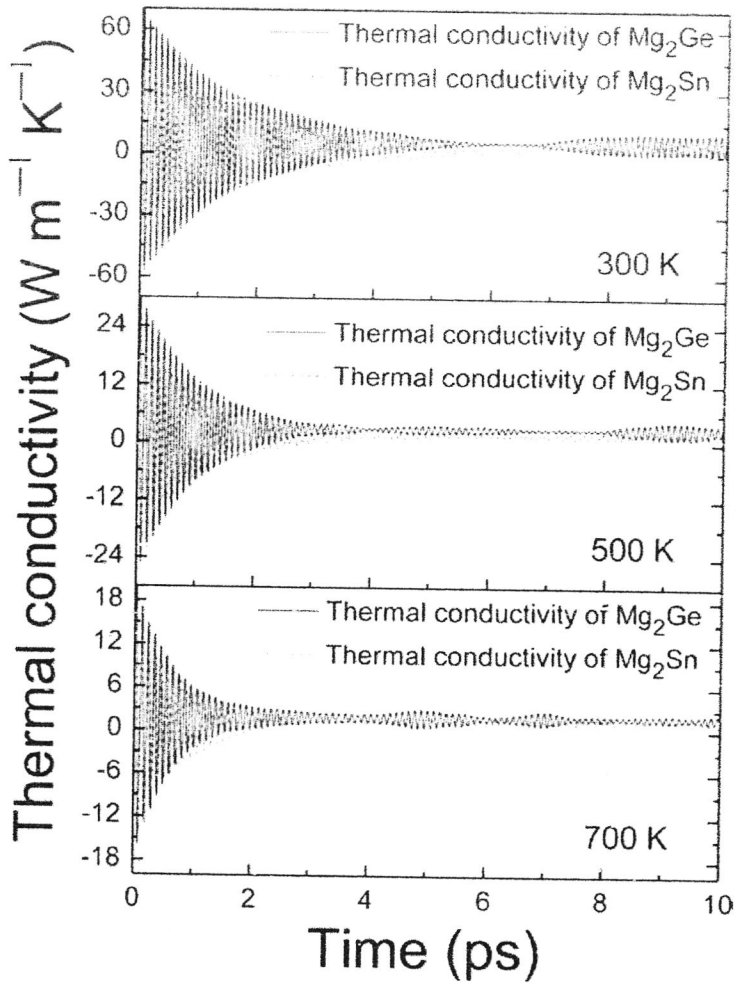

Figure 12. Thermal conductivity of Mg_2Ge and Mg_2Sn at 300 K, 500 K and 700 K versus time.

heat capacity for Mg_2Ge and Mg_2Sn can be evaluated by equations;

$$C_{\mathrm{d}} = \frac{(3\alpha_{lin})^2 V_m(T)}{\beta} T \tag{13}$$

$$C_{\mathrm{V}} = \left(\frac{\partial E(\mathrm{T})}{\partial T}\right)_V \tag{14}$$

$$C_{\mathrm{P}} = C_{\mathrm{V}} + C_{\mathrm{d}} \tag{15}$$

where C_{d}, $V_m(T)$, C_{V}, $E(\mathrm{T})$ and C_{P} are heat capacity of lattice dilatational term, molar volume at temperature T (K), heat capacity at volume constant, total internal energy and heat capacity at pressure, respectively.

The thermal conductivity (κ) could be evaluated by sum of electrical contribution to thermal conductivity term (κ_{el}), lattice contribution to thermal conductivity term (κ_{lat}) and orther contribution to thermal conductivity term κ_{other}. This MD result presents the lattice contribution to thermal conductivity; hence $\kappa \approx \kappa_{lat}$. The κ_{lat} was evaluated from time integral of the heat flux auto–correlation function (ACF), by using the Green–Kubo

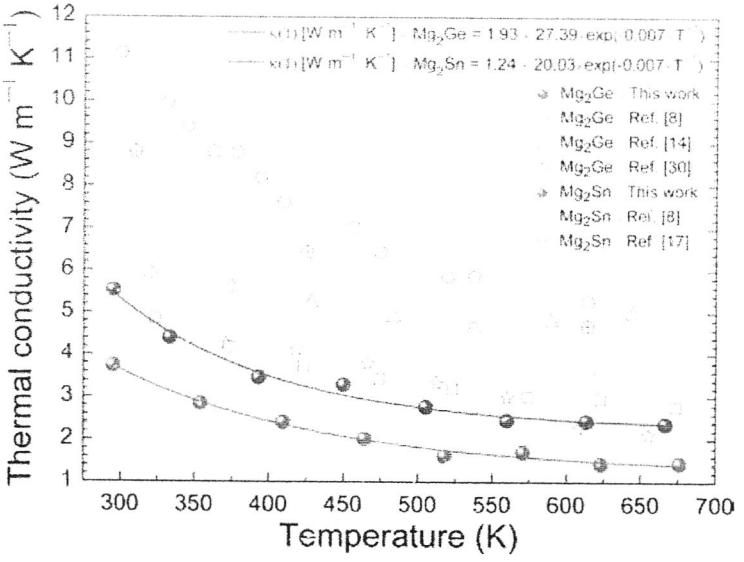

Figure 13. Thermal conductivity of Mg_2Ge and Mg_2Sn at various temperatures.

relation [29], as shown in equations;

$$\kappa_{lat} = \frac{V}{3k_B T^2} \int_0^\infty \langle S(t)S(0)\rangle dt \tag{16}$$

$$S(t) = \frac{1}{V}\left[\sum_j E_j v_j + \frac{1}{2}\sum_j \sum_{i\neq j} r_{ij}\left(f_{ij} v_j\right)\right] \tag{17}$$

$$E_j = \left\{\frac{1}{2} m_i v_j^2 + \frac{1}{2}\sum_{i\neq j} U_{ij}\left(r_{ij}\right)\right\} - E_{av} \tag{18}$$

where κ_{lat}, k_B, V, $S(t)$, E, m, v, r_{ij}, f_{ij}, $U_{ij}\left(r_{ij}\right)$ and E_{av} are lattice thermal conductivity, Boltzmann constant, volume, auto–correlation function, energy, mass, velocity, interatomic distance between atom i and j, force between atom i and j, the Busing–Ida potential between atom i and j, and average energy of the system, respectively.

From the calculation, it was found that the relationship of κ_{lat} dependent ACF and inverse temperature. ACF inverse of time (ps and dependent of temperature, as shown in Fig. 12 and 13). The thermal conductivity of Mg_2Ge and Mg_2Sn have values 5.53 W m^{-1} K^{-1} and 3.37 W m^{-1} K^{-1} at 300 K, which decrease to 1.78 W m^{-1} K^{-1} and 1.44 W m^{-1} K^{-1} at 700 K, respectively. Mg_2Sn is more interesting to enhance thermoelectric performance because it has thermal conductivity less than Mg_2Ge. The lattice thermal conductivity (κ_{lat}) of Mg_2Ge and Mg_2Sn were compared with the total thermal conductivity (κ_{tot}) [8, 14, 17, 30] as shown in Fig. 13. In addition, this κ_{lat} was less than the reference data because the reference shows total conductivity composing of orther contribution to thermal conductivity term (κ_{other}). However, the κ_{lat} of Mg_2Ge had a good agreement with M. Akasaka [14].

4. Conclusion

Molecular dynamics was used to calculate lattice expansion, elastic and thermal properties of Mg_2Ge and Mg_2Sn. The lattice expansion showed that Mg_2Sn had structure, linear expand and area of vibration better than Mg_2Ge. The elastic properties showed that Mg_2Ge had better elasticity than Mg_2Sn. Thermal properties reported that Mg_2Sn had the heat capacity, and the thermal conductivity better than Mg_2Ge. This work found that Mg_2Sn was attractive for thermoelectric performance study. However, it should be further study of electrical properties for evaluating thermoelectric properties to confirm materials before experiment.

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หนังสือยินยอม

ข้าพเจ้า นายมีนา ฤทธิร่วม เป็นผู้เขียนชื่อแรกในบทความเรื่อง "Predication of Thermal Conductivity of Mg_2X (X = Ge and Sn) by Molecular Dynamics" ตีพิมพ์ในวารสาร Integrated Ferroelectrics An International Journal เล่มที่ (Vol) 15 ฉบับที่ (No.) ISSUE 1 เดือนตุลาคม ปี ค.ศ. 2015 เลขหน้า (pp) 61-72 นั้น ขอยินยอมให้ นายไวรุจ อิ่มโพธิ์ ซึ่งเป็น ผู้เขียนร่วม (co-author) ในบทความดังกล่าว เป็นผู้ขอรับเงินสนับสนุนการตีพิมพ์เผยแพร่บทความวิจัยในวารสารระดับนานาชาติ

ลงชื่อ.....ผู้ยินยอม

(นายมีนา ฤทธิร่วม)

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Predication of Thermal Conductivity of Mg_2X (X = Ge and Sn) by Molecular Dynamics

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Materials Chemistry	Q4	Q4	Q4	Q4	Q4	Q4	Q4	Q4	Q4	Q4	Q4	Q3	Q3	Q3	Q3	Q3
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