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Lili Liu*, Xiaozhi Wu, Weiguo Li, Rui Wang, and Qing Liu

High temperature and pressure effects on the elastic properties of B2 intermetallics AgRE

Abstract: The high temperature and pressure effects on the elastic properties of the AgRE (RE=Sc, Tm, Er, Dy, Tb) intermetallic compounds with B2 structure have been performed from first principle calculations. For the temperature range 0-1000 K, the second order elastic constants for all the AgRE intermetallic compounds follow a normal behavior: they decrease with increasing temperature. The pressure dependence of the second order elastic constants has been investigated on the basis of the third order elastic constants. Temperature and pressure dependent elastic anisotropic parameters *A* have been calculated based on the temperature and pressure dependent elastic constants.

Keywords: rare-earth intermetallics; elastic properties; temperature; pressure; first principles calculation

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1 Introduction

Over the past few decades, the B2 structure (CsCl-type structure) intermetallic compounds have attracted considerable attention owing to their high strength and melting temperature combined with a low specific weight and high oxidation resistance [1, 2]. However, few practical uses have materialized because of their brittle nature at ambient temperature [3]. In 2003, a new class of highly ordered, ductile intermetallic compounds with composition MRE (where RE indicates a rare-earth element, and M denotes a late transition metal or an early p-element) at room temperature was discovered by Gschneidner *et al.* [4]. These MRE compounds are "line-compounds" with exact 1:1 stoichiometry, and they are formed from high M and RE without the addition of a third element. Thereafter, a great deal of work (including theory and experiment) has been performed to understand their various properties [5–15]. Recently, some properties such as mechanical, electronic structure and thermal properties of the AgRE intermetallics have been studied by using the projector augmented-wave (PAW) method within the generalized gradient approximation (GGA) [16].

In general, the elastic constants of a solid are important since they relate to various fundamental solid-state properties such as interatomic potentials, equation of state, Young's modulus, Poisson's ratio, thermal expansion, Debye temperature, melting point, Grüneisen parameter and so on. In linear elastic theory were infinitesimal deformations are assumed, the second-order elastic constants (SOECs) are sufficient to describe the linear elastic stress-strain response [17]. There have been many reports of first principles calculations of the SOECs of materials by the total energy approach [18, 19], stress-strain approach [20–23] and density functional perturbation theory (DFPT) [24–26]. However, all of these calculations are restricted to a temperature of 0 K. Obtaining the corresponding temperature dependent SOECs is still an arduous challenge [27]. The temperature dependent SOECs are very important for understanding the mechanical strength, stability and phase transition of a material. Fortunately, Wang *et al.* [28, 29] proposed a quasistatic approach based on the assumption that the temperature dependent elastic constants mainly result from volume change with increasing temperature to determine the temperature dependent SOECs from first principles calculations. Excellent agreement between their predicted values and existing experimental measurements was found. In this work, we employ this method [28, 29] to investigate the temperature dependent SOECs of intermetallic compounds AgRE (RE=Sc, Tm, Er, Dy, Tb) with B2 structure.

***Corresponding Author: Lili Liu:** College of Physics and Institute for Structure and Function, Chongqing University, 401331, P.R. China, Email: liulili0612@163.com
Xiaozhi Wu: College of Physics and Institute for Structure and Function, Chongqing University, 401331, P.R. China, E-mail: xiaozhiwu@cqu.edu.cn
Xiaozhi Wu: College of Materials Science and Engineering, Chongqing University, 400044, P.R. China
Weiguo Li: College of Aerospace Engineering, Chongqing University, 400044, P.R. China
Rui Wang: College of Physics and Institute for Structure and Function, Chongqing University, 401331, P.R. China
Qing Liu: College of Materials Science and Engineering, Chongqing University, 400044, P.R. China, E-mail: qingliu@cqu.edu.cn

The pressure dependence of the SOECs is also very useful for AgRE intermetallics since there are no experimental values available. The pressure dependent SOECs can be obtained through the third order elastic constants (TOECs). TOECs are useful not only in describing the mechanical response of crystals under high stress and strain, but they also serve as a basis for describing anharmonic properties such as thermal expansion, phonon-phonon interaction and Grüneisen parameter, amongst others [30, 31]. As is well known, it is rather difficult to obtain a complete set of TOECs for crystals with low-yield stress from experimental methods. Several theoretical approaches have been introduced to calculate the TOECs of solids. These methods include the empirical interatomic force-constant model [32, 33], molecular-dynamics simulations using fluctuation formulas [34, 35], and the first-principles quantum mechanics calculations [36, 37]. The use of first-principles mechanics calculations method to determine TOECs was first introduced by Nielson and Martin [38]. They employed the method of homogeneous deformation strain combined with the first-principles strain-energy relations calculations to determine the elastic constants. The homogeneous deformation strains used are usually simple deformation modes such as uniaxial tensor or compression, simple or pure shear, and other combinations of homogeneous strains. Recently, the same method of the fist-principles quantum mechanics calculations has been employed to determine the TOECs in single crystals [39–41]. Their results show good agreement with experiments. In this work, we employ the method of homogeneous deformation combined with first-principles total-energy calculations to calculate the TOECs of rare-earth intermetallic compounds AgRE (RE=Sc, Tm, Er, Dy, Tb) with B2 structure. For more details of TOECs calculations, see [39–42].

2 Computational methodology

The Helmholtz free energy per atom of intermetallics at a constant volume V and T within the framework of quasi-harmonic approach (QHA) can be expressed as

$$F(V,T) = U_{\text{static}}(V) + \sum_{\kappa}\left[\frac{1}{2}\hbar\omega_{\kappa} + k_B T \ln\left(1 - e^{-\hbar\omega_{\kappa}/k_B T}\right)\right], \quad (1)$$

where $U_{\text{static}}(V)$ is the static total energy at 0 K, k_B is the Bolzmann's constant, $\hbar$ represents the reduced Planck constant, and ω_{κ} is the frequency of an individual phonon.

The isothermal elastic constants are obtained by expanding the Helmholtz free energy as a Taylor series in Lagrangian strain tensor η at constant temperature [43, 44]

$$F(V,\eta,T) = U(V,0,T) + \frac{V}{2!}\sum_{ijkl} C^T_{ijkl}\eta_{ij}\eta_{kl} + \frac{V}{3!}\sum_{ijklmn} C^T_{ijklmn}\eta_{ij}\eta_{kl}\eta_{mn} + \ldots. \quad (2)$$

The elastic behavior of cubic crystals is specified by three independent elastic constants C^T_{11}, C^T_{12} and C^T_{44} (in Voigt notation). The bulk modulus $B^T = (C^T_{11} + 2C^T_{12})/3$ is the resistance to deformation by a uniform hydrostatic pressure and is also obtained from fitting the Vinet equation of state [45]. The strain matrix for the calculation of $C^T_{11} - C^T_{12}$ combination has the following form

$$\eta(\delta) = \begin{pmatrix} \delta & 0 & 0 \\ 0 & \delta & 0 \\ 0 & 0 & (1+\delta)^2 - 1 \end{pmatrix}, \quad (3)$$

and the free energy expression is

$$F(V,\delta) = F(V,0) + 3(C^T_{11} - C^T_{12})V\delta^2 + O(\delta^3),$$

where $F(V,0)$ refers to the free energy of the equilibrium configuration. We use a volume-conserving tetragonal strain to determine C^T_{44}:

$$\eta(\delta) = \begin{pmatrix} 0 & \delta & 0 \\ \delta & 0 & 0 \\ 0 & 0 & \delta^2/(1-\delta^2) \end{pmatrix}, \quad (4)$$

and the Helmholtz free energy related to this strain is $F(V,\delta) = F(V,0) + 2C^T_{44}V\delta^2 + O(\delta^4)$.

In the present work, we employ a quasistatic approximation developed by Wang *et al.* [28, 29] to calculate the temperature dependence of the elastic constant C^T_{ij}. The quasistatic method is based on the assumption that the temperature dependence of elastic constant mainly results from a volume change due to thermal expansion, and the contribution of vibrational free energy to these second derivation can be neglected. The quasistatic method has the following three-step procedure [28]. The first step in this procedure is to the determine equilibrium volume $V(T)$ at given T. This is calculated using the first-principles quasiharmonic approach. In the second step, we obtain the volume-dependent elastic constants $C^T_{ij}(V)$ at T = 0 K. They are defined as the second derivatives of the Helmholtz free energy F with respect to the elements of the infinitesimal strain tensor by employing the energy-strain relation based on Equations (2)–(6). In the third step, the elastic constants calculated from the second step,

at the volume $V(T)$, are approximated as those at finite temperature. To compare with experiment, the isothermal elastic constants must be converted to the isentropic elastic constants. The isothermal elastic constants and the isentropic elastic constants have the relations $C_{44}^S = C_{44}^T$ and $C_{11}^S - C_{11}^T = C_{12}^S - C_{12}^T = \frac{TV}{C_v}\alpha^2 B^{T^2}$, where C_V and α are the specific heat at constant volume and the thermal expansion coefficient, respectively.

In our third order elastic constants (TOECs) calculations, deformations are applied under isothermal conditions $T = 0K$, $F = U - TS = U$, so $C^S = C^T$. We will not distinguish those two types of elastic constants in the following. There are six independent TOECs (C_{111}, C_{112}, C_{123}, C_{144}, C_{155} and C_{456}) for AgRE. The number of applied strain tensors must be as large as the number of independent TOECs for solving the TOECs. Hence, we need consider six sets of deformation [41]:

$$\eta_A = \begin{pmatrix} \delta & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \eta_B = \begin{pmatrix} \delta & 0 & 0 \\ 0 & \delta & 0 \\ 0 & 0 & 0 \end{pmatrix},$$
$$\eta_C = \begin{pmatrix} \delta & 0 & 0 \\ 0 & \delta & 0 \\ 0 & 0 & \delta \end{pmatrix},$$
$$\eta_D = \begin{pmatrix} \delta & 0 & 0 \\ 0 & 0 & \frac{\delta}{2} \\ 0 & \frac{\delta}{2} & 0 \end{pmatrix}, \quad \eta_E = \begin{pmatrix} \delta & 0 & \frac{\delta}{2} \\ 0 & 0 & 0 \\ \frac{\delta}{2} & 0 & 0 \end{pmatrix},$$
$$\eta_F = \begin{pmatrix} 0 & \frac{\delta}{2} & \frac{\delta}{2} \\ \frac{\delta}{2} & 0 & \frac{\delta}{2} \\ \frac{\delta}{2} & \frac{\delta}{2} & 0 \end{pmatrix}. \tag{5}$$

The corresponding elastic energy on deformation parameter δ for each stain tensor can be written as [41]

$$\Delta U(\eta_A) = \tfrac{1}{2}C_{11}\delta^2 + \tfrac{1}{6}C_{111}\delta^3,$$
$$\Delta U(\eta_B) = (C_{11} + C_{12})\delta^2 + (\tfrac{1}{3}C_{111} + C_{112})\delta^3,$$
$$\Delta U(\eta_C) = (\tfrac{3}{2}C_{11} + 3C_{12})\delta^2 + (\tfrac{1}{2}C_{111} + 3C_{112} + C_{123})\delta^3,$$
$$\Delta U(\eta_D) = (\tfrac{1}{2}C_{11} + \tfrac{1}{2}C_{44})\delta^2 + (\tfrac{1}{6}C_{111} + \tfrac{1}{2}C_{144})\delta^3,$$
$$\Delta U(\eta_E) = (\tfrac{1}{2}C_{11} + \tfrac{1}{2}C_{44})\delta^2 + (\tfrac{1}{6}C_{111} + \tfrac{1}{2}C_{155})\delta^3 \text{and}$$
$$\Delta U(\eta_F) = \tfrac{3}{2}C_{44}\delta^2 + C_{456}\delta^3. \tag{6}$$

In the present work, the computational approach is based on the density functional theory (DFT) as implemented in the highly efficient Vienna ab initio simulation package (VASP) developed at the Institute für Materialphysik of Universität Wien [46–48]. The effects of the exchange-correlation functional are treated with the generalized gradient approximation (GGA) of Perdew-Burke-Ernzerhof (PBE) [49]. A plane-wave basis set is employed within the framework of the projector augmented wave (PAW) method [50]. Since high accuracy is needed to evaluate the TOECs, the k-point meshes ($23 \times 23 \times 23$) and the 600 eV energy cutoff of the wavefunction based on our test are employed to calculate the temperature dependent SOECs and TOECs for all our calculated AgRE (RE=Sc, Tm, Er, Dy, Tb) intermetallics. The total energy is converged numerically to less than 1×10^{-6} eV/atom with respect to electronic self-consistency.

Phonon calculations are performed for intermetallic compounds AgRE (RE=Sc, Tm, Er, Dy, Tb) by using the supercell method with the force constants predicted by the VASP code [1] in the framework of density-functional perturbation theory (DFPT) while the phonon properties are calculated by the PHONOPY package[2] [51]. The chosen supercell size strongly influence the thermal properties. To obtain a reasonable supercell size, we compared the vibrational free energies of the $3 \times 3 \times 3$ supercell with those of a $5 \times 5 \times 5$ supercell at 300 K and 1000 K. We discovered that the energy fluctuations between the $3\times3\times3$ and $5 \times 5 \times 5$ supercells are less than 0.01%. Hence, the supercell size consisting of $3\times3\times3$ unit cells with 54 atoms and the k-point scheme with $7\times7\times7$ grid meshes for Brillouin zone are employed to calculate the phonon frequency. In addition, a smearing with 0.05 eV is employed to deal with the possible convergence problems for all the intermetallic compounds. For more details of the temperature dependent SOECs calculations, see Ref. [28, 29].

3 Results and discussion

3.1 High temperature effect on the SOECs

The calculated equilibrium lattice constants a, elastic constants C_{ij}, and the elastic anisotropy factors A at $T = 0$ K for B2-AgRE (RE=Sc, Tm, Er, Dy, Tb) have been listed in Table 1 along with the available experimental data [5, 52, 53] and other theoretical values [16]. As can be seen from Table 1, the present calculated lattice constants increase with decreasing rare-earth atom number. Comparison with experimental lattice constants [5], the present calculated lattice constants are in fairly good agreement with the exper-

1 G. Kresse, M. Marsman, J. Furthmüller, VASP the Guide, http://cms.mpi.univie.ac.at/vasp/

2 A. Togo, Phonopy, http://phonopy.sourceforge.net/

imental data within 1.0%. The lattice constants of AgSc, AgTm, AgEr, AgDy and AgTb obtained by Tao *et al.* [16] are 3.436 Å, 3.586 Å, 3.601 Å, 3.633 Å and 3.649 Å, respectively. Obviously, the present lattice constants of AgRE are almost exactly the same as the results obtained by Tao *et al.* [16]. The present calculated elastic constants for B2-AgRE (RE=Sc, Tm, Er, Dy, Tb) are also in good agreement with the theoretical values [16]. However, for AgTm and AgDy, the present calculated elastic constants C_{11} and C_{12} are smaller than the experimental values [52, 53], but the elastic constants C_{44} are very close to the experimental data [52, 53]. All the differences between the calculations and experiments are within 13%. It should be mentioned that most of the experimental data of elastic constants are usually reported as isentropic elastic constants, therefore, the isothermal elastic constants obtained here must be converted to the isentropic elastic constants [15]. The calculated isentropic elastic constants C_{11}^S, C_{12}^S and C_{44}^S as a function of temperature in the range of 0-1000 K for B2-AgRE (RE=Sc, Tm, Er, Dy, Tb) are shown in Figure 1. To judge that our calculations are reasonable, the temperature dependent C_{ij}^S for benchmark metal Ag have also been calculated, and our calculated results are shown in Figure 1(a) along with the available experimental values taken from ultrasonic measurements [54]. Comparing our calculated results with the experimental values for the benchmark metal Ag, we can test the accuracy of the method and the precision of our calculations for the unknown values of temperature dependent C_{ij}^S for B2-AgRE (RE=Sc, Tm, Er, Dy, Tb). As shown in Figure 1, it is apparent that the elastic constants C_{ij}^S for all calculated AgRE intermetallics decrease monotonically with increasing temperature, since thermal expansion may soften the elastic moduli at high temperature. There is abundant experimental evidence that lends support to the approximation, e.g. observations of the temperature dependent isothermal bulk modulus [55], Elinvar effect [56] and the isentropic bulk modulus and shear modulus [57]. We also find that the trend of C_{ij}^S is close to linearity at higher temperature and zero slope at zero temperature. Besides, it is found that the values of C_{11}^S decrease to slightly larger than C_{12}^S and C_{44}^S. The elastic constant C_{11}^S represents elasticity in length. A longitudinal strain causes a change in C_{11}^S. However, the elastic constants C_{12}^S and C_{44}^S are related to the elasticity in shape, which is a shear constant. The requirement of mechanical stability in a cubic crystal leads to the following relations on the elastic constants, $C_{11} - C_{12} > 0$, $C_{11} > 0$ and $C_{44} > 0$ [58]. Our values of the elastic constants for all researched AgRE intermetallics as shown in Figure 1 are satisfied with these stability conditions in the temperature range of 0-1000 K.

As is well known, cubic crystals have elastic anisotropy as a result of the fourth rank tensor property of elasticity. The elastic anisotropic parameter is related to the elastic constants as $A = 2C_{44}^S/(C_{11}^S - C_{12}^S)$. It is convenient to obtain the elastic anisotropic parameters A as a function of temperature for B2-AgRE (RE=Sc, Tm, Er, Dy, Tb) from the calculated temperature dependent elastic constants. In Figure 2, we show the temperature dependence of the elastic anisotropic parameters A in the temperature range of 0-1000 K, from which we can see that the elastic anisotropic parameters A of B2-AgRE (RE=Sc, Tm, Er, Dy, Tb) decrease with increasing temperature. We also find AgRE (RE=Sc, Tm, Er, Dy, Tb) exhibit high elastic anisotropy at zero temperature and the degree of the anisotropy decreases with increasing temperature.

3.2 High pressure effect on the SOECs via the TOECs

As far as calculations of TOECs are concerned, extremely good convergence of parameters included cutoff energy and k-points gird size governing the accuracy of computations is required. Taking AgEr as an example, Figure 3(a) and (b) show that two sample elastic constants C_{111} and C_{112} converge with the k-point grid size and the cutoff energy, respectively. For the selected parameters ($E_{\text{cutoff}}^{\text{AgEr}}$ = 600eV and $23 \times 23 \times 23$ k-point mesh size) in our calculations, the relative difference between successive values of examined constants is lower than 1 GPa. The convergence tests of k-point grid size and cutoff energy (see in Figure 3) show that we obtain very reliable information of the TOECs for our researched rare-earth intermetallic compounds AgRE (RE=Sc, Tm, Er, Dy, Tb) with B2 structure. The usage of PAW formalism chosen to solve the Kohn-Sham (KS) equations seems not to influence the results significantly [39]. In addition, we use the GGA-PBE exchange-correlation functional which is commonly considered to be one of the best in the market [39]. In essence, we provide very reliable information of the TOECs for intermetallic compounds AgRE (RE=Sc, Tm, Er, Dy, Tb) in Table 2. Unfortunately, there are no experimental data and theoretical values of the TOECs for comparison until now. Our results need to be verified accurately in future work.

We employ the method of homogeneous deformation strain combined with the first-principles strain-energy relations calculations to determine the TOECs. The homogeneous deformation strains used are usually simple deformation modes such as uniaxial tensor or compression, simple or pure shear, and other combinations of homogeneous strains. Interested reader should refer to [39–41] for

Table 1: The present calculated lattice constants a (Å), elastic constants C_{ij} (GPa) and elastic anisotropy parameters A for B2-AgRE (RE=Sc, Tm, Er, Dy, Tb) at $T = 0$ K compared to previous computed results and experimental data. Note that $C_{ij}^S = C_{ij}^T = C_{ij}$ at T=0K.

	AgSc	AgTm	AgEr	AgDy	AgTb
a	3.440[a], 3.436[b], 3.412[c]	3.580[a], 3.586[b], 3.550[c]	3.608[a], 3.601[b], 3.584[c]	3.617[a], 3.633[b], 3.612[c]	3.653[a], 3.649[b], 3.627[c]
C_{11}	108.9[a], 106.6[b]	103.2[a], 100.1[b], 110.4[d]	101.0[a], 102.7[b]	95.9[a], 98.1[b], 106.9[e]	93.03[a], 94.8[b]
C_{12}	64.7[a], 70.2[b]	54.9[a], 58.3[b], 60.4[d]	53.9[a], 57.1[b]	52.2[a], 55.3[b], 59.8[e]	51.5[a], 54.6[b]
C_{44}	43.6[a], 42.4[b]	38.5[a], 37.1[b], 39.0[d]	37.2[a], 36.5[b]	35.6[a], 35.3[b], 36.1[e]	34.5[a], 34.5[b]
A	1.97[a], 2.33[b]	1.59[a], 1.78[b], 1.56[d]	1.58[a], 1.60[b]	1.63[a], 1.65[b], 1.53[e]	1.66[a], 1.71[b]

[a] This work.
[b] Ref. [16] from first-principles calculations.
[c] Ref. [5] from experiment.
[d] Ref. [52] from experiment.
[e] Ref. [53] from experiment.

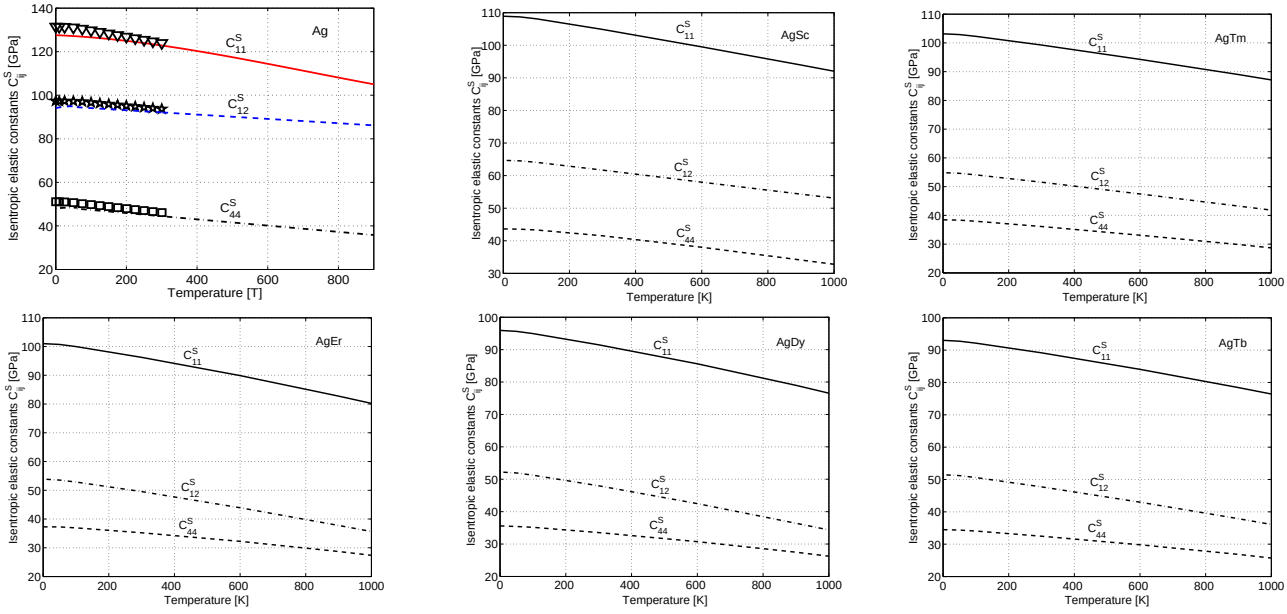

Figure 1: The isentropic elastic constants as a function of temperature for Ag, AgSc, AgTm, AgEr, AgDy, AgTb. The solid, dashed-dotted, and dashed curves denote the present values of C_{11}^S, C_{12}^S and C_{44}^S, respectively. For Ag, the open symbols represent the corresponding values of ultrasonic measurements by Neighbours and Alers [54].

Table 2: The predicted results of the third-order elastic constants (TOECs) for B2-AgRE (RE=Sc, Tm, Er, Dy, Tb) intermetallic compounds. All data are in GPa.

	AgSc	AgTm	AgEr	AgDy	AgTb
C_{111}	-956.6	-920.0	-857.8	-773.3	-690.1
C_{112}	-304.6	-260.1	-242.7	-252.9	-240.2
C_{144}	-341.7	-339.5	-174.0	-332.1	-305.7
C_{155}	-222.4	-193.8	-217.5	-176.6	-161.9
C_{123}	-210.1	-206.3	-326.8	-189.3	-176.2
C_{456}	-161.7	-159.5	-149.6	-151.1	-141.0

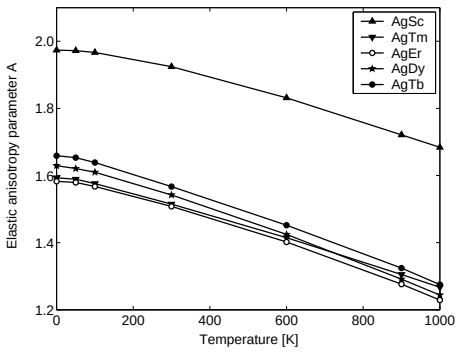

Figure 2: The elastic anisotropy parameters A as a function of temperature for AgSc, AgTm. AgEr, AgDy and AgTb.

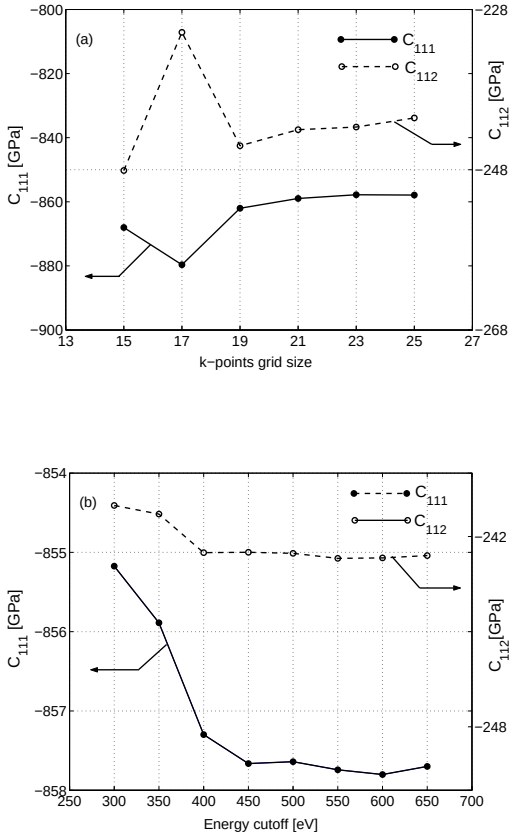

Figure 3: Sample convergence tests for the TOECs in AgEr. (a) The dependence of the TOECs C_{111} and C_{112} on the density of k-points mesh (energy cutoff of 600 eV is applied for all points). (b) The dependence of the TOECs C_{111} and C_{112} on the cutoff energy (Monkhorst-Pack sampling $23 \times 23 \times 23$ is used for all points).

further details on the calculations. Another interesting issue is to examine the range of deformations that the third-order effects dominant the properties of solids. In Figure 4, we compare energy values obtained within linear and nonlinear elasticity and DFT results for six sets of deformation in AgEr crystal. The six sets of deformation employed here are similar to those in Ref. [42]. It is apparent to see that linear elasticity is not sufficient for strains larger than approximately 2.5% and the third-order effects must be considered. It is also worth noting that for AgEr and examined Lagrangian strains up to 8.0%, our fitted curves are in good agreement with the DFT data from first-principles calculations. The other intermetallic compounds AgRE have the properties similar to those in AgEr.

The pressure dependence of the SOECs is also very useful for AgRE intermetallics since there are no experimental values available. Usually, it is sufficient to consider only linear terms in the external hydrostatic pressure and the pressure dependent C_{ij} can be expressed as $C_{ij}(P) \approx C_{ij} + C'_{ij}P$ [39]. Naturally, the information about pressure derivative C'_{ij} can be recovered from TOECs and they can be expressed as $C'_{11} = -(C_{111} + 2C_{112} + 2C_{11} + 2C_{12})/(C_{11} + 2C_{12})$, $C'_{12} = -(2C_{112} + C_{123} - C_{11} - C_{12})/(C_{11} + 2C_{12})$ and $C'_{44} = -(2C_{155} + C_{144} + C_{11} + 2C_{12} + C_{44})/(C_{11} + 2C_{12})$. The calculated pressure derivatives C'_{ij} based on our estimates for SOECs and TOECs are presented in Table 3. In Ref. [59], the following method for the determination of the pressure-dependent SOECs has been used. First, applying the hydrostatic strain to a crystal, and then additionally deforming to the same crystal obtain the pressure dependent elastic constants. The first principles calculations for the total elastic energy combined with the strain-energy relations will enable us to determine $C_{ij}(P)$. Łopuszyński *et al.* [39] have employed the ab initio calculations to determine the pressure derivatives for selected semiconductors. Therefore, we believe that the method used in our paper is accurate. The static elastic constants as a function of pressure are presented in Figure 5. Obviously, all the elastic constants increase monotonically with increasing pressure and the requirement of mechanical stability in the pressure range of 0-10 GPa is satisfied for AgRE. Further, the elastic anisotropy parameters $A = 2C_{44}/(C_{11} - C_{12})$ as a function of pressure can be calculated on the basis of the pressure dependent SOECs. In Figure 6, we show the pressure dependence of the elastic anisotropic parameters A in the range of 0-10 GPa, from which we can infer that all the AgRE intermetallic compounds exhibit low elastic anisotropy at zero pressure and that the degree of anisotropy increases with pressure.

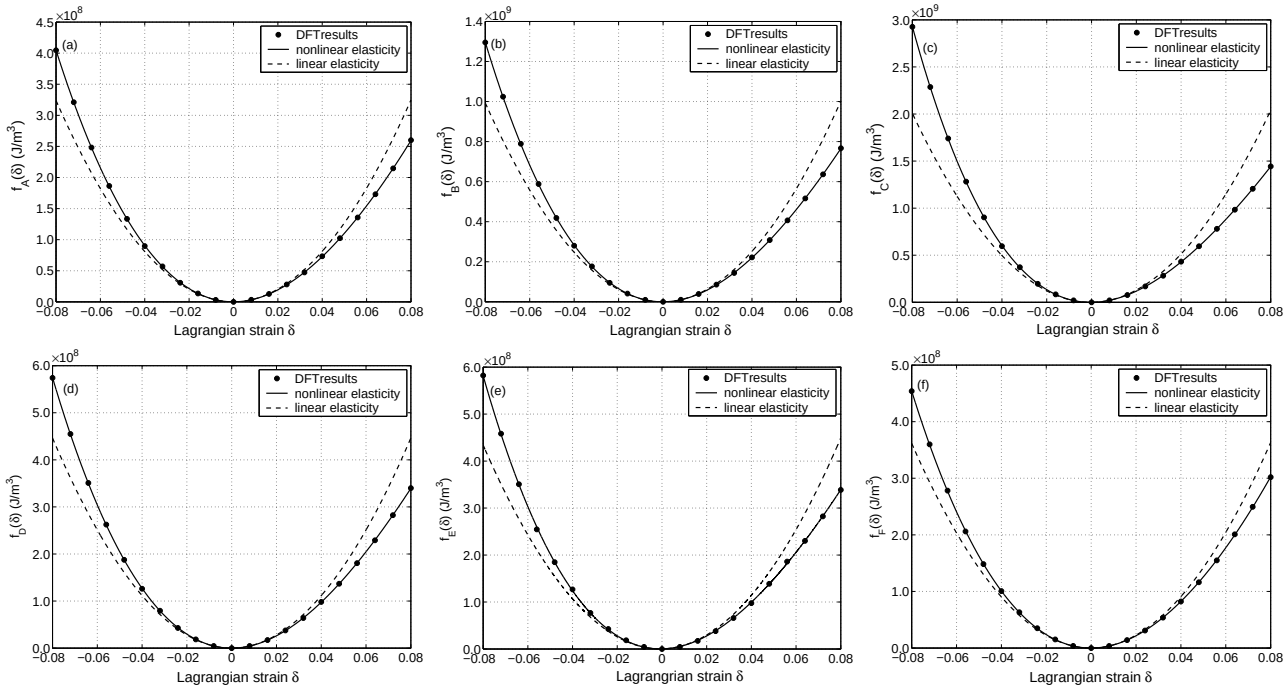

Figure 4: The strain energy relations as a function of linear strain parameter δ for AgEr cubic crystal. Circle points denote results of DFT computations; solid and dashed lines represent the curves obtained from nonlinear and linear elasticity theory, respectively. (a), (b), (c), (d), (e), and (f) describe Lagrangian strains η_A, η_B, η_C, η_D, η_E, and η_F, respectively.

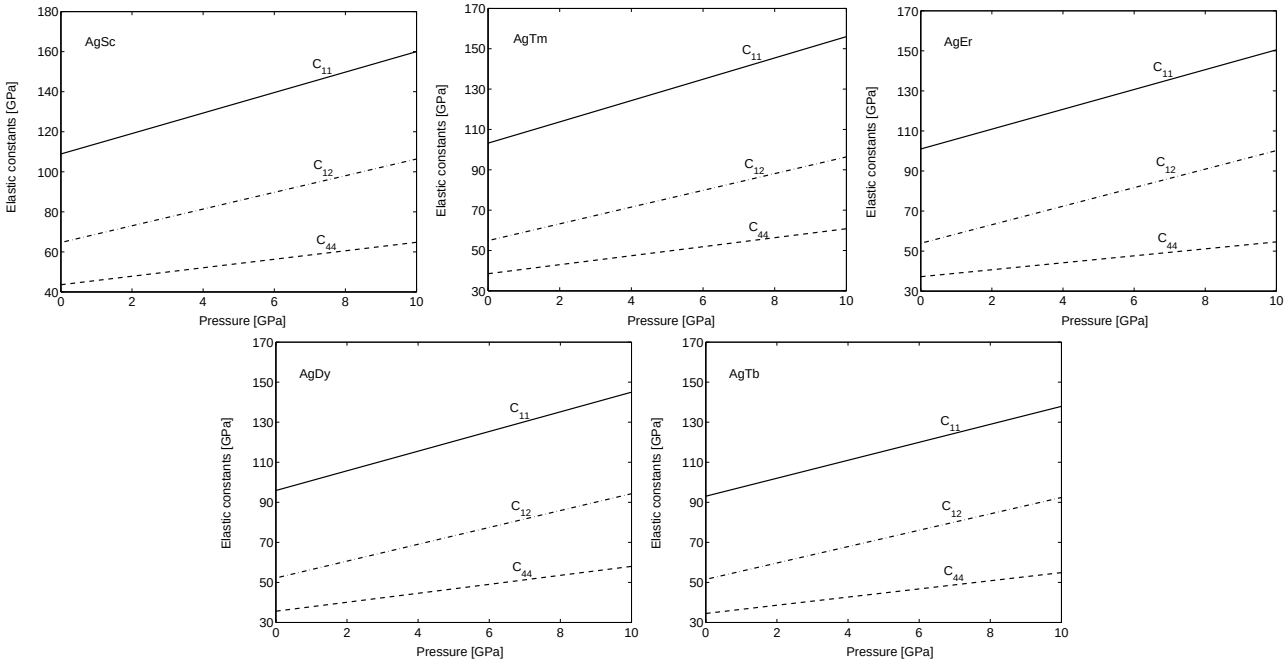

Figure 5: The static elastic constants of AgSc, AgTm, AgEr, AgDy and AgTb as a function of pressure. The solid, dashed-dotted, and dashed curves denote the present values of C_{11}, C_{12} and C_{44}, respectively.

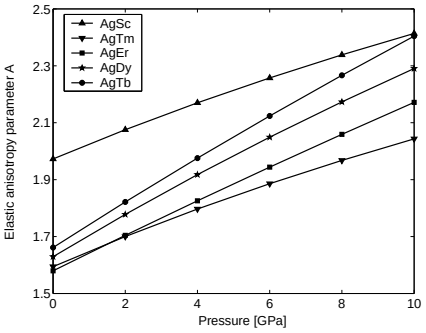

Figure 6: The elastic anisotropy parameters A as a function of pressure for AgSc, AgTm, AgEr, AgDy and AgTb.

Table 3: Theoretical predictions for the pressure derivatives of second-order elastic constants (SOECs) for B2-AgRE (RE=Sc, Tm, Er, Dy, Tb) intermetallic compounds.

	AgSc	AgTm	AgEr	AgDy	AgTb
C'_{11}	5.11	5.28	4.95	4.91	4.49
C'_{12}	4.17	4.15	4.63	4.21	4.09
C'_{44}	2.12	2.23	1.74	2.24	2.04

4 Conclusions

In summary, the first principles calculations have been performed to investigate high temperature and pressure effects on the elastic properties of the AgRE (RE=Sc, Tm, Er, Dy, Tb) intermetallic compounds with B2 structure. In the temperature range of 0-1000 K, the SOECs follow a normal behavior that those decrease with increasing temperature and approach linearity at higher temperature and zero slope at 0 K. The temperature dependence of the elastic anisotropic parameters A in the range of 0-1000 K has been calculated from the temperature dependent SOECs. The elastic anisotropic parameters A of B2-AgRE (RE=Sc, Tm, Er, Dy, Tb) decrease with increasing temperature and the degree of the anisotropy decreases with temperature. Pressure dependent SOECs have also been investigated on the basis of the TOECs. Convergence tests of k-point grid size and cutoff energy show that we obtain very reliable information of the TOECs for our researched rare-earth intermetallic compounds AgRE (RE=Sc, Tm, Er, Dy, Tb) with B2 structure. We also calculate the pressure dependence of the elastic anisotropic parameters A in the range of 0-10 GPa, and find that all the AgRE intermetallic compounds exhibit low elastic anisotropy at zero pressure and that the degree of anisotropy increase with pressure.

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