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CODEN: IAASCA **ORIGINAL ARTICLE**

Thermoelastic Behaviour : A Critical Analysis In Solids

Sanjay Singh
Department of Physics, Chintamani College of Arts and Science Gondpipri (MS)-India
E-Mail:sanjay2010.in@rediffmail.com

ABSTRACT

In this work, the elastic and thermodynamic properties of Pt3Al under high pressure are investigated using density functional theory within the generalized gradient approximation. The results of bulk modulus and elastic constants at zero pressure are in good agreement with the available theoretical and experimental values. Under high pressure, all the elastic constants meet the corresponding mechanical stability criteria, meaning that Pt3Al possesses mechanical stability. In addition, the elastic constants and elastic modulus increase linearly with the applied pressure.

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INTRODUCTION

According to the Poisson's ratio σ and elastic modulus ratio (B/G), Pt3Al alloy is found to be ductile, and higher pressure can significantly enhance the ductility. Those indicate that the elastic properties of Pt3Al will be improved under high pressure. Through the quasi-harmonic Debye model, we first successfully report the variations of the Debye temperature θ_D, specifc heats C_p , thermal expansion Coeffcient α, and Grüneisen parameter under pressure range from 0 to 100 GPa and temperature range from 0 to 1000 K.In order to understand the thermoelastic behaviour of solids adequately under the effect of high pressures and at high temperatures, we have to develop models for estimating the variations of thermal expansivity and bulk modulus. The pressure dependence of thermal expansivity and temperature dependence of bulk modulus are directly related to each other and defined in terms of the Anderson-Grüneisen parameters. It is therefore of central importance to study the variations of the Anderson-Grüneisen parameter under the effect of pressure and temperature. The knowledge of the volume dependence of the Grüneisen parameter and the Debye temperature is also very useful for understanding the thermodynamic behaviour of solids. In particular the volume dependence of the Grüneisen parameter is required for investigating the equation of state at high pressure . At elevated temperatures, the thermal energy can be elevated using the values of Debye temperature and the Grüneisen parameter. It is desirable to develop an equation of state using the expansion of potential energy functions in powers of changes in volume. For studying the variations of thermal expansivity and bulk modulus with pressure and temperature we formulated models by taking into account the dependence of Anderson–Grüneisen parameter on the change in pressure or volume. In order to evaluate the pressure derivative of bulk modulus we use interatomic potential functions and equations of state derived from them in particular, we use, the Vinet EOS based on the Rydberg potential energy function The magnitude of thermal pressure increases continuously with the increase in temperature. The product of thermal expansivity and isothermal bulk modulus is equal to the temperature derivative of thermal pressure at constant volume. By evaluating the thermal pressure we study the thermal expansivity, isothermal bulk modulus, Grüneisen parameter and thermodynamic properties of solids. The range of temperatures shall be extended from room temperature upto the melting temperatures of solids. The relationship between thermodynamic properties and melting of solids under high pressure is of considerable importance. We review and critically examine the existing theories of the Grüneisen parameter and suitably modify them for studying the thermoelastic behaviour of solids under high pressures.

Functionally graded materials (FGMs) are new of branch of materials which can be used for various conditions such as thermal and mechanical load applications. The FGMs are microscopically non-homogeneous materials where the composition of the constituents of materials is changed continuously.

The mechanical benefits obtained by a material gradient may be significant, as can be seen by the excellent structure performance of some of these materials. Hence, there has been considerable interest in recent years in the application of such materials in areas such as light weight armors, high temperature applications and industrial fields such as electronics, biomaterials and so on Among some articles which dealt with the subject of stress analysis of functionally graded structures the following papers may be referenced. Kwon et al. studied the case of a graded sphere under non-uniform temperature variations by using a numerical integration procedure. Obata and Nod used a perturbation approach to study the thermal stresses in functionally graded hollow sphere that was uniformly heated. Lutz and Zimmerman solved the problem of uniform heating of spherical body whose elastic modulus and thermal expansion coefficients each vary linearly with radial position. Eslami et al. analytically solved the governing equation of a functionally graded spherical vessel and investigated the temperature, displacement and relevant thermal stresses due to the thermal and mechanical loads Wang and Mai considered the finite element method to analyze one-dimensional transient heat conduction problems. Durodola and Adlington presented the use of numerical methods to assess the effect of various forms of gradation of material properties to control deformation and stresses in rotating axisymmetric components such as disks and rotors. Nadeau and Ferrari presented a one-dimensional thermal stress analysis of a transversely isotropic layer that was inhomogeneous along its thickness. Using the infinitesimal theory of elasticity, Naki and Murat obtained close-form solution for stresses and displacements in functionally graded cylindrical and spherical vessels subjected to internal pressure. Fukui et al. studied the problem of uniform heating of a radial inhomogeneous thick walled cylinder.

METHODS

In the present work, all the calculations were performed based on the plane wave pseudopotential density-function theory method as implemented in CASTEP package . The exchange correlation energy is described in the generalized gradient approximation (GGA) for the exchange correlation functional.

Pt $5d94s1$ and Al $3s23p1$ were treated as valence electrons. A plane wave cutoff energy of 400 eV was employed. The Brillouin zone was sampled by a 14θ uniform k-point mesh according to the Monkhorst-Pack scheme grids. In this work, the quasi-harmonic Debye model implemented in the Gibbs program is used to obtain the thermodynamic properties of Pt3Al. This model is Sufficiently flexible in giving all thermodynamic quantities by incorporating the obtained results of energy and volume. The non-equilibrium Gibbs function $G^*(V,P,T)$ is described in the following form:

$G^*(V,P,T)$ Æ $E(V)$ÅPV Å $A_{\text{vib}}(\theta,T)$

Here, $E(V)$ represents total energy/formula of Pt3Al, P is the hydrostatic pressure, $A_{\text{vib}}(\theta,T)$ is used to represent lattice vibration Helmholtz free energy and is taken as:

$$A_{\text{vib}}(\Theta,T) = nk_{\text{B}}T\left[\frac{9\Theta}{8T} + 3\ln\left(1-e^{-\Theta/T}\right) - D(\Theta/T)\right], \qquad \text{..........(1)}$$

where $D(\theta/T)$ stands for the Debye integral, n is the number of atoms per formula unit, and θ is expressed by

$$\Theta = \frac{\hbar}{k_{\text{B}}}\left(6\pi^2 V^{\frac{1}{2}} n\right)^{\frac{1}{3}} f(\nu)\sqrt{\frac{B_{\text{S}}}{M}}. \qquad \text{............(2)}$$

In relation, M is the molecular mass per formula unit, B_S is a representative for adiabatic bulk modulus, which is estimated in terms of static compressibility by using the following relation:

$$B_{\text{S}} = V\left(\frac{d^2E(V)}{dV^2}\right). \qquad \text{............................(3)}$$

And $f(v)$ is defined as follows:

$$f(\nu) = \left\{3\left[2\left(\frac{21+\nu}{31-\nu}\right)^{3/2} + \left(\frac{1}{3}\frac{1+\nu}{1-\nu}\right)^{3/2}\right]^{-1}\right\}^{1/3}, \qquad \text{.....(4)}$$

Hence, the non-equilibrium Gibbs function $G^*(V\ ;P,T\ )$ as a function of $(V\ ,P,T\ )$ can be minimized with respect to the volume as follows:

$$\left(\frac{\mathrm{d}G^*(V;P,T)}{\mathrm{d}V}\right)_{P,T}=0.$$

…………………(5)

In order to obtain the thermal equation of states, we should solve the equation (5) After the equilibrium state of a given $V\ (P,T\ )$ has been obtained, the isothermal bulk modulus and other thermodynamic properties, such as the heat capacity, vibrational internal energy, and thermal expansion can be evaluated using the relations given as below:

$$C_V=3nk_\mathrm{B}\left[4D(\Theta/T)-\frac{3\Theta/T}{\mathrm{e}^{\Theta/T}-1}\right],$$

………(6)

……(7)

$$C_P=3nk_\mathrm{B}\left[4D(\Theta/T)-\frac{3\Theta/T}{\mathrm{e}^{\Theta/T}-1}\right](1+\alpha\gamma T),$$

$$\alpha=\frac{\gamma C_V}{BV},$$

$$\gamma=-\frac{\mathrm{d}\ln\Theta(V)}{\mathrm{d}\ln V},$$

where γ is the Grüneisen parameter. This method has already been successfully used to investigate the thermodynamic properties of a series of compounds.

Estimating the effective thermal and mechanical properties of fg sphere

In present study, two methods are used to estimate the effective mechanical properties of FG sphere. One of the simplest methods in estimation of the effective mechanical and thermal properties of a mixture of two constituent materials is the Rule of Mixture (R-M) scheme. Another scheme for estimating the mechanical properties is due to the work of Mori-Tanaka. When the mechanical properties of FG sphere are estimated by using the Mori-Tanaka scheme, thermal material properties of FG body may be determined utilizing the R-M or the other methods which will be discussed as follows.

Rule of mixture (R-M) scheme

In rule of mixture scheme, the fractions of mixtures are only considered and the forces between the phases are not included in consideration. The R-M scheme states that the material properties of a matrix phase and particulate phase in a mixture can be determined by application of only the effect of volume fraction of each phase on material properties.

RESULTS AND DISCUSSIONS

Structure property

As we know, Pt3Al has two kinds of structures including cubic phase and tetragonal phase. For cubic phase, Pt3Al alloy has a Cu3Au-type structure (space group: Pm3m, No: 221), with lattice parameters: *a* Æ *b* Æ *c* Æ 3.876 Å . The Pt and Al atoms are located at the site (0, 0, 0) and (0.5, 0, 0), respectively. Each Al atom is surrounded by twelve Pt atoms. For tetragonal phase, Pt3Al has a space group: P4/mmm (No: 123) with experimental lattice parameters: *a* Æ *b* Æ 3.832 Å and *c* Æ 3.894 Å. There are two types of Pt: 1c (0.5, 0.5, 0) and 2e (0, 0.5, 0.5), respectively. The Al atom is in the site 1a (0, 0, 0).We have calculated the formation enthalpies of tetragonal and cubic phase as the pressure increasing from 0 GPa to 100 GPa. Our results show that the formation enthalpies of cubic structure are lower than that of tetragonal structure below 100 GPa. This means that cubic Pt3Al is stable under high pressure which is consistent with the result of Liu . To obtain equilibrium structural parameters, the atom position and structure of Pt3Al were optimized. At 0 GPa, the calculated lattice parameters of cubic phase *a* is 3.86 Å. We note a very good agreement between our results and experimental data. This offers the reliability and accuracy to our further investigation.

Elastic property

To the best of our knowledge, the elastic properties define the behavior of a solid under different stress and strain conditions. The elastic stiffness parameters can describe the bonding characteristics, mechanical deformations, and structural stability. To obtain the elastic constants, a small strain should be loaded to the crystal. They can be got by calculating the total energy as a function of appropriate lattice deformation, which are expanded as the Taylor expansion for a system with respect to a small strain ±and volume V_0[20, 21]. The elastic strain energy $E(V)$ is expressed as follows:

$$E(V) = E(V_0, 0) + \frac{1}{2}\sum_{i}^{6}\sum_{j}^{6} C_{ij}\delta_i\delta_j . \qquad \text{………………..(8)}$$

Here, $Ci\,j$ are elastic constants, ±*i* and ±*j* are related to the strain on the crystal. For cubic symmetry, there are three independent elastic constants, that are $C11$, $C12$, $C44$. The calculated elastic constants $Ci\,j$ of Pt3Al are shown in figure 1. At 0 GPa, the calculated elastic constants of Pt3Al ($C11$ Æ 400.8,$C12$ Æ 205.27, $C44$ Æ 131.71, and B Æ 270.46) are consistent with the experimental values (B Æ 277) and other theoretical results ($C11$ Æ 395, $C12$ Æ 210, $C44$ Æ 118) [8]. In general, the requirements of mechanical stability in a cubic crystal lead to the following restrictions on the elastic constants: $C11$ È 0, $C12$ È 0, $C11$ ¡$C12$ È 0, $C11$ Å2$C12$ È 0 [22, 23]. Obviously, our results in figure 1 (a) show that all the elastic constants satisfy the stabilities criteria up to 100 GPa. This clearly indicates that Pt3Al under high pressure possesses mechanical stabilities. There is no doubt that the elastic constants of a solid are strongly affected by the pressure. It should be noted that the elastic constants $C11$, $C12$, $C44$ increase linearly with the pressure increase because the lattice parameters of Pt3Al become shorter under pressure.

Table 1. The Poisson's ratio v and B/G of Pt_3Al under high pressure.

Pressure (GPa)	0	10	20	30	40	50	60	70	80	90	100
B/G	2.289	2.356	2.410	2.436	2.462	2.480	2.506	2.527	2.543	2.577	2.592
v	0.309	0.314	0.318	0.319	0.321	0.322	0.324	0.325	0.326	0.328	0.329

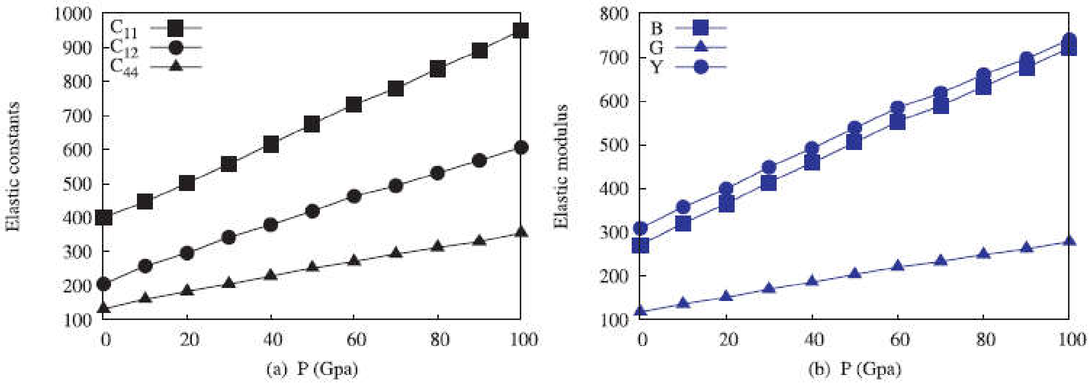

Figure 1. The calculated elastic constants C_{ij} and the elastic modulus of cubic Pt_3Al under pressure from 0 GPa to 100 GPa.

It is acknowledged that bulk modulus B and shear modulus$G$ can measure the hardness in an indirect way. The calculated bulk modulus B, shear modulus G, and Young's modulus Y under different pressures are shown in figure 1 (b). It is found that bulk modulus B, shear modulus G, and Young's modulus Y of Pt3Al gradually increase as pressure increases, indicating that Pt3Al becomes more and more difficult to be compressed as the pressure increases. In addition, all the elastic modulus can be used as a measure of the average bond strength of atoms for a given crystal. A larger bulk modulus B and Young's modulus Y respond to the more covalent and stronger bond strength. Hence, it can be expected that Pt and Al atom can form covalent bonds under high pressure. The shear modulus G is the relationship between the resistance to reversible deformations and the shear stress. A high shear modulus G is mainly due to the elastic constants $C44$, because a large $C44$ implies a stronger resistance to shear in the (1 0 0) plane. For a further analysis, the deformation behavior of Pt3Al, the value of B/G and Poisson's ratio □ which are related with the brittleness and hardness of the materials are shown in table 1. Generally, the B/G ratio is used to predict the brittle or ductile behavior of materials. The critical value which separates ductile and brittle material is 1.75. The material exhibits a ductile behaviour when the value B/G È 1.75; otherwise, the material behaves in a brittle manner. We found that the B/G is 2.89 at 0 GPa and increases with the pressure increase. It means that the Pt3Al belongs to a ductility material and the pressure can improve the ductility of Pt3Al. Another important property is the Poisson's ratio σ which is defined as the absolute value of the ratio of transverse strain to longitudinal strain. It is used to quantify the stability of the crystal against shear. The larger is the Poisson's ratio σ the better is the plasticity.

Thermodynamic properties

To our knowledge, Debye temperature θ_D is one of the most important parameters describing the thermal characteristics of compounds. The Debye temperature correlates with many physical properties of material, which are derived from elastic properties under pressures. Some detailed information of a solid, such as the melting temperature and specific heat can be found by calculating the Debye temperature. We obtain the thermodynamic properties of Pt3Al at various temperatures and pressures from the energy-volume relations using the quasi-harmonic Debye model. The Debye temperature θ_D as a function of temperature at different pressures is shown in figure 2 (a). It can be clearly seen that θ_D in the range of temperatures from 0 to 1000 K approximately remains unaltered with the temperature increase, meaning that it is insensitive to temperature. Figure 2 (b) shows the Debye temperature as a function of pressure at different temperatures of T 0, 300, 600, and 900 K. It is noted that θ_D linearly increases and further compression slows down the increase. As the pressure goes higher, the decreased magnitude of Debye temperature θ_D becomes small. This is because the Debye temperature is related to the volume V and adiabatic bulk modulus. Figure 2 (b) shows that when the temperature is constant, the Debye temperature in θ_D creases non-linearly with the applied pressures, indicating the change of the vibration frequency of particles under pressure. Hence, the temperature has a more significant effect on the Debye temperature th θ_D an pressure, and the temperature exhibits a smaller and smaller effect on the Debye temperature with an increase of pressure. To describe the thermal properties of a material, the volume thermal expansion coefficient α is another essential parameter. The dependence of the volume thermal expansion coefficient α of Pt3Al on the temperature and pressure is illustrated in figure 3. We noted that in α creases rapidly with T 3 at zero or low pressure when the temperature is below 200 K and gradually approaches a very low linear increase above 400 K for a given pressure. Moreover, we can also see that the values of at α zero pressure are much greater than those at other pressures. Figure 3 (b) gives α as a function of pressure at different temperatures of T 0, 300, 600, 900 K. It can be seen that for a given temperature, the thermal expansion coefficient α is zero at 0 K and rapidly decreases with the pressure α increase, and it becomes at under high pressure. Moreover, the higher is the temperature, the faster the decreases. There is observed a larger thermal expansion α at a higher temperature and at a lower pressure, and it provides less sensitivity of α at high temperature and high pressure for Pt3Al. As another important thermodynamic parameter of solids, the heat capacity C_p is of key importance for linking thermodynamics with microscopic structures and dynamics. Moreover, the knowledge of the heat capacity of a substance not only provides an essential insight into its vibrational properties but also is mandatory for many applications. Figure 4 shows the calculated heat capacity C_p as a function of temperature and pressure. It is obvious that CP follows the relationship of the Debye model $[C(T)/T\,3]$ up to 200 K. Then, it monotonously increases with the temperature increase and converges to a constant Dulong-Petit limit, which is common to all solids at high temperatures.We note that the heat capacity C_p slowly decreases with the pressure increase, and the high temperature will slow down this trend seen in figure 4 (b). Figure 4 implies that temperature and pressure have an opposite effect on the heat capacity, while the temperature has a greater effect on the heat capacity than the pressure. In the quasi-harmonic Debye model, the Grüneisen parameter γ is of a great significance. It describes the anharmonic effects of the crystal lattice thermal vibration and has been widely used to characterize the thermodynamic behavior of a material at high pressure. The calculated Grüneisen parameter γ with pressure and temperature are presented in figure 5. It can be observed that the Grüneisen parameter γ almost keeps unchanged with the temperature increase at a fixed pressure in figure 5 (a), while it quickly decreases with the applied pressure. This is because the Grüneisen parameter γ is as function of the volume which is affected by the pressure in the quasi-harmonic model. And, there is a larger thermal expansion at low pressure. Those results suggest that the effect of the temperature on the Grüneisen parameter γ is not as significant as that of the pressure P. Furthermore, the Grüneisen parameter γ increases more slowly at high pressure than at low pressure.

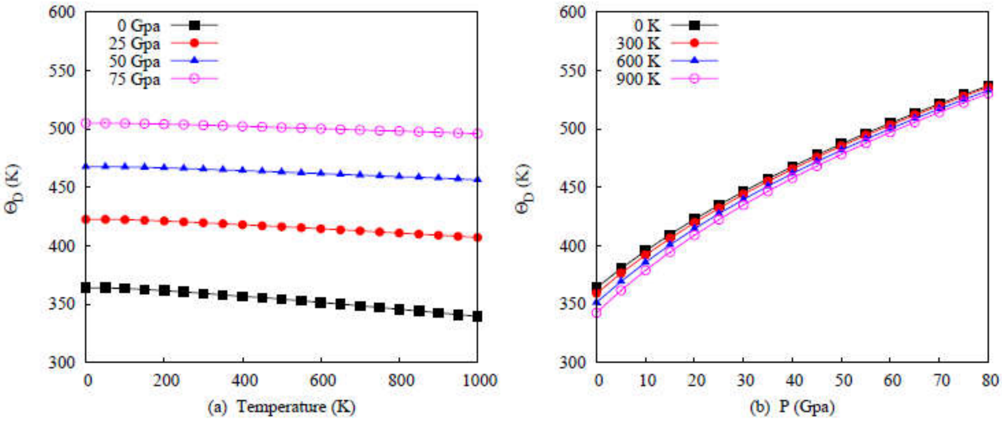

Figure 2. (Color online) The Debye temperature as a function of temperature and pressure. (a) $P = 0, 25, 50$, and 75 GPa, respectively; (b) $T = 0, 300, 600$, and 900 K, respectively.

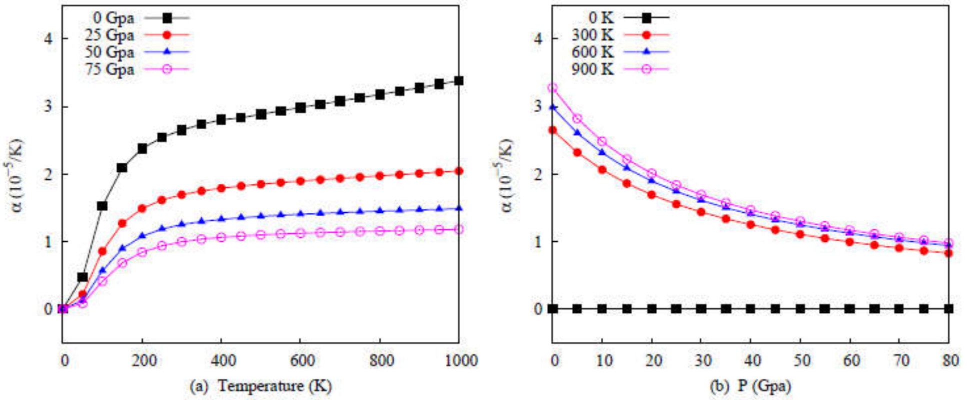

Figure 3. (Color online) The volume thermal expansion coefficient as a function of temperature and pressure. (a) $P = 0, 25, 50$, and 75 GPa, respectively; (b) $T = 0, 300, 600$, and 900 K, respectively.

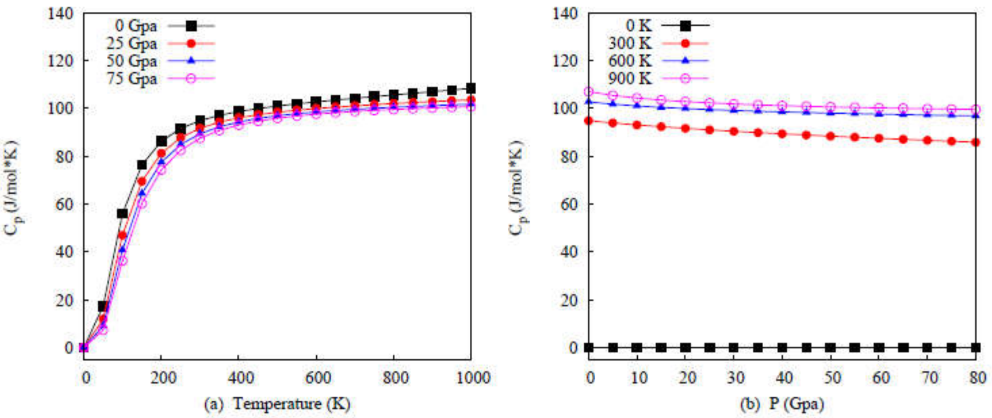

Figure 4. (Color online) The heat capacity as a function of temperature and pressure. (a) $P = 0, 25, 50$, and 75 GPa, respectively; (b) $T = 0, 300, 600$, and 900 K, respectively.

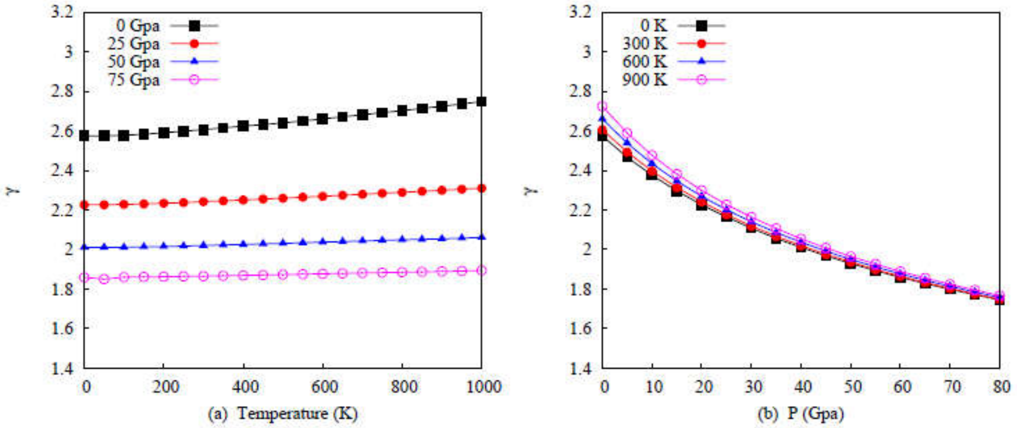

Figure 5. (Color online) The Grüneisen parameter γ as a function of temperature and pressure. (a) $P = 0$, 25, 50, and 75 GPa, respectively; (b) $T = 0$, 300, 600, and 900 K, respectively.

CONCLUSIONS

First principles calculations are performed to investigate the elastic and thermodynamic properties of L12 phase Pt3Al alloy under high pressure and high temperature. The elastic constants, bulk modulus B, shear modulus G, and Young's modulus Y as a function of the pressure have been systematically investigated. The results show that all the elastic constants meet the corresponding mechanical stability criteria and the elastic modulus increases linearly with the applied pressure. The Poisson's ratio σ and the elastic modulus ratio (B/G) show that L12 phase Pt3Al alloy is found to be ductile and higher pressure can significantly enhance the ductility. This means that the elastic properties of Pt3Al will be improved under high pressure. To study the thermal and vibrational effects, the quasi-harmonic Debye is used. The dependence of Debye temperature θ_D , specific heats C_p , thermal expansion coefficient α , and the Grüneisen parameter γ are systematically explored in the ranges of 0–100 GPa and 0–1000 K.We find that the temperature has a more significant effect on the Debye temperature θ_D and the heat capacity C_p than pressure. Furthermore, the thermal expansion coefficient α becomes insensitive to high temperature and high pressure.

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