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First-principles Study on Effect of Pressure and Temperature on Mechanical, Thermodynamic Properties, and Electronic Structure of Ni₃Al Alloy

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Abstract: The influence of temperature and pressure on the electronic, elastic, structural, and thermodynamic properties of Ni₃Al alloy was investigated by performing a first-principles study. The calculated elastic constants, equilibrium lattice constants, and elastic modulus agree well with the recorded theoretical and experimental data. The calculated elastic constants indicate that C_{11} is more sensitive than C_{12} and C_{44} to pressure. The Young's modulus, bulk modulus, and shear modulus increase with the increase of pressure. The ratio of bulk to shear modulus (B/G) and anisotropy factor A were also analyzed. The Debye temperature was obtained by calculating the elastic constants, and it changes with the change in the pressure. The thermal expansion coefficient, normalized volume, heat capacity, bulk modulus, and Debye temperature Θ_D were determined and analyzed using the quasi-harmonic Debye model at pressures of 0~60 GPa and temperatures of 0~1600 K. Finally, the density of states and Mulliken population were investigated and the effect of pressure on these was analyzed.

Key words: Ni-based alloys; electronic structure; mechanical properties; thermodynamics properties; first-principles

Because of the high strength, elevated thermal stability, high work hardening rate at room temperature, and high temperature oxidation resistance of Ni-based alloys, they have been widely applied in practical production and life[1-3]. The L1₂-ordered phase Ni₃Al is an important intermetallic compound in Ni-based alloys[4], exhibiting excellent physical properties that make them attractive for high temperature structural materials applications.

Recently, many theoretical and experimental studies have been performed on the structure and mechanical properties of Ni₃Al. For example, Hou et al[5] calculated the elastic, structural, and electronic properties of Ni₃X (X=Al, Ga, Ge) under pressure using first-principles calculations. Guo et al[6] recorded the mechanical, structural, and magnetic characteristics of Ni₃Al from first-principles and experimental studies. Boucetta et al[7]

studied the mechanical properties of Ni₃Al under high pressures using the plane-wave pseudo potential (PWPP) method. Yasuda et al[8] confirmed the elastic stiffness of Ni₃Al at room temperature using the rectangular parallelepiped resonance method. However, to our knowledge, neither experimental nor theoretical studies have been conducted on the elastic, thermodynamic, and electronic properties of the Ni₃Al alloy at different temperatures and pressures. As far as we know, the pressure and temperature have an important influence on the physical properties of the material. However, the effects of temperature on physical and mechanical properties of Ni₃Al have seldom been reported. Thus, systematic investigation on structural, elastic, thermodynamic and electronic properties of Ni₃Al under temperature and pressure can determine the value

of the basic parameters, such as lattice parameters, elastic constants and Debye temperature, and provide insight into the nature of the solid-state theory. It would be useful for understanding and designing the relevant alloys[9].

Here, we studied the elastic, thermodynamic, structural, and electronic properties of Ni_3Al. The relationships between the pressure and the anisotropy factor A, Young's modulus E, shear modulus G, bulk modulus B, Debye temperature Θ, and Poisson's ratio v were systematically studied. Second, the relationships among the pressure, temperature, and thermo-dynamic properties were studied using the quasi-harmonic Debye model. Finally, the pressure dependence of the electronic properties of Ni_3Al alloy was calculated. The results enable the valuable assessment of some properties that are difficult to measure by experimental methods.

1 Computational Methods

The elastic, structural, thermodynamic, and electronic properties of Ni_3Al alloy were calculated using the Cambridge sequential total energy package (CASTEP)[10] based on the density functional theory (DFT)[11,12]. The electronic exchange-correlation potential energy was determined using the generalized gradient approximation (GGA)[13] of the Perdew-Wang (PW91)[14] version. The value of the kinetic cut-off energy for plane waves was set to 330 eV[15]. The k-points were $8\times8\times8$ and the total energy was less than 5.0×10^{-7} eV/atom[16]. The Pulay schemes[17] of density mixing and a finite basis set correction were used to evaluate the stress and energy. The positions of the atoms had been relaxed in the model using the total force and energy by the BFGS scheme[18], considering the criterion of cell optimization (displacement of 5.0×10^{-5} nm, RMs force of 5.0×10^{-5} eV/nm, and stress of 0.01 GPa). The electronic structure and total energy were recorded using cell optimization with a SCF tolerance of 5.0×10^{-7} eV. The states Ni $3d_8$ $4s_2$ and Al $3s_2$ $3p_1$ were taken as the fundamental setting for the calculations.

Using the quasi-harmonic Debye model[19] to study the thermodynamic properties of the Ni_3Al alloy, the non-equilibrium Gibbs function $G^*(V; P, T)$ is as follows:

$$G^*(V;P,T) = E(V) + PV + A_{vib}(\Theta(V);T) \qquad (1)$$

where, A_{vib} represents the Helmholtz free energy of the lattice vibrations, $E(V)$ represents the all of the energy of every unit cell, PV represents the requirement of constant hydrostatic pressure, and $\Theta(V)$ represents the Debye temperature. The details of the calculations can be found in Ref. [20].

2 Results and Discussion

2.1 Structural properties

Ni_3Al has the structure of ordered C15-type with group Pm3m (No. 221), the highest point symmetry O_h^7, and the Pearson symbol cP4. The Ni atoms occupy the 3c site (0, 1/2, 1/2) and the Al atoms take up the 1a site (0, 0, 0), as shown in Fig.1.

The calculated lattice parameters a_0, volume V_0, pressure derivative B_0', and the bulk modulus B_0 at 0 GPa are shown in
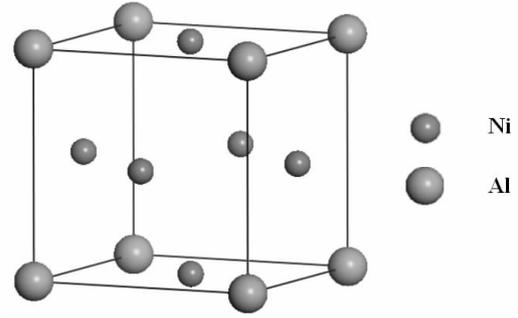
Fig.1   Crystal structure of Ni_3Al alloy

Table 1, together with the available theoretical[21,22] and experimental data[23]. The obtained results of the lattice parameter coincide with the previous theoretical and experimental records, and the pressure derivative and bulk modulus accord with a previous report. Our experimental data agree with the theoretical results, proving that our calculated results are accurate.

In order to obtain the pressure derivative B_0' and the bulk modulus B_0, geometry optimization of the cell volume at different pressures was performed using generalized gradient approximation (GGA). The recorded volume and pressure coincided with the result obtained using the third-order Birch-Murnaghan equation as follows[24]:

$$P = \frac{3}{2}B_0[(\frac{V}{V_0})^{-7/3} - (\frac{V}{V_0})^{-5/3}]\cdot\left\{1 + \frac{3}{4}(B'-4)\cdot[(\frac{V}{V_0})^{-2/3}-1]\right\} \qquad (2)$$

The changes in the cell volume V/V_0 and the lattice parameter a/a_0 of Ni_3Al are plotted in Fig.2. It is easy to observe the decrease in V/V_0 and a/a_0 with increasing pressure. However, there is no available reference to compare this to. The functions of Ni_3Al can be obtained by the V/V_0 and a/a_0 curve:

$$a/a_0 = 0.9992 - 0.00165P + 1.6792\times10^{-5}P^2 \qquad (3)$$

$$V/V_0 = 0.9982 - 0.00475P + 2.8537\times10^{-5}P^2 \qquad (4)$$

In order to obtain the steady state structure of Ni_3Al, the cell volume and total energy were calculated using several lattice constant values. The relationship between the calculated energy and volume is shown in Fig.3. By coincide with it to the Birch-Murnaghan equation of states (EOS)[24], the calculated total energy and cell volume of the steady-state structure are

Table 1   Recorded equilibrium lattice constant a_0, volume V_0, bulk modulus B_0 and its first pressure deriva-tive B_0' from the Birch-Murnaghan equation of states (EOS) of Ni_3Al

	a_0/nm	V_0/$\times10^{-3}$ nm^3	B_0/GPa	B_0'
Present	0.3578	45.769	185.247	4.75
Exp. [21]	0.3572	45.576	171	-
Cal. [22]	0.3574	45.652	182.0	4.70
Cal. [23]	-	-	179.9	4.73
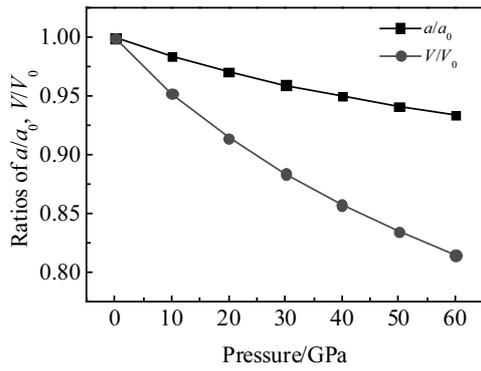
Fig.2   Variations of lattice parameter a/a_0, cell volume V/V_0 of Ni$_3$Al at different pressures
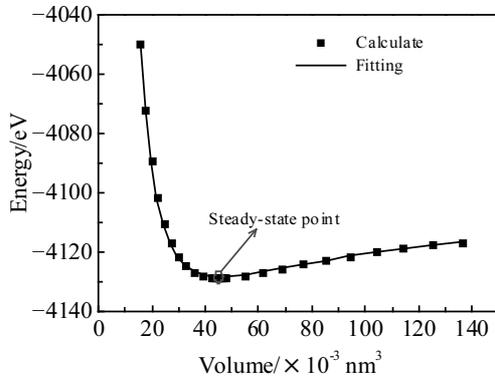
Fig.3   Curve of calculated total energy versus primitive cell volume of Ni$_3$Al

–4128.6335 eV and 45.4993×10^{-3} nm^3, respectively, which agree well with the geometry optimization results.

2.2   Elastic properties

The elastic constant is a significant material parameter, and can provide important details regarding the mechanical stability[25]. The elastic constants are very important for studying the mechanical properties of Ni-Al alloys under various pressures. By geometry optimization, we can determine the elastic constant of a single crystal.

The calculated Ni$_3$Al phases in the present study are cubic crystal. The elastic constants are C_{11}, C_{12}, and C_{44}. The related mechanical stability requirements are as follows[26]: $C_{11}+2C_{12}>0$ and $C_{11}>|C_{12}|$, $C_{44}>0$. The recorded results of the elastic constants are listed in Table 2 at 0 pressure, together with

theoretical[5,7] and experimental values[8]. The mechanical stability requirements are obtained for Ni$_3$Al, and the calculated values of the elastic constants agree well with the experimental and theoretical data. Hence, selection of the requirements and calculations of the elastic constants should be done appropriately.

The changes in the elastic constants with pressure are shown in Fig.4a. We determine that C_{11}, C_{12}, and C_{44} increase with the increasing pressure, while the change in C_{11} with pressure is more significant than those of C_{12} and C_{44}. This is because C_{11} represents the elasticity in length, while C_{44} and C_{12} represent the elasticity in shape. The transverse strain could result in shape changes, but cannot lead to volume changes[27]. Hence, C_{11} is more significant than C_{44} and C_{12}.

The Cauchy pressure (C_{11}–C_{44}) is usually used to study the angular characteristics of atomic bonding in metals even than in compounds[25]. When the Cauchy pressure is negative (positive), it indicates that the object is nonmetallic (metallic). Ni$_3$Al has a positive Cauchy pressure, indicating that it is a ductile material. Furthermore, the Cauchy pressure increases when the pressure increases (Fig.4a), i.e., the ductility of Ni$_3$Al increases when the pressure increases.

The shear moduli G, bulk moduli B, Poisson's ratio v, and Young's moduli E of Ni$_3$Al were calculated using the Voigt-Reuss-Hill (VRH) formula[28]. For the cubic system, the calculation formulas are as follows[29]:

$$B = \frac{1}{3}(C_{11} + 2C_{12}) \tag{5}$$

$$G_V = \frac{1}{5}(3C_{44} + C_{11} - C_{12}) \tag{6}$$

$$G_R = \frac{5(C_{11} - C_{12})C_{44}}{3(C_{11} - C_{12}) + 4C_{44}} \tag{7}$$

$$G = \frac{1}{2}(G_V + G_R) \tag{8}$$

$$E = \frac{9GB}{3B + G} \tag{9}$$

$$v = \frac{(E - 2G)}{2G} \tag{10}$$

The calculated results of the polycrystalline Young's modulus E, shear modulus G, and bulk modulus B under various pressures are shown in Fig.4b. It was determined that the calculated G, E, and B increase when the external pressure

Table 2   Recorded Cauchy pressure (C_{12}–C_{44}), elastic constants C_{ij}, Poisson's ratio v, elastic modulus and anisotropy factor A of Ni$_3$Al at 0 GPa

	C_{11}/GPa	C_{12}/GPa	C_{44}/GPa	C_{12}–C_{44}/GPa	B/GPa	G/GPa	E/GPa	G/B	v	A
Present	235.22	163.35	121.67	41.67	187.31	74.82	198.09	0.399	0.324	2.017
Exp. [8]	221.0	146.0	124.0	22.0	171	76.9	200.73	0.449	0.304	-
Cal. [5]	225.3	157.6	121.1	36.5	180.2	72.9	192.74	0.405	0.321	-
Cal. [7]	228.4	160.4	123.8	36.6	183.1	74.1	195.73	0.404	0.322	-
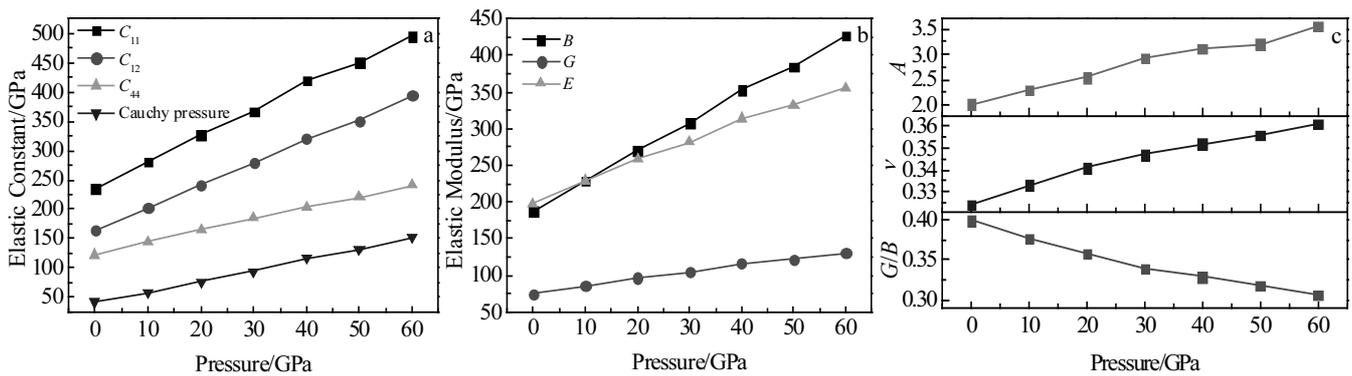
Fig.4   Parameters variations of Ni₃Al with the changing of pressure: (a) elastic constants, (b) elastic modulus, and (c) *B/G*, Poisson's ratio *v*
        and anisotropy factor *A*

increases, indicating that with the increasing pressure, the hardness can be improved. It is generally known that the material resistance to volume and shape changes can be measured using the bulk modulus *B* and the shear modulus *G*[30]. It was found that the calculated bulk modulus is much larger than the shear modulus, which means that the resistance to volume change of Ni₃Al is much better than the resistance to shape change.

The ratio of *G/B*, Poisson's ratio *v*, and anisotropy factor *A* are shown in Fig.4c. Pugh[30] reported the ductile and brittle characteristics of materials are predicted using the ratio of shear modulus to bulk modulus (*G/B*) of polycrystalline phases. The high (low) *G/B* values are related to the brittleness (ductility). The critical value is a very important value, and is about 0.57 for the brittle-ductile transition. The recorded *G/B* values of Ni₃Al are lower than 0.57, indicating ductility. The recorded *G/B* values of Ni₃Al decrease with an increase in pressure, illustrating that ductility would be better than before with the pressure increase. It is an important parameter of Poisson's ratio *v* to quantify the stability resist shear[24], and the value of the Poisson's ratio *v* ranges from 0.25~0.5. The recorded Poisson's ratio values of Ni₃Al at different pressures are in the range of 0.32~0.37 and increase with the increasing pressure, indicating that the interatomic forces are the central forces.

The elastic anisotropy of the crystal is widely used in engineering science because it is possible to induce microcracks. *A*=1 indicates an absolutely isotropic material. When the value becomes larger or smaller than the standard value, it predicts the level of elastic anisotropy[31]. The changes in the anisotropy factor with the changes in pressure are shown in Fig.4c. It was determined that the value of *A* increases with the increasing pressure, and Ni₃Al can be considered as an elastically anisotropic material because its *A* value is larger than 1.0.

The heat capacity and Debye temperature Θ_D at low temperature could be obtained using the electronic structures and the elastic constants of the compound. The Debye temperature provides some insights into the thermodynamic

properties of an elastic material[32]; it can be used to distinguish the low and high temperature areas of the solid. For $T > \Theta_D$, the material has an energy of $k_B T$; and for $T < \Theta_D$ it is predicted that high-frequency materials would be frozen in the foreseeable future[33]. Θ_D is calculated by the average values of sound velocity as follows[34,35]:

$$\Theta_D = \frac{h}{k_B} \left[\frac{3n}{4\pi} \left(\frac{N_A \rho}{M} \right) \right]^{1/3} v_m \tag{11}$$

$$v_m = \left[\frac{1}{3} \left(\frac{2}{v_s^3} + \frac{1}{v_l^3} \right) \right]^{-1/3} \tag{12}$$

$$v_l = \sqrt{\left(B + \frac{4}{3} G \right) \frac{1}{\rho}} \tag{13}$$

$$v_s = \sqrt{G/\rho} \tag{14}$$

where, k_B represents the Boltzmann constant, *h* represents the Planck's constant, *n* represents the number of atoms in a molecular formula, N_A represents the Avogadro constant, *M* represents molecular mass, ρ represents the density, v_l represents the longitudinal sound velocity, v_s represents the shear sound velocity, and v_m represents the average sound velocity.

The dependence of density (ρ), shear (v_s) and average wave velocity (v_m), longitudinal sound velocities (v_l), and Debye temperature (Θ_D) under various pressures from 0 to 60 GPa are listed in Table 3. It was determined that the Debye temperature increases with an increase in the pressure. The Debye temperature of Ni₃Al at 0 GPa and 0 K is 471.67 K, which agrees with the available experimental data of 462±5 K[36] and 460.0±10 K[37] obtained from elastic constants at room temperature. These values are close to our results, indicating that the previous results were precise and the present calculated results are accurate. However, it is difficult to compare the calculated and experimental data of the Debye temperature of Ni₃Al under various pressures. Therefore, the present calculated results can be used to predict the results of the experiments in future.

2.3 Thermodynamic properties

The quasi-harmonic Debye model was used to study the

Table 3 Pressure (*P*) dependence of density (*ρ*), shear (*v*s) and average wave velocity (*v*m), longitudinal sound velocities (*v*l) and Debye temperature (*Θ*D) for Ni3Al

P/GPa	$\rho/\times 10^3$ kg·m⁻³	v_m/m·s⁻¹	v_l/m·s⁻¹	v_s/m·s⁻¹	Θ_D/K
0	7.369	3570.07	6241.49	3186.42	471.67
10	7.738	3739.36	6658.81	3333.56	502.15
20	8.057	3890.16	7038.84	3464.61	529.48
30	8.338	3980.05	7324.87	3541.18	547.95
40	8.595	4136.93	7689.63	3678.72	575.32
50	8.831	4186.86	7872.26	3720.82	587.54
60	9.048	4279.13	8154.51	3800.18	605.39

thermodynamic properties of Ni3Al at high pressures and temperatures. The effects of pressure and temperature were studied over the range of 0~60 GPa and 0~1600 K. Fig.5a shows the volume as a function of temperature and pressure. It was found that the calculated volume recorded by the quasi-harmonic Debye model is 133.05 bohr³ at 0 GPa and 0 K, which agrees with the experimental value of 131.26 bohr³[21] and calculated value of 131.48 bohr³[22]. Furthermore, the volume increases smoothly with the increasing temperature, while the volume decreases smoothly when the pressure increases, with the temperature being a constant, indicating that the crystal structure of Ni3Al becomes stable with the increasing pressure. The ratio of volume V/V_0 agrees with the pressure and temperature, as shown in Fig.5b. It was observed that the V/V_0 curves become steeper with the increasing pressure, indicating that Ni3Al is compressed more easily with the increasing pressure.
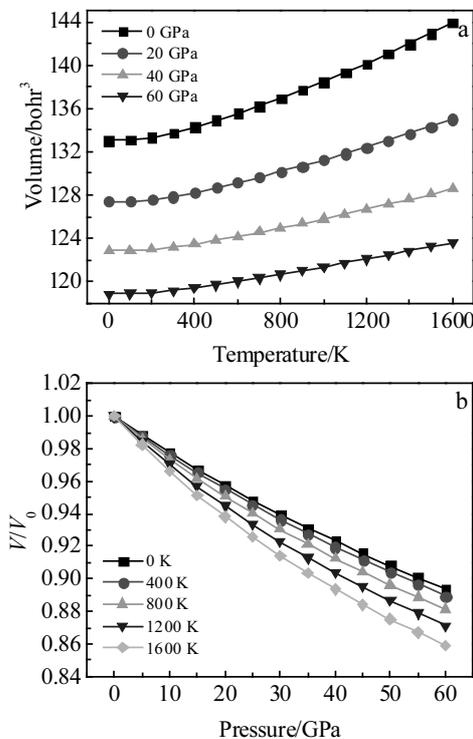
The bulk modulus with the change in pressure and temperature is plotted in Fig.6. The calculated value of the bulk modulus using the quasi-harmonic Debye model is 185.42 GPa at 0 GPa and 0 K, which agrees with the experimental value of 171.0 GPa[21] and calculated value of 182.0 GPa[22]. Furthermore, the bulk modulus decreases with an increase in temperature when the pressure is a constant, while it increases with increasing pressure. The hardness of Ni3Al can be represented by the bulk modulus, and the changes in the bulk modulus can be used to define the changes in the hardness. Therefore, we concluded that the hardness of Ni3Al increases with an increase in pressure, but it increases with the decreasing temperature.

The heat capacity C_v change with the change in the pressure and temperature is shown in Fig.7. It was determined that C_v increases with an increase in temperature, and it increases with a decrease in pressure, indicating that C_v is more sensitive to pressure, and C_v increases rapidly at temperatures below 800 K at a constant pressure. This increase in C_v obeys Debye's law[38]. The C_v is approximate to the constant data at very high temperatures, and this is known as the Dulong-Petit limit[39]. However, there are no experimental values or theoretical calculations of the heat capacity of Ni3Al available currently, which can be used for comparison. Therefore, the calculated values in the present study can be used as a reference for further experimental studies.

The changes in the thermal expansion coefficient α by changing the pressure and temperature are displayed in Fig.8. For a given pressure, it was found that α increases rapidly at temperatures below 500 K, while its value at 800 K is only slightly smaller than that at 1000 K, indicating that the rate of increase in α becomes slower at high temperatures. Furthermore, when $T<500$ K, α increases slowly with the decreasing pressure, but α decreases quickly with the increasing pressure at high temperatures.

The temperature dependences of the Debye temperature Θ_D are shown in Fig.9. It was found that the calculated Θ_D obtained by the quasi-harmonic Debye model is 475.82 K at 0

Fig.5 Variations of volume (a) and V/V_0 (b) of Ni3Al with the changing of temperature and pressure
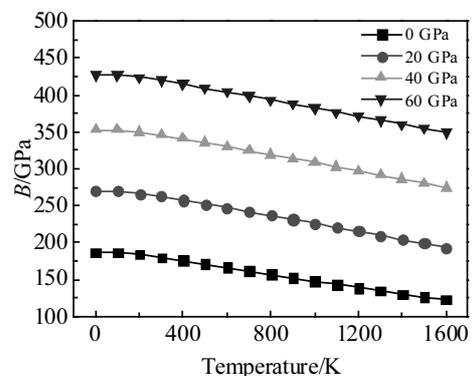
Fig.6 Variations of bulk modulus of Ni3Al with the changing temperature at different pressures
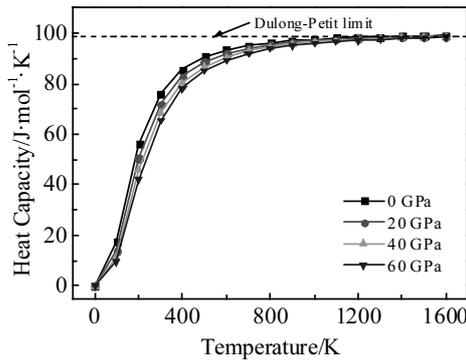
Fig.7 Variations of heat capacity of Ni$_3$Al with the changing of temperature at different pressures
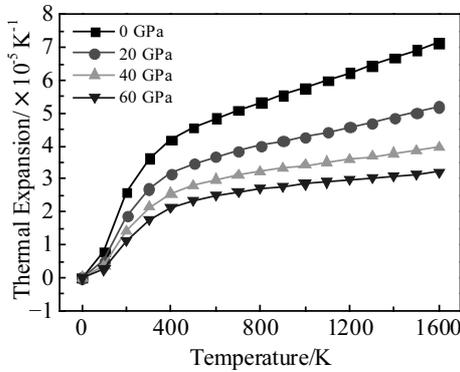
Fig.8 Variations of thermal expansion coefficient of Ni$_3$Al with the changing of temperature at different pressures

GPa and 0 K, which agrees with the calculated results (465.36 K)[5] and experimental values (462±5 K)[36] derived from the elastic data. Furthermore, the Θ_D increases markedly but decreases slowly with an increase in pressure. These results

agree with the general behavior that the Debye temperature decreases with an increase in the temperature in intermetallic compounds[40]. The influence of temperature on Θ_D is obviously smaller than that of the pressure. We hope that the thermodynamic properties obtained by the quasi-harmonic Debye model can provide more insight into the physical properties of the Ni$_3$Al alloy.

2.4 Electronic properties

It is important to understand the influence of pressure on the electronic structure and bonding. To understand this better, the local density of states (PDOS) and total density of states (TDOS) of the Ni$_3$Al alloy were calculated. The PDOS of Ni-Al alloy is illustrated in Fig.10a, and TDOS, plotted at pressures of 0, 30, and 50 GPa is shown in Fig.10b.

As shown in Fig.10a, we found that the energy states were higher than the Fermi level, indicating that the Ni$_3$Al phases have metallic properties. Furthermore, most of the bonding peaks usually show an energy range from –10 eV to 20 eV, because the valence electron numbers of the Ni(s), Ni(d), Al(s), and Al(p) orbits. Moreover, it is obvious that hybridization
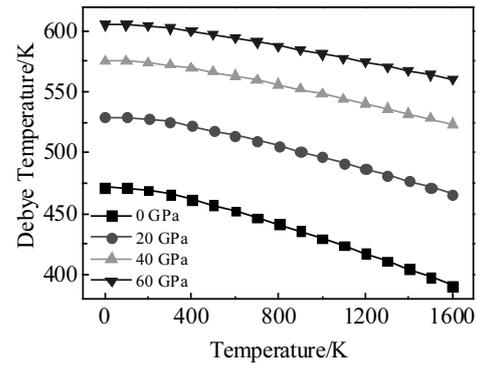
Fig.9 Variations of Debye temperature with the changing of temperature under different pressures
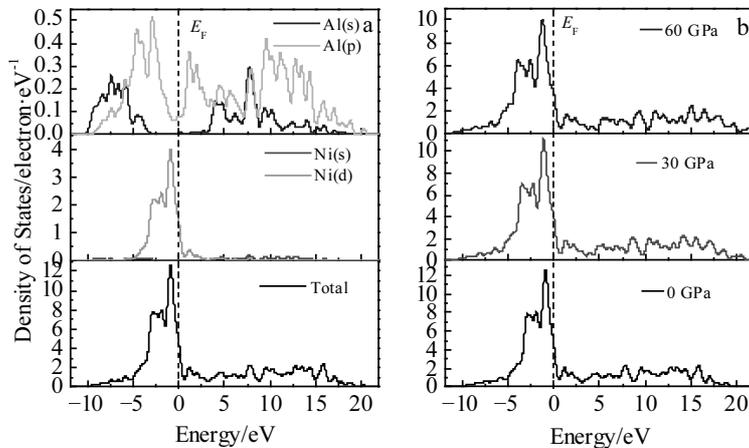
Fig.10 Variations of density of states of Ni$_3$Al under various pressures: (a) zero pressure and (b) high pressure (vertical dotted lines are the Fermi level)

Table 4   Mulliken charges and bond length of Ni₃Al phases at different pressures

Pressure/GPa	Mulliken Charge/e	Bond length/nm	Pressure/GPa	Mulliken Charge/e	Bond length/nm
0	$Ni^{-0.09}Al^{+0.26}$	0.252935	40	$Ni^{-0.07}Al^{+0.22}$	0.240292
10	$Ni^{-0.08}Al^{+0.25}$	0.248849	50	$Ni^{-0.07}Al^{+0.20}$	0.238135
20	$Ni^{-0.08}Al^{+0.24}$	0.245523	60	$Ni^{-0.06}Al^{+0.19}$	0.236206
30	$Ni^{-0.08}Al^{+0.23}$	0.242730			

between the Ni and Al atoms forms a covalent bond.

The TDOS at pressures of 0, 30, and 60 GPa is depicted for understanding the TDOS of the Ni₃Al phases at different pressures, as shown in Fig.10a. It was found that the shape change of the TDOS curves is slight, indicating that the Ni₃Al phases maintain the stability of the structure and show no structural changes for pressures up to 60 GPa. Besides, the TDOS decreases with an increase in the external pressure. It can be deduced that there is a variation in the interaction potentials in the Ni₃Al phases because the interatomic distances shrink under pressure, which results in a decrease in the entire electronic energy levels.

For further understanding the relative covalence and ionicity of the Ni₃Al phases at different pressures, the Mulliken charge and bond length were also calculated, as displayed in Table 4. The (+) and (−) represent the gains and losses of electronic charge, respectively. The calculated values demonstrate that the velocity of charge transport from the Ni atom to the Al atom decreases with an increase in pressure, and bond lengths decrease with the increasing pressure. This data can be used as a comparison for experimental studies. It is remarkable that the absolute magnitudes of the atomic charges rely heavily on the fundamental setting[41]. However, the recorded bond lengths and charge transfer trend are important for a better understanding of the bonding characteristics.

3   Conclusions

1) The structural, elastic, electronic, and thermodynamic properties of Ni₃Al at different temperatures and pressures were analyzed by performing a first-principles study. The calculated elastic constants, equilibrium lattice constants, and elastic modulus coincide well with other theoretical and experimental records. The bulk modulus B_0 and its pressure derivative B_0' for Ni₃Al is 185.247 GPa and 4.75, respectively.

2) The shear modulus, Poisson's ratio, bulk modulus, elastic constants, Young's modulus, and anisotropy factor of Ni₃Al were determined at various pressures. Under applied pressure, the elastic stiffness constant C_{11} changes to a greater extent than C_{12} and C_{44} do. The shear modulus, Young's modulus, and bulk modulus increase with an increase in pressure. B/G and the anisotropy factor A were also determined.

3) The Debye temperature was obtained by calculating the elastic constants, and it changes with a change in the pressure. The normalized volume, heat capacity, Debye temperature, thermal expansion coefficient, and bulk modulus were

obtained and analyzed using the quasi-harmonic Debye model at temperatures of 0~1000 K and pressures of 0~50 GPa, and the results were interpreted.

4) The DOS and Mulliken population analysis were performed. Ni₃Al is structurally stable and the velocity of charge transport from the Ni atom to the Al atom increases with the increasing pressure.

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第一性原理研究压力和温度对 Ni₃Al 合金力学性能、热力学性能和电子结构的影响

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摘 要：采用基于密度泛函理论的第一性原理研究了压力和温度对 Ni₃Al 合金的力学性能、热力学性能和电子结构的影响。计算结果表明：弹性常数、晶格常数和弹性模量的计算值与理论值和实验值十分吻合，其中压力对弹性常数 C_{11} 的影响比 C_{12} 和 C_{44} 更明显，杨氏模量（E）、体模量（B）和剪切模量（G）随着压力的增加而增大。同时还对 Ni₃Al 合金的泊松比和各向异性因子做了分析，计算了德拜温度与压力关系。采用准谐德拜模型，预测了 Ni₃Al 合金在压力（0~60 GPa）、温度（0~1600 K）下的热膨胀系数、热焓、体模量和德拜温度。最后就压力对 Ni₃Al 合金的态密度和电荷密度的影响做了分析。

关键词：镍基合金；电子结构；力学性能；热力学性能；第一性原理