First-principles investigation of elastic, mechanical, electronic and thermodynamic properties of Al₃Li compound under pressure

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Keywords: first-principles, Al₃Li compound, properties under pressure

Abstract

First-principles calculations are employed to study the elastic, mechanical, electronic and thermodynamic properties of Al₃Li compound under pressure up to 25.9 GPa. Based on the elastic constant and phonon calculations, we found that Al₃Li has mechanical and dynamical stability in the considered pressure range. The elastic constants and mechanical properties of Al₃Li under pressure are calculated. The values of hardness, thermal conductivity and melting temperature under ambient pressure are compared with that of the pure Al and Al₃Sc. The wave velocities, Debye temperatures, phonon vibrational frequencies positively increase with the increasing pressure. The results from the analysis of electronic density of states exhibit a metallic bonding behavior of Al₃Li. Finally, the temperature dependent behaviors of thermodynamic properties of Al₃Li as a function of temperature are determined within the quasi-harmonic approximation theory and compared with the available experimental and theoretical data.

1. Introduction

Al–Li alloys have attracted significant attention in cryogenic applications and aerospace industry because of the advantages of low density and high strength [1, 2]. The strengthening of Al–Li alloy can be attributed to the spherical precipitations, δ’ phase of Al₃Li with L1₂-ordered structure which is formed in heat treatment [3, 4]. The mechanical properties of Al₃Li could be further improved by the addition of Sc, which can enhance the grain refinement of the alloys and improve its low-cycle fatigue properties [5]. On the other hand, the addition of Li in Al-Sc alloys can lead to higher hardness, which is introduced by the Al₃X (X = Sc, Li) precipitates [6]. Recently, the metastable phase Al₃Li is also experimentally observed in the Al–Cu–Li compounds [7].

Plenty of works have investigated the various properties of L1₂-Al₃Sc, under ambient pressure [4, 8, 9] and high pressure [10]. At the side of Al₃Li compound with δ’ phase, the temperature dependence of elastic constants have been uncovered experimentally more than a half century ago [11]. After that, the mechanical, electronic and thermodynamic properties under ambient pressure have been extensively investigated. Noble et al [1] estimated the Young’s moduli of Al₃Li at room temperature, 96 GPA. Hu et al [4] performed a comparative study between Al₃Sc and Al₃Li compounds under 0 pressure and reported vast useful information, including energy, mechanical parameters as well as the properties based on elastic constants. Mao et al [12] studied the nucleation and stability of L1₂-ordered precipitates in Al–Sc–Li alloys. Their study suggested that the contribution of strain energy to free energy is small due to the small lattice parameter difference between Al and Al₃Li compound. Guo et al [13] calculated the elastic constants of Al₃Li compound. The calculated Young’s modulus showed a good agreement with the experimental observation when the experimental values are extrapolated to 0 K. The vibrational and thermal properties of Al₃Li were studied by the first-principles pseudo-potential calculations [14].

Aluminides compounds are always used as structural materials, and their work environment may be under pressure. There are many reported investigations to exhibit that the pressure has significant impacts on the
various properties in aluminides [10, 15–19]. The above statements indicate that a systematic investigation of aluminides under pressure is of great necessity and importance. However, to the best of our knowledge, properties of Al3Li under pressure are rarely studied. Therefore, in this paper, the first-principles calculations are performed to clarify and understand the elastic, mechanical, thermodynamic and electronic properties of Al3Li under high pressure up to 25.9 GPa.

2. Calculation methods

We used the Vienna Ab-initio Simulation Package (VASP) [20, 21] to perform the first-principles calculations. Exchange correction function was treated by adopting the generalized gradient approximations of the Perdew-Burke-Ernzerhof form [22]. The Brillouin zone (BZ) of the unit cell was sampled by using the Monkhorst-Pack scheme and the BZ integration was performed by the Methfessel-Paxton method for stress calculations or by tetrahedron method for density of state calculations. The summation over the BZ is performed on a 0.1 Å−1 spacing k-point mesh with smearing of 0.08 eV. The kinetic cut-off energy of 500 eV has been tested to be sufficient for convergence. The structure relaxation convergence was set as $1 \times 10^{-6}$ eV. The Bader charge analysis code [23] was used to explore the volume of each atom [24]. The elastic constants were directly obtained based on the stress-strain relationship. The PHONOPY code [25] was employed to perform the calculations of phonon frequencies with a $2 \times 2 \times 2$ supercell for Al3Li. The thermal properties under different pressures were calculated by using the quasi-harmonic approximation theory [26].

There are two schemes to realize the pressurization on the Al3Li unit cell. The first method is that the destination hydrostatic pressurization is set in the feed file of VASP code, i.e. setting PSTRESS tag in INCAR file. The second one is that the lattice constant of unit cell is changed to simulate the hydrostatic pressurization. These two schemes are all successfully employed in previous works [17]. Based on the consideration of computational cost, we picked the second scheme in this paper. Of course, no matter which scheme is employed, the law induced by pressure should be the same.

3. Result and discussion

3.1. Lattice constant and cohesive energy

In this paper, Al3Li in L12 structure belongs to cubic crystal structure, with space group Pm3m (No. 221). In a unit cell, the Li and Al atoms occupy the 1a (0, 0, 0) and 3c (0.0, 0.5, 0.5) sites. The relaxed lattice constant under ambient pressure is 4.026 Å, which agrees well with the experimental data (3.972 Å) [14] and theoretical data (4.021 Å [12], 4.035 Å [4]).

The calculated pressure dependence of the relative volume, $V / V_0$ ($V_0$ and $V$ stand for the volume of cell under ambient and various pressures, respectively) of the unit cell for Al3Li is shown in figure 1(a). It reveals that the ratio of $V / V_0$ becomes more and more smaller with the increasing pressure, which indicates that the internal atomic distances in this compound should be more and more smaller. The obtained pressure-volume data are fitted to a third order Birch-Murnaghan equation of state as follows:

$$P = \frac{3}{2} B_0 \left[ \left( \frac{V}{V_0} \right)^{-\frac{3}{2}} - 1 \right] - \frac{3}{2} B_0' \left( \frac{V}{V_0} \right)^{-\frac{3}{2}} - \frac{3}{4} B_0' \left( \frac{V}{V_0} \right)^{-\frac{3}{2}} \left[ \left( \frac{V}{V_0} \right)^{-\frac{3}{2}} - 1 \right] + \frac{3}{4} B_0' \left( \frac{V}{V_0} \right)^{-\frac{3}{2}} \left[ \left( \frac{V}{V_0} \right)^{-\frac{3}{2}} - 1 \right] \right] \times \left( \frac{V}{V_0} \right)^{-\frac{3}{2}} - 1 \right],$$

where $B_0$ is the bulk modulus, $B_0'$ is the first pressure derivative of $B_0$, and $V_0$ is the equilibrium volume.

Figure 1. (a) Pressure-volume relation of Al3Li; (b) pressure induced cohesive energy increasing for Al3Li.
The fitting parameter \( B_0 \) is the bulk modulus and \( B'_0 \) is the first-order derivative of \( B_0 \). The fitting is based on the least-squares fitting method, where the root-mean-square deviation \( \sigma \) is estimated by

\[
\sigma = \sqrt{\frac{1}{n-1} \sum_{i=1}^{n} \left( \frac{V_{fit}(P_i) - V(P_i)}{V(P_i)} \right)^2},
\]

The variables \( P_0 \), \( V \), and \( V_{fit} \) are the pressure, volume of optimized geometry, and volume of fitting amount, respectively. The minimum \( \sigma \) can be achieved with an excellent agreement between \( V \) and \( V_{fit} \). Thus, the optimal value of \( B_0 \) can be obtained. A Fortran program has been developed to perform this fitting work [27, 28].

The calculated values of \( B_0 \) and \( B'_0 \) are 64.3 GPa and 4.2, with value of \( \sigma \) less than 0.002, which agrees well with the experimental value of \( B_0 \), 63.1 GPa [11].

Based on the Bader charge analysis, the volume of Al and Li atoms in Al3Li unit cell could be obtained. Their volume ratios under different pressure are presented in figure 1(a). It is seen that Li atom has a smaller compressive trend than Al atom in Al3Li compound.

The cohesive energy of atom in compound can be directly obtained by dividing the system total energy by the number of atom in system. The additional cohesive energy is the energy introduced by the external pressure. It can be described by the difference between the energy of the unit cell under various pressures \( (E) \) and under ambient pressure \( (E_0) \).

Figure 1(b) plots the additional cohesive energy introduced by external pressure. It is obvious that an external hydrostatic pressure up to 25.9 GPa results in an increase of about 0.22 eV/atom for the cohesive energy, which does not destroy the cubic stability of Al3Li.

The formation enthalpy per formula unit (f.u.) is defined as the total energy difference between the compound and its constituents in proportion to the composition, which can be obtained by the following equation:

\[
H = E_{Al, Li} - 3E_{Al} - E_{Li},
\]

Where \( E_{Al, Li} \) is the total energy of an Al3Li f.u. with different lattice parameters under various pressures, \( E_{Al} \) and \( E_{Li} \) are the cohesive energy per atom of pure element solids with their ground state, i.e. Al in FCC, Li in BCC under ambient pressure.

Our calculated formation enthalpy of Al3Li is \(-0.39\) eV f.u., which is in good line with the previous theoretical results, \(-0.39\) eV f.u. within GGA [12] and \(-0.41\) eV f.u. within LDA [29].

### 3.2. Elastic constant and mechanical behavior

As listed in table 1, the elastic constants at ambient pressure agree well with the experimental observations[11] and previous theoretical findings [4, 9, 12–14]. Figure 2(a) presents these elastic constants for Al3Li under various pressures. All elastic constants positively increase with the increasing pressure, which is understandable because the interaction between atoms is enhanced by the external pressure. The mechanical stability criterion, Born criterion, for elastic constants is: \( C_{11} - C_{12} > 0 \), \( C_{44} > 0 \), \( C_{11} + 2C_{12} > 0 \) [17, 30–34]. As seen in table 1, the elastic constants meet that criteria, suggesting that Al3Li is mechanically stable under pressure up to 25.9 GPa.

The bulk modulus \( B \), shear modulus \( G \), and Young’s modulus \( E \) can be obtained with these elastic constants by the Voigt-Reuss-Hill method [35]. The calculation for Poisson ratio \( \nu \) also has been performed. For the cubic system, the formulas used are summarized as follows:

\[
B = \frac{1}{3} (G_{11} + 2G_{12}), \\
G_V = \frac{1}{5} (G_{11} - G_{12} + 3G_{44}), \\
G_R = \frac{5(G_{11} - G_{12})G_{44}}{3(G_{11} - G_{12}) + 4G_{44}}, \\
G = \frac{1}{2} (G_V + G_R), \\
E = \frac{9GB}{3B + G}, \\
\nu = \frac{3B - 2G}{2(3B + G)}.
\]

The calculated values of \( B \) and \( G \) at ambient pressure are 64.5 and 43.1 GPa, which agree well with the experimental values of 63.1 and 40.3 GPa [11]. The value of \( E \) is 105 GPa, which is 9.7 GPa larger than the experimental value obtained at 293 K [1], and it is in line with other theoretical results, as listed in table 1. It is obvious that the values of \( B, G \) and \( E \) increase with increasing pressure as shown in figure 2(b), which exhibits similar behavior to the elastic constants. This indicates that the elevated external pressure could improve the hardness of materials [36].

The ratio of \( B/G \) was proposed by Pugh to quantitatively describe the brittle or ductile behavior of materials [37]. A high \( B/G \) ratio is associated with ductility nature, vice versa. The critical value which separates ductile
and brittle material is 1.75 [16]. The B/G ratio for Al3Li is 1.497 at zero pressure, meeting the experimental result 1.5 [11]. The B/G ratio positively increases with the increasing external pressure and reaches 1.570 at the pressure of 25.9 GPa. It illustrates that Al3Li is a brittle compound even if the pressure is up to 25.9 GPa.

The Cauchy pressure \((C_{12}-C_{44})\) can also provide the brittle or ductile nature of materials [38]. Based on the values of \(C_{12}\) and \(C_{44}\) listed in table 1, the Cauchy pressures for Al3Li in the pressure range of 0–25.9 GPa are all negative, which suggests the brittle behavior of Al3Li under pressure.

Poisson ratio is employed to quantitatively describe the stability of crystals against shear deformation. The larger Poisson ratio \((\nu)\) suggests the better plasticity in materials. The value of \(\nu\) of ductile material is larger than 0.26, while that value of brittle materials is less than 0.26 [39]. Poisson ratio of Al3Li increases from 0.227 to 0.242 when the pressure increases from 0 to 25.9 GPa, indicating Al3Li keeps brittle property in the considered pressure range. This is exactly consistent with the predictions from the B/G relationship and Cauchy pressure. Furthermore, Poisson ratio provides useful information about the characteristics of bonding forces in solid [40]. The values of \(\nu\) for the minimum and maximum limits for central force solids are 0.25 to 0.5, respectively. As

![Figure 2. Pressure dependence of (a) the elastic constants \(C_{ij}\) and (b) the bulk modulus (B), shear modulus (G) and Young’s modulus (E).](image)

| Pressure | \(C_{11}\) | \(C_{12}\) | \(C_{44}\) | \(\nu\) | B | G | E | B/G | \(A^a\) | \(H_u\) | \(H_m\) |
|----------|-----------|-----------|-----------|-------|---|---|---|---|-----|-----|-----|
| Al3Li    |           |           |           |       |   |   |   |   |     |     |     |
| 0a       | 123.3     | 33.5      | 42.4      | 0.221 | 63.5| 43.5| 106.1| 1.462| 0.034|     |     |
| 0b       | 123.6     | 37.2      | 42.8      | 0.230 | 63.1| 40.3| —   | 1.500| —    |     |     |
| 0c       | 123.6     | 34.6      | 39.2      | 0.236 | 64.4| 41.5| —   | 1.56  | —    |     |     |
| 0d       | 122       | 33.3      | 52.3      | —     | 62.9| 49.2| —   | —    | —    |     |     |
| 0e       | 158.0     | 29.4      | 57.7      | —     | 72.3| 60.3| 141.5| —    | —    |     |     |
| 0f       | 120.0     | 57.1      | 70.4      | —     | —   | —   | —   | —    | —    |     |     |
| 0g       | —         | —         | —         | —     | —   | —   | —   | —    | —    |     |     |
| 0h       | 0.0       | 130.9     | 31.3      | 39.1  | 0.227| 64.5| 43.1| 105.7| 1.497| 0.071| 8.271| 7.844|
| 1.2      | 142.3     | 35.8      | 43.8      | 0.228 | 71.3| 47.4| 116.3| 1.505| 0.046| 8.839| 8.586|
| 4.4      | 154.3     | 40.7      | 49.0      | 0.229 | 78.6| 52.0| 127.8| 1.511| 0.026| 9.444| 9.393|
| 7.6      | 165.2     | 47.0      | 54.8      | 0.232 | 86.4| 56.5| 139.1| 1.530| 0.007| 9.880| 10.106|
| 11.0     | 181.6     | 54.9      | 62.6      | 0.234 | 97.1| 62.9| 155.2| 1.544| 0.000| 10.565| 11.166|
| 12.8     | 188.4     | 58.4      | 66.1      | 0.234 | 101.7| 65.7| 162.1| 1.549| 0.000| 10.856| 11.624|
| 14.7     | 195.4     | 62.0      | 69.6      | 0.235 | 106.5| 68.4| 169.1| 1.556| 0.002| 11.125| 12.072|
| 16.6     | 202.6     | 65.8      | 73.3      | 0.236 | 111.4| 71.3| 176.3| 1.562| 0.006| 11.399| 12.537|
| 18.8     | 210.2     | 69.8      | 77.1      | 0.237 | 116.6| 74.3| 183.8| 1.570| 0.011| 11.662| 13.005|
| 21.0     | 217.5     | 74.3      | 81.2      | 0.239 | 122.0| 77.2| 191.3| 1.580| 0.019| 11.885| 13.449|
| 23.4     | 224.3     | 79.1      | 85.5      | 0.240 | 127.5| 80.1| 198.7| 1.592| 0.032| 12.076| 13.864|
| 25.9     | 231.8     | 84.1      | 89.9      | 0.242 | 133.3| 83.1| 206.4| 1.605| 0.047| 12.265| 14.293|

Table 1. The calculated elastic constants and related material properties of Al3Li as a function of pressure. \(\nu\) represent Poisson ration. \(A^a\) stands for the universal elastic Anisotropy index and \(H_u/m\) is on behalf of hardness. The available values for comparison are also included.

* GGA-PBE (CESTEP) calculations from [4].
* Experimental data at 294 K from [11].
* GGA-PBE (VASP) calculations from [9].
* GGA-PAW (VASP) calculations from [12].
* FLAPW-LDA calculations from [13].
* LDA with pseudopotentials (VASP) calculations from [14].
* Experimental data at 293 K from [1].

and brittle material is 1.75 [16]. The B/G ratio for Al3Li is 1.497 at zero pressure, meeting the experimental result 1.5 [11]. The B/G ratio positively increases with the increasing external pressure and reaches 1.570 at the pressure of 25.9 GPa. It illustrates that Al3Li is a brittle compound even if the pressure is up to 25.9 GPa.

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Poisson ratio is employed to quantitatively describe the stability of crystals against shear deformation. The larger Poisson ratio \((\nu)\) suggests the better plasticity in materials. The value of \(\nu\) of ductile material is larger than 0.26, while that value of brittle materials is less than 0.26 [39]. Poisson ratio of Al3Li increases from 0.227 to 0.242 when the pressure increases from 0 to 25.9 GPa, indicating Al3Li keeps brittle property in the considered pressure range. This is exactly consistent with the predictions from the B/G relationship and Cauchy pressure. Furthermore, Poisson ratio provides useful information about the characteristics of bonding forces in solid [40]. The values of \(\nu\) for the minimum and maximum limits for central force solids are 0.25 to 0.5, respectively. As
this criterion and the values of ν listed in table 1, the interatomic forces of Al3Li is not central force. Additionally, the values of Poisson ratio increase accordingly along with increasing pressure.

The universal anisotropy index $A^U$ can be calculated by [41]:

$$A^U = 5\frac{G_V}{G_R} + \frac{B_V}{B_R} - 6,$$

where $B_V = B_R$ for cubic structures. The material is isotropy if $A^U = 0$. As seen in table 1, the values of $A^U$ approach 0, suggesting Al3Li exhibits isotropy property under the considered pressure. It is worth to notice that, the value of $A^U$ declines with the increasing pressure when the pressure is less than 11 GPa and increases again when the pressure is larger than 12.8 GPa. The Al3Li shows exact isotropy in the pressure range of 11.0–12.8 GPa.

In order to understand the elastic isotropy, we plot the directional dependences of the Young’s modulus at different pressures in figure 3 [42–45]. We can note that this result is consistent with the analyses of $A^U$ under pressure. The difference between the upper and lower limits for Al3Li under the pressure of 11.0 and 12.8 GPa is only 2 GPa, which shows a good isotropic behavior as shown in figures 3(b) and (c). The decreasing and increasing behavior of the values of $A^U$ before and after 11 GPa is illustrated vividly in figure 3.

### 3.3. Anisotropic wave velocity and Debye temperature

The wave velocities in solid are related to their elastic constants. The wave velocities of both longitudinal and transverse along three different crystal directions, including [100], [110] and [111], were calculated for Al3Li.

The equations used for these calculations are given by [46]:

$$[100]v_l = \sqrt{\frac{G_{11}}{\rho}}, [010]v_{l1} = [001]v_{l2} = \sqrt{\frac{C_{44}}{\rho}},$$

$$[110]v_l = \sqrt{\frac{(G_{11} + G_{12} + 2C_{44})}{2\rho}}, [110]v_{l1} = \sqrt{\frac{(G_{11} - G_{12})}{\rho}}, [001]v_{l2} = \sqrt{\frac{C_{44}}{\rho}},$$

$$[111]v_l = \sqrt{\frac{(G_{11} + 2G_{12} + 4C_{44})}{3\rho}}, [112]v_{l1,2} = \sqrt{\frac{(G_{11} - G_{12} + 3C_{44})}{3\rho}}.$$  

The calculated wave velocities in different directions are listed in table 2, the results for Al at ambient pressure are also included. Our results for Al are in good agreement with the available experimental [10] and theoretical results [10, 18, 47]. Obviously, the wave velocities in different directions for Al3Li are larger than those of Al, and increase with the increasing pressure.

Debye temperature ($\theta_D$) is the highest temperature that can be achieved due to a single normal vibration for a compound [48, 49]. It gives insight into several important physical properties, such as specific heat, ultrasonic wave velocity. The method for estimating the value of $\theta_D$ is as [50]:

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

where $h$ and $k_B$ are the Plank’s constant and Boltzmann’s constant. $n$ and $N_A$ present the total number of atoms in the cell and Avogadro’s number, $\rho$ and $M$ are the mass density and molecular weight of the compound. Moreover, $v_m$ can be approximately calculated from the longitudinal wave velocity $v_l$ and transverse wave velocity $v_t$ [50].

$$v_m = \left[ \frac{1}{3} \left( \frac{2}{v_l^2} + \frac{1}{v_t^2} \right) \right]^{\frac{1}{2}}, v_l = \sqrt{\frac{3B + 4G}{3\rho}}, v_t = \sqrt{\frac{G}{\rho}}$$

where $B$ and $G$ are bulk and shear modulus.
The \( v_l \), \( v_t \), \( v_m \) and \( \theta_D \) for Al\(_3\)Li as a function of pressure are shown in Figure 4. At ambient pressure, our results agree well with the values obtained under GGA-PBE scheme in [4]. However, the value of \( \theta_D \) from [13] is much higher than our result. According to the computational formulas of \( v_l \), \( v_t \) and \( \theta_D \), the value of \( \theta_D \) strongly depends on the bulk modulus and shear modulus. Those values in [13] are significantly higher than this paper, as listed in Table 1. For Al\(_3\)Li under other pressures, the wave velocity and Debye temperature all increase with the increasing external pressure up to 25.9 GPa, as shown in Figure 4. The increasing Debye temperature corresponds to the increasing vibrational frequency with increasing pressure. Future experimental work could test our prediction since there are no experimental data or theoretical results available in literature on these properties for Al\(_3\)Li under pressure.

### 3.4. Thermal conductivity, hardness and melting temperature

The thermal conductivity is often used to quantify the thermal transportation behavior of materials. Since the thermal conductivity will change with the external conditions, it is meaningful to determine the thermal conductivity of Al\(_3\)Li under different pressures. Both Clark’s model and Cahill’s model were developed for studying the minimum thermal conductivity \( (k_{\text{min}}) \) of crystals based on phonon-model but with different

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**Table 2.** Wave velocity along different directions for Al\(_3\)Li under different pressures. The results for Al at 0 GPa are also included. Units of pressure, velocity and mass density are in GPa, Km/s and g/cm\(^3\).

| P   | \( \rho \) | \( [100]v_l \) | \( [001]v_{1,2} \) | \( [110]v_l \) | \( [1\bar{1}0]v_l \) | \( [001]v_{1,2} \) | \( [111]v_l \) | \( [112]v_{1,2} \) |
|-----|-----|-------|-------|-------|-------|-------|-------|-------|
| Al  | 0   | 2.721 | 6.303 | 3.169 | 6.442 | 4.069 | 3.169 | 6.488 | 2.978 |
|     | 0a  | 6.325 | 3.220 | 6.469 | 4.128 | 3.220 | 6.517 | 3.023 |        |
|     | 0b  | 5.943 | 3.503 | 6.173 | 4.354 | 3.503 | 6.248 | 3.226 |        |
|     | 0c  | 6.009 | 3.325 | 6.226 | 4.098 | 3.325 | 6.297 | 3.047 |        |
|     | 0d  | 2.732 | 6.006 | 3.358 | 6.239 | 4.106 | 3.325 | 6.318 | 3.032 |        |
| Al\(_3\)Li | 0.0  | 2.220 | 7.452 | 4.374 | 7.379 | 6.358 | 4.374 | 7.355 | 4.456 |        |
|     | 0    | 2.235 | 7.653 | 4.183 | 7.334 | 6.676 | 4.183 | 7.224 | 4.548 |        |
|     | 2.1  | 2.303 | 7.860 | 4.361 | 7.595 | 6.800 | 4.361 | 7.504 | 4.664 |        |
|     | 4.4  | 2.375 | 8.061 | 4.543 | 7.855 | 6.917 | 4.543 | 7.785 | 4.778 |        |
|     | 7.1  | 2.449 | 8.214 | 4.731 | 8.106 | 6.948 | 4.731 | 8.070 | 4.833 |        |
|     | 8.6  | 2.487 | 8.309 | 4.821 | 8.236 | 6.992 | 4.821 | 8.212 | 4.904 |        |
|     | 11.0 | 2.546 | 8.446 | 4.959 | 8.428 | 7.054 | 4.959 | 8.422 | 4.978 |        |
|     | 12.8 | 2.586 | 8.553 | 5.056 | 8.560 | 7.090 | 5.056 | 8.568 | 5.027 |        |
|     | 14.7 | 2.627 | 8.624 | 5.147 | 8.688 | 7.125 | 5.147 | 8.709 | 5.075 |        |
|     | 16.6 | 2.670 | 8.712 | 5.240 | 8.817 | 7.159 | 5.240 | 8.851 | 5.122 |        |
|     | 18.8 | 2.712 | 8.803 | 5.332 | 8.947 | 7.195 | 5.332 | 8.994 | 5.170 |        |
|     | 21.0 | 2.756 | 8.883 | 5.428 | 9.077 | 7.208 | 5.428 | 9.141 | 5.209 |        |
|     | 23.4 | 2.801 | 8.949 | 5.525 | 9.202 | 7.200 | 5.525 | 9.285 | 5.240 |        |
|     | 25.9 | 2.847 | 9.023 | 5.620 | 9.331 | 7.203 | 5.620 | 9.431 | 5.275 |        |

* Experimental result from [10].
* Theoretical result by LDA + U from [47].
* Theoretical result by LDA from [10].
* Theoretical result by GGA + PBE from [18].
* Theoretical result by GGA + PBE from [4].

The \( v_l \), \( v_t \), \( v_m \) and \( \theta_D \) for Al\(_3\)Li as a function of pressure are shown in Figure 4. At ambient pressure, our results agree well with the values obtained under GGA-PBE scheme in [4]. However, the value of \( \theta_D \) from [13] is much higher than our result. According to the computational formulas of \( v_l \), \( v_t \) and \( \theta_D \), the value of \( \theta_D \) strongly depends on the bulk modulus and shear modulus. Those values in [13] are significantly higher than this paper, as listed in table 1. For Al\(_3\)Li under other pressures, the wave velocity and Debye temperature all increase with the increasing external pressure up to 25.9 GPa, as shown in Figure 4. The increasing Debye temperature corresponds to the increasing vibrational frequency with increasing pressure. Future experimental work could test our prediction since there are no experimental data or theoretical results available in literature on these properties for Al\(_3\)Li under pressure.

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approaches [51]. They work well for many materials and give an intuitive description of the phonon limit of thermal conductivities [52]. The formulas used in this work are:

In Clark’s model [53],

\[
k_{\text{Clark}}^{\text{min}} = 0.87k_B \left[ \frac{M}{3nN_A} \right]^{1/2} E^2 / \rho^{1/3},
\]

and in Cahill’s model [35],

\[
k_{\text{Cahill}}^{\text{min}} = \frac{k_B}{2.48} \rho^2 (\nu_l + 2\nu_t),
\]

where \( k_B \) is the Boltzmann’s constants, \( M \) is the molar weight, \( n \) is the total number of atoms per f.u., \( E \) is the Young’s modulus, \( \rho \) is the density mass, \( \rho \) is the density of number of atom per volume, and \( \nu_l \) and \( \nu_t \) are the longitudinal and transverse wave velocities, respectively. The \( k_{\text{min}} \) values based on these two models are usually above the experimental observation because of the influence of temperature on phonon propagation. More information can be found in [51].

The values of \( k_{\text{min}} \) obtained by Cahill’s model are slightly larger than that of Clark’s model at a given pressure throughout the whole pressurization process. At the pressure of 0 GPa, the value of \( k_{\text{min}} \) for Al\(_3\)Li is 1.28–1.40 Wm\(^{-1}\)K\(^{-1}\), which is higher than that of pure Al (0.84–1.08 Wm\(^{-1}\)K\(^{-1}\)), but slightly lower than Al\(_3\)Sc, as listed in table 3. The minimum thermal conductivity is 40%–50% improved by alloying Li in Al to form Al\(_3\)Li compound. The values of \( k_{\text{min}} \) for Al\(_3\)Li increase with the increasing pressure, as shown in figure 5(a), and it reaches 1.87–2.04 Wm\(^{-1}\)K\(^{-1}\) when the pressure is up to 25.9 GPa.

Moreover, the melting temperature (\( T_m \)) of Al\(_3\)Li can be estimated by the empirical function [55]:

\[
T_m^1 = (553 + 5.91G_{11}) \pm 300,
\]

or another empirical relation [56]:

\[
T_m^2 = 607 + 9.3B \pm 553,\text{ The } T_m \text{ of Al}_3\text{Li at } 0 \text{ GPa is } 1326 \pm 300 \text{ and } 1207 \pm 300 \text{ K for } T_m^1 \text{ and } T_m^2,
\]

respectively. The estimated \( T_m \) based on the theoretical and experimental elastic constants for Al and Al\(_3\)Sc are listed in table 3. We can see the melting temperature of Al\(_3\)Li is similar to that of pure Al and lower than that of Al\(_3\)Sc.

The calculated \( T_m \) of Al\(_3\)Li as a function of pressure is shown in figure 5(b). The \( T_m \) calculated by \( T_m^1 \) and \( T_m^2 \) follows the same varying trend of pressure, that is the gradual increase with the increasing external pressure. It should note that the two empirical functions for \( T_m \) might have potential risk in predicting the crystals melting point under pressure, one should be very cautious on the range of applicability of empirical function in the future study.

To obtain the hardness of Al\(_3\)Li under pressure, we adopted the empirical scheme to evaluate their Vicker’s hardness [57, 58], which is determined by \( B \) and \( G \) as:

\[
H_V = 2(k^2G)^{0.585} - 3, \text{ where } k = G/B,
\]
Another relation for calculating microhardness \( (H_m) \) based on the Poisson ratio \( (\nu) \) and Young’s modulus \( (E) \) is [39]:

\[
H_m = \frac{(1 - 2\nu)E}{6(1 + \nu)}.
\]

The calculated hardness for Al, Al\(_3\)Sc and Al\(_3\)Li under ambient pressure are listed in table 3. The values obtained by these two methods are close to each other for all these three systems. We can see that the hardness of Al\(_3\)Sc, the other important precipitate in Al-Sc-Li alloy, is higher than Al\(_3\)Li, and both of them are significantly higher than pure Al. Our result answers the peak hardness introduced by the precipitates of Al\(_3\)Li and Al\(_3\)Sc in Al-Li-Sc alloys [6]. From the last two columns in table 1, we find that the hardness \( H_m \) of Al\(_3\)Li at ambient pressure is 8.271 (7.844) GPa, and it increases with the pressure, up to 12.265 (14.293) GPa at pressure 25.9 GPa. The reason is that the bond lengths gradually become shorter with the increasing pressure.

### 3.5. Electronic structure and chemical bonding

To analyze the bonding characteristics of the Al\(_3\)Li compound, the electronic densities of states (DOS) were calculated under different pressures, which are presented in figure 6. At the ambient pressure, figure 6(a), Al\(_3\)Li exhibits a metallic character because there is no energy gap near the Fermi level. The Li atom has one valence electron and Al atom has three. However, the electronic density of the Li atom is lower than 1/3 of Al, indicating that partial of Li electronic charge is transferred to Al atoms. This is consistent with the Born electronegative of Al and Li (Al: 1.61, Li: 0.98). The main bonding peaks of Al\(_3\)Li are predominantly derived from Al\(_s\) with a little contribution from Li\(_s\) sp states at the energy region below -3.5 eV. Al\(_p\) and Li\(_p\) states dominate the bonding peaks at the energy region of -3.5 to 0 eV. The increasing pressure hardly affects the bonding character of Al\(_3\)Li in the considered pressure range, as shown in figures 6(b) and (c). The shape of DOS curves exhibits relatively few changes, and it is expanded in the energy scales introduced by the increasing of pressure.
3.6. Phonon dispersion and density of states

Lattice dynamics plays an important role in the understanding of physical properties of solids, such as phase stability. Phonon dispersions in materials are also interesting because of the anomalous electronic screening \[60,61\]. Therefore, the phonon dispersion has been calculated to investigate the lattice dynamic properties of \(\text{Al}_3\text{Li}\) under pressure, as shown in figure 7. No imaginary frequency has been observed, suggesting that \(\text{Al}_3\text{Li}\) is dynamically stable under pressure up to 25.9 GPa. There are 4 atoms in \(\text{Al}_3\text{Li}\) cell, phonon spectra curves consists of 12 phonon branches, which contain 3 acoustic branches and 9 optical branches \[18\]. Generally, the frequency of optical models is higher than that of acoustic models\[17\]. The highest optical branches are separated clearly from the rest branches at 0 GPa because of the large mass difference between Al and Li elements.

Four multi-band degenerations at the Gamma point are presented in the phonon dispersion curves, as shown in figure 7, and their frequencies are also printed. The type of degeneration does not change with pressure which reflects the stability of \(\text{Al}_3\text{Li}\) under pressure. The frequencies of those degenerated bands are enhanced as the external pressure increase. This phenomenon can be explained by the shorter bond length when pressure increases. The shorter bond length can lead to the larger force constants, resulting in higher phonon frequencies \[62\]. At the meantime, the external pressure limits the vibration range of the atoms and increases the lattice vibration frequencies to consume the internal energy \[18\].

To further understand the lattice dynamic behavior of \(\text{Al}_3\text{Li}\) under pressure, we calculated the phonon density of states (PDOS), presented in figure 8. We can see that the 3 separated optical branches are mainly derived from Li atoms and other branches are dominated by Al atoms at 0 GPa, as shown in figure 8(a). The increasing pressure lowers the absolute value of PDOS and increases their vibration frequency. With the increase of the pressure, the branches with low frequency, lower than the frequency at the pseudogap marked by an arrow, are always dominated by Al atoms with a constant contribution from Li while the branches with high frequency, higher than the frequency at the pseudogap, are dominated by Li atoms with a slightly increasing contribution from Al atoms, as shown in figures 8(b) and (c). Al atoms are more sensitive than Li to the effects introduced by external pressure.

3.7. Thermodynamic properties

The data of thermodynamic properties under high pressure and temperature can provide the valuable information for industrial applications of materials under extreme conditions\[18\]. The thermal properties of \(\text{Al}_3\text{Li}\) as a function of temperature are calculated by the quasi-harmonic approximation theory\[26\].

![Figure 7. The phonon dispersion curves for \(\text{Al}_3\text{Li}\) under 0 GPa (a), 12.8 GPa (b) and 25.9 GPa (c). The frequencies of the degenerated multi-band at the Gamma point are given and in THz.](image1)

![Figure 8. The phonon density of states for \(\text{Al}_3\text{Li}\) under 0 GPa (a), 12.8 GPa (b) and 25.9 GPa (c).](image2)
Figure 9(a) shows the bulk modulus of Al\(_3\)Li along with the available experimental and theoretical data under the pressure of 0 GPa. We can see that our result is in good agreement with the results obtained in [14] with a constant difference about 4 GPa. This difference can be explained by the different value of C\(_{12}\), as listed in table 1, which leads to the 4 GPa difference of bulk modulus at 0 K. On the other hand, the limited experimental value of bulk modulus versus temperature apparently decreases faster than our calculations and [14]. It might be because Al\(_3\)Li is a metastable phase in Al-Li alloy [1] and it is difficult to obtain reliable experimental results for such a phase. On the other hand, our result is obtained with the help of DFT calculation and quasi-harmonic approximation theory [26], which are widely employed in this field, wish the future solution could give new explanation on this mismatch. The thermal expansion coefficient of Al\(_3\)Li at 0 GPa was shown in figure 9(b) along with the theoretical results from [14]. We can see the good agreement between them, especially when temperature is lower than 500 K.

The volume expansion coefficient, volume expansion and bulk modulus under pressure versus temperature are shown in figures 9(b)–(d), respectively. We can see that the thermal expansion coefficient increases exponentially with temperature below 200 K, and gradually approaches linear behavior beyond 300 K at ambient pressure. At a given temperature, the expansion coefficient decreases with the external pressure, as shown in figure 9(b). The similar phenomenon also presented in the volume expansion, figure 9(c). We can conclude that the external pressure weakens the thermal effect on volume expansion of Al\(_3\)Li. The values of bulk modulus decrease accordingly with the increasing temperature, as shown in figure 9(d). At the same temperature, the bulk modulus increases along with the increasing external pressure, exhibiting the same trend as that of elastic constants.

The calculated free energies, entropies for Al\(_3\)Li compound as a function of temperature under different pressures are displayed in figures 10(a) and (b). We can see that the free energy decreases gradually with increasing temperature under a certain pressure and increases with the increasing pressure at a given temperature. The entropies just possess the opposite varying trend of free energy on temperature, which the entropy increases with the increasing temperature under a given pressure and decreases with the increasing pressure at a certain temperature.

The variation of the isochoric heat capacity (C\(_V\)) with temperature is shown in figure 10(c). It can be seen that at low temperature, C\(_V\) is proportional to third power of temperature. Whereas in the range of high temperature, C\(_V\) approaches the Dulong-Petit limit of 99 J mol\(^{-1}\)K\(^{-1}\). Figure 10(d) illustrates the calculated isobaric heat
capacity \((C_p)\) as a function of temperature under pressures up to 25.9 GPa. The results of \(C_p\) for Al\(_3\)Li under 0 GPa from [14] are also presented. It is obvious that our results agree well with that from [14]. The \(C_p\) follows the similar behavior as \(C_v\) except at the very high temperature. The values of \(C_p\) at 800 K for Al\(_3\)Li under the pressures of 0, 12.8 and 25.9 GPa are 111.6, 101.8 and 99.4 J mol\(^{-1}\) K\(^{-1}\), respectively.

One should note that there is electronic contribution to free energy, entropy, heat capacity and thermal conductivity of Al\(_3\)Li as other metals. The electronic contribution to free energy, \(F_{el}\), could be given by [63]:

\[ F_{el} = U_{el}(T) - T S_{el}(T), \]

where \(U_{el}(T)\) and \(S_{el}(T)\) indicate the electronic contribution to the internal energy and entropy. The effects of temperature give a negligible contribution to \(U_{el}(T)\) under a self-consistent field finite temperature DFT calculation [63], while \(S_{el}(T)\) could be determined by [64]:

\[ S_{el}(T) = \frac{1}{3} \pi^3 k_B^2 T \eta_F, \]

where \(\eta_F\) is the DOS at Fermi level. From the above two equations we could get that a large DOS at the fermi energy implies a largely negative free energy contribution [63]. Obviously, the electronic contribution to entropy is proportional to the DOS at fermi level at a given temperature.

For heat capacity, the vibration contribution is shown in figure 10(c), \(C_v\) is proportional to the third power of temperature at low temperature, i.e. \(C_v \sim T^3\); the electronic contribution to \(C_v\) could be given by [65]:

\[ C_{v,el} = T \left( \frac{\partial S_{el}(T)}{\partial T} \right)_{v}, \]

which means \(C_{v,el} \sim T\). Therefore, the influence of electronic contribution to heat capacity should be significantly at low temperature.

There is also electronic contribution to thermal conductivity due to the phonon and electron coupling. One can find more information from [66].

\[ \text{Figure 10. The temperature dependence of (a) free energy, (b) entropy, (c) isochoric heat capacity (} C_v(\text{)), (d) isobaric heat capacity (} C_p), \] including the results at ambient pressure from [14], for Al\(_3\)Li under different pressures. \]
4. Conclusion

In this study, we have comprehensively studied the elastic, mechanical, electronic and thermodynamic properties of Al₃Li compound under pressure based on the first-principles calculations. The conclusions of this work may be summarized as following:

1. The calculated elastic constants for Al₃Li show increase with the increasing pressure and satisfy the Born’s criteria, indicating the mechanical stability is well even if the pressure is up to 25.9 GPa. There is no imaginary frequency presented in the calculation of the phonon dispersion spectrum also suggests the stability of Al₃Li under pressure.

2. The bulk modulus, Yang’s modulus and shear modulus are 64.5, 105.7 and 43.1 GPa at 0 pressure and they increase accordingly to 133.3, 206.4 and 83.1 GPa as the pressure increases to 25.9 GPa. The Poisson ratio and Cauchy pressure both suggest that Al₃Li sustains brittle nature in the whole considered pressure range. The universal elastic anisotropy index firstly declines with the increasing pressure when the pressure is less than 11 GPa, and it increases with the increasing pressure when the pressure is larger than 12.8 GPa. Based on the good agreement between the calculated wave velocities and experimental observation for pure Al, the wave velocities for Al₃Li under pressure were calculated. The Debye temperature was also obtained further. They all accordingly increase along with the increasing pressure.

3. According to empirical functions, the thermal conductivity, melting temperature and hardness were all predicted, and they show the same reaction to pressure as that of wave velocities. These quantities for Al, Al₃Sc and Al₃Li are compared when the pressure is 0. Al₃Sc has the best hardness and the highest melting temperature, the Al₃Li and Al present the similar melting temperature, Al has the worst thermal conductivity. The results from the analysis of electronic density of states exhibit a metallic bonding behavior of Al₃Li.

4. We gave a prediction of the bulk modulus, thermal expansion coefficient, isochoric heat capacity, isobaric heat capacity, free energy and entropy under various pressures for Al₃Li as a function of temperature. The presented study would be helpful to future experimental and theoretical explorations.

Acknowledgments

This research was funded by the National Natural Science Foundation of China (Grant No. 51801091), the Provincial Natural Science Foundation of Liaoning of China (Grant No. 20180550484), and the Research Funds from the Education Department of Liaoning Province of China (Grant No. JL201613405). The authors declare that there are no conflicts of interest related to this work.

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