A first-principles study on the site occupancy behavior of transition metals in \(L1_2-Al_3Li\) phase

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Abstract

The main strengthening mechanism in Al-Li alloys is generally achieved by the existence of a high volume fraction of the \(L1_2\)-Al\(_3\)Li precipitation from Al matrix. In this work, we do density functional theory (DFT) total energy calculations on the site occupancy behaviour of transition metals in \(L1_2\)-Al\(_3\)Li compound. The ground state properties of \(L1_2\)-Al\(_3\)Li, fcc-Al, and bcc-Li are determined and compared to the available literature data. The formation energies of intrinsic point defects in \(L1_2\)-Al\(_3\)Li phase as well as Al\(_3\)LiX alloy formation energy are calculated and identified. We show that the Li antisite is preferential to from in the \(L1_2\)-Al\(_3\)Li phase. Finally, the site occupancy behaviour of transition metals in \(L1_2\)-Al\(_3\)Li as well as the solute atomic volume effect on the solute site preference and lattice expansion of the \(L1_2\)-Al\(_3\)Li have been studied, the later results can be used for an indirect estimation of the site substitution behaviour of the alloying elements in \(L1_2\)-Al\(_3\)Li phase.

1. Introduction

Al-Li alloys are mainly used for aerospace industry due to the light weight and high strength. It has been known that the strengthening mechanism of Al-Li alloys is associated with the precipitation of the metastable ordered \(\delta^\prime\)-Al\(_3\)Li phase, which has a \(L1_2\) structure and forms as coherent spherical particles from the Al matrix \([1-6]\). It has been confirmed that \(\delta^\prime\)-Al\(_3\)Li phase has a large intrinsic modulus, which could be the main reason of high elastic modulus in Al-Li alloys \([7-9]\). At the same time, one of the major problems associated with Al-Li alloys is the decreased ductility due to the presence of the shearable strengthening phase \(\delta\)-Al\(_3\)Li \([10-12]\). It was reported experimentally that rapidly solidified powder metallurgy could improve the ductility and fracture resistance of Al-Li alloy \([10-12]\). Other approaches, for instance, grain refinement through additions of alloying elements and minimization of tramp elements through composition control, have been also used to increase the ductility of Al-Li alloys \([13]\).

From alloy chemical design aspect, one potential way to improve the ductility of the alloys is to introduce metallic alloying elements into the materials \([14, 15]\). The transition metals have been used to modify the thermodynamic and mechanical properties of \(\delta^\prime\)-Al\(_3\)Li phase according to previous investigations \([16-25]\). However, in order to identify the effect of alloying elements on the improvement of the thermodynamic and mechanical properties of Al\(_3\)Li, knowing of the solute elements site occupancy behaviour in ordered \(L1_2\)-Al\(_3\)Li is of great importance. Despite the fact that the mechanical and thermodynamic properties \([16-25]\) as well as the site preference behaviour \([26]\) of a list of elements in \(L1_2\)-Al\(_3\)Li have been investigated previously in the literature, there is no systematic calculation of alloying elements site occupancy behaviour for the whole transition metals in \(L1_2\)-Al\(_3\)Li phase. Particularly, Tian \textit{et al}\([26]\) have studied the site preference of a list of alloying elements (8 elements) in \(L1_2\)-Al\(_3\)Li by using first-principles calculations, they have used the enthalpy of formation of alloyed \(L1_2\)-Al\(_3\)Li to predict the 0 K site preference of solute. In fact, most of the 3d, 4d, and 5d elements are used in Al-Li based alloys as alloying solutes \([4]\) in Al-Li alloys. Therefore, the knowledge of the intrinsic defect and alloys formation enthalpies as well as site preference of the alloying elements of transition metals can be used to evaluate the role of the selected elements on the thermodynamic and mechanical properties of Al-Li alloys.
The main focus of present work is to study the site preference behaviour of 3$d$, 4$d$, and 5$d$ transition metal elements in L12-Al3Li using the first-principles calculations based on density functional theory. The formation of intrinsic defects and site occupancy behaviours of transition metals in L12-Al3Li phase will be investigated by using supercell models with dilute limit of defects, the correlation between solute atomic volume and the site occupancy as well as the lattice expansion will be fully considered at 0 K. Furthermore, we compare our results to existing literature results and show a good agreement.

2. Methodology

2.1. Computational details
Spin polarized density functional theory calculations have been performed using the projector-augmented-wave (PAW) [27, 28] method as implemented in the Vienna Abinitio simulation package (VASP) [29, 30]. The Perdew–Burke–Ernzerhof (PBE) form of generalized gradient approximation (GGA) has been used for the exchange-correlation potential [31] calculations. The plane-wave basis set cutoff energy has been set to 500 eV after convergence test of total energy of Al. The convergence criteria of self-consistent calculations have been set to $10^{-5}$ eV/cell for the total energy. The relaxed configurations have been obtained from the conjugate gradient method that the optimization search is terminated when the force on all atoms was reduced to $9 \times 10^{-3}$ eV/Å. The integration over the Brillouin zone has been done using the $6 \times 6 \times 6$ Monkhorst–Pack k-mesh [32] for the $3 \times 3 \times 3 \times$ [conventional L12 cell] supercell calculations. The lattice parameter has been fixed to the equilibrium value for the intrinsic defect formation and the site occupancy behaviour calculations while only the ions have been allowed to relax within the supercells.

2.2. Formation of the intrinsic defects and the L1$_2$Al$_3$LiX alloys
The L1$_2$-Al$_3$Li is a fcc-base ordered structure. In stoichiometric Al$_3$Li, there are three Al sublattices located at the face centers and one Li sub-lattice located at the corner of the cubic. The crystallographic point defects (e.g., vacancies, antisites, and ternary substitutional atoms) in L1$_2$-Al$_3$Li can be on one or both sublattices and show a site preference behavior. Moreover, the crystallographic defects affect the atomic arrangement of L1$_2$-Al$_3$Li and which contribute to the thermodynamic and mechanical properties of L1$_2$-Al$_3$Li as well as Al-Li alloys.
Furthermore, the intrinsic defects also interact with external solutes and at the end affect the solute solubility and site occupancy in the alloys. In figure 1(a), we show the perfect L12-Al3Li unit cell containing three Al atoms and one Li atom, we also show the supercell geometries with Al vacancy, Li vacancy, Al antisite, Li antisite, and Al-Li exchange antisite defects in figures 1(b), (c), (d), (e), and (f) respectively.

In the ordered L12-Al3Li phase with dilute limit of defect, one can assume that the formation enthalpy (per atom) \( \Delta H_d \) of a ternary L12 Al3LiX alloy is a linear function of the point defect formation enthalpy concentrations \([34–36]\), which can be written as following:

\[
\Delta H_d = \Delta H_{\text{Al,Li}} + \sum_d H_d x_d,
\]

here \( \Delta H_{\text{Al,Li}} \) is the formation enthalpy of stoichiometric Al3Li, \( H_d \) is the formation enthalpy of a point defect. \( x_d \) is the fraction of defect \( d \) with \( d = \text{Vac}_{\text{Al}}, \text{Vac}_{\text{Li}}, \text{Al}_{\text{Li}}, \text{Al}_{\text{Al}}, \text{Li}_{\text{Li}} \), and \( \text{X}_{\text{X}} \), where X denotes the ternary alloy element and Vac denotes a vacancy, here \( x_d = 1/108 \) for the antisites and the ternary alloying elements and \( x_d = 1/107 \) for the vacancies. The formation enthalpy of a point defect type \( d \) in stoichiometric L12-Al3Li can be obtained by using \([34–36]\)

\[
H_d = \frac{\partial \Delta H}{\partial x_d} \approx \frac{\Delta H_d - \Delta H_{\text{Al, Li}}}{x_d}.
\]

The formation enthalpy of a Al_{1-x-b} Li_{x} X sub-lattice is the energy difference between the alloy and the reference state components of the alloy, which can be calculated per atom from the following equation:

\[
\Delta H (\text{Al}_{1-x-b} \text{ Li}_{x} \text{ X}) = E (\text{Al}_{1-x-b} \text{ Li}_{x} \text{ X}) - (1 - a - b) E (\text{Al}) - a E (\text{Li}) - b E (\text{X}),
\]

where \( E (\text{Al}), E (\text{Li}), E (\text{X}), \) and \( E (\text{Al}_{1-x-b} \text{ Li}_{x} \text{ X}) \) are the calculated total energies (per atom) of the pure elements, and the corresponding alloy. Here a and b are the mole fractions of Li and X in the Al_{1-x-b} Li_{x} X alloy respectively. In this paper, a negative formation enthalpy indicates the formation tendency of a alloy.

2.3. Site occupancy of solute in L12-Al3Li

When an impurity is introduced into the ordered L12-Al3Li alloy, it exhibits a site preference behaviour on two non-equivalent site, i.e., Al sublattice and Li sublattice. For the determination of the site substitution behaviour of solute in L12-Al3Li, we use the follow formalisms which have been introduced in \([35, 36]\) for evaluating the 0 K site preference of alloying elements in L12-Al3Li:

(i) \( H_{X_a} - H_{X_b} = H_{Al_b} > 0 \) (equivalently \( H_{X_b} - H_{X_a} + H_{Li_a} > H_{Al_b} + H_{Li_b} \)) : X always has a strong Al site preference in Al-rich, Li-rich and stoichiometric L12-Al3Li alloys;

(ii) \( H_{X_a} - H_{X_b} + H_{Li_b} < 0 \) X always has a strong Li site preference in Al-rich, Li-rich and stoichiometric L12-Al3Li alloys;

(iii) \( H_{X_b} - H_{X_a} < 0 \) and \( H_{X_b} - H_{X_a} + H_{Li_b} > 0 \) : X prefers the Al sublattice in Li-rich and the Li sublattice in Al-rich L12 Al3Li, and shows no site preference in stoichiometric L12-Al3Li.

The aforementioned formation enthalpies of the point defects can be obtained by equation (3) and supercell calculations as shown in the figure 1. The calculations have been done in the dilute limit of defect by supercells, thereby the solute-solute interaction can be neglected in this study.

3. Results

3.1. Ground state properties of Al3Li

Using the experimental crystallographic data of the Al, Li, and L12-Al3Li phases from Ref. \([37]\) as the initial configurations, the lattice parameters as well as the bulk moduli of the fcc-Al, bcc-Li, and L12-Al3Li phases are optimized via the Birch-Murnaghan equation of state \([38]\). As shown in table 1, the predicted lattice constants of fcc-Al, bcc-Li, and L12-Al3Li phases at their ground states are listed with comparison of available theoretical and experimental results \([39–41]\). Obviously, all of the calculated lattice parameters are in good agreement with the previous literature results, which demonstrate that the computational methodologies and parameter choices utilized in our current work are suitable and reliable. Therefore, the equilibrium lattice constants obtained from equation of state will be used for the site preference behaviour study later.

3.2. Formation of intrinsic defects in L12-Al3Li

In the ordered L12 Al3Li phase, there exist following elementary intrinsic defects: Al and Li antisites at the sublattices (Al Li and Li Al), Al-Li exchange anti-site defect, and vacancies (Vac Al and Vac Li) at the Li and Al
Formations of L12 Al3LiX alloy

Our calculations for Al3LiX alloy, namely, sublattices. Their energies of formation have been calculated using a 108-atom supercell at the same time, one notices that the formation enthalpy of AlLi is slightly higher than that of LiAl, indicating that the formation enthalpy is predicted for all solute-doped Al3LiX alloys, indicating the stability of those structures.

Generally, a lower value of the formation enthalpy means the material is more stable. We have also compared our calculated formation enthalpies to literature data [26], showing a good agreement in the formation enthalpies of X locating at Al site or Li site. However, one also notices the large discrepancies between ours and the literature results. For example, our calculated formation enthalpy of a Sc atoms locating at Li site of L12-Al3Li is −0.111 eV, while the literature result [26] is −0.180 eV, namely, there is a discrepancy of 0.07 eV/atom. The reason for the discrepancy is that the formation enthalpies in [26] are obtained by a 16-atom [1 × 1 × 4] L12-Al3Li supercell, meaning that there is a concentration-dependent formation enthalpy discrepancy between our calculations for Al3LiX alloy, namely, xX = 1/108 in this study and xX = 1/16 in the [26] make this discrepancy. Moreover, the interactions between defects in neighboring [1 × 1 × 4] L12-Al3Li supercells may induce such energy discrepancies [43].

### Table 1. The calculated lattice constant (a0) and bulk modulus (B) with literature comparison for Al, Li, and Al3Li.

| Structure | a0 (Å) | B (GPa) | Method | Reference |
|-----------|--------|---------|--------|-----------|
| fcc-Al    | 4.04   | 76.4    | VASP-PAW | This work |
|           | 4.05   | −       | Expt. (x-ray) | [39] |
|           | 4.04   | 79.3    | VASP-PAW | [40] |
|           | 4.05   | 78.0    | CASTEP-PAW | [41] |
| bcc-Li    | 3.44   | 13.4    | VASP-PAW | This work |
|           | 3.51   | −       | Expt. (x-ray) | [39] |
|           | 3.43   | 11.8    | VASP-PAW | [40] |
|           | 3.51   | 15.0    | CASTEP-PAW | [41] |
| L12-Al3Li | 4.03   | 62.5    | VASP-PAW | This work |
|           | 4.03   | 62.9    | VASP-PAW | [40] |
|           | 4.01   | 63.0    | CASTEP-PAW | [41] |

### Table 2. First-principles calculated formation enthalpies (ΔH, eV/atom) of the alloy and formation enthalpies (Hd, eV/defect) of the intrinsic point defects in L12-Al3Li.

| Defect | None | AlLi | LiAl | VacLi | VacAl | Al ↔ Li |
|--------|------|------|------|-------|-------|---------|
| ΔH     | −0.0998 | −0.0944 | −0.1007 | −0.0921 | −0.0924 | −0.0955 |
| Hd     | −0.583 | −0.088 | 0.823 | 0.791 | 0.472 |

### 3.3. Formation of L12 Al3LiX alloy

The predicted formation enthalpies of Al3LiX (X = transition metals) are listed in table 3. A negative formation enthalpy is predicted for all solute-doped Al3LiX alloys, indicating the stability of those structures. Generally, a lower value of the formation enthalpy means the material is more stable. We have also compared our calculated formation enthalpies to literature data [26], which shows a good agreement in the formation enthalpies of X locating at Al site or Li site. However, one also notices the large discrepancies between ours and the literature results. For example, our calculated formation enthalpy of a Sc atoms locating at Li site of L12-Al3Li is −0.111 eV, while the literature result [26] is −0.180 eV, namely, there is a discrepancy of 0.07 eV/atom. The reason for the discrepancy is that the formation enthalpies in [26] are obtained by a 16-atom [1 × 1 × 4] L12-Al3Li supercell, meaning that there is a concentration-dependent formation enthalpy discrepancy between our calculations for Al3LiX alloy, namely, xX = 1/108 in this study and xX = 1/16 in the [26] make this discrepancy. Moreover, the interactions between defects in neighboring [1 × 1 × 4] L12-Al3Li may induce such energy discrepancies [43].
3.4. Site preferences of transition metals in L12 Al3Li phase

When a substitutional impurity is introduced into an ordered alloy, it has a certain site preference. The site preference of the impurity plays a key role of determining thermodynamic and mechanical properties of the ordered phase. It can be seen that a single parameter \( E_{X \rightarrow Al} \) is already sufficient in completely describing the \( T = 0 \) K site preference behavior of any ternary element in L12 Al3Li. Here the parameter \( E_{X \rightarrow Al} \) can be seen as the transfer energy \( [44, 45] \) and it characterizes the energy required to transfer an X atom from the Al sublattice to the Li sublattice while the Li atom goes to the Al sublattice where the X atom occupied, the reaction can be written via:

\[
X_{Al} + Li_{Li} \rightarrow X_{Li} + Li_{Al},
\]

and its absolute value is independent of the choice of reference states for the pure elements. In this study, we obtained \( E_{X \rightarrow Al} \) by using equations (2) and 3.

As shown in figure 2, the site preference behavior are following: Cu, Zn, Pd, Ag, Cd, Pt, and Au fall into type (i), Co, Ni, Rh, Ir fall into type (ii), and other elements Sc-Fe, Y-Ru, and La-Os fall into type (iii). A general trend can be seen that the site preference for the Al sublattice increases as the atomic number increases along a series. Such a trend is obeyed by all 3d, 4d and 5d elements. Our site preference results are also in good agreement with the previous DFT study from Ref. [26], however, according to our calculated transfer energy, Co shows no site preference in stoichiometric Al3Li, while Co has a Al-sublattice preference in the study of Ref. [26] by formation enthalpies of alloys. It has been show that the formation enthalpies \( \Delta H_{X_{Al}} \) and \( \Delta H_{X_{Li}} \) are insufficient to
Table 3. First-principles calculated formation enthalpy (eV/atom) of the Al3LiX alloy with literature comparison [26].

| Element | This $\Delta H_{X\text{Al}}$ | This $\Delta H_{X\text{Li}}$ | Ref. [26] $\Delta H_{X\text{Al}}$ | Ref. [26] $\Delta H_{X\text{Li}}$ |
|---------|--------------------------|---------------------------|----------------------------|--------------------------|
| Sc      | -0.101                   | -0.111                    | -0.127                     | -0.180                   |
| Ti      | -0.098                   | -0.110                    | -0.108                     | -0.169                   |
| V       | -0.093                   | -0.104                    |                            |                          |
| Cr      | -0.090                   | -0.098                    |                            |                          |
| Mn      | -0.094                   | -0.099                    |                            |                          |
| Fe      | -0.098                   | -0.100                    |                            |                          |
| Co      | -0.103                   | -0.101                    | -0.152                     | -0.140                   |
| Ni      | -0.106                   | -0.102                    |                            |                          |
| Cu      | -0.102                   | -0.096                    | -0.111                     | -0.075                   |
| Zn      | -0.101                   | -0.093                    | -0.098                     | -0.057                   |
| Y       | -0.097                   | -0.107                    |                            |                          |
| Zr      | -0.099                   | -0.113                    | -0.118                     | -0.191                   |
| Nb      | -0.095                   | -0.109                    | -0.094                     | -0.150                   |
| Mo      | -0.095                   | -0.106                    | -0.075                     | -0.107                   |
| Tc      | -0.102                   | -0.108                    |                            |                          |
| Ru      | -0.109                   | -0.110                    |                            |                          |
| Rh      | -0.118                   | -0.114                    |                            |                          |
| Pd      | -0.116                   | -0.110                    |                            |                          |
| Ag      | -0.103                   | -0.094                    |                            |                          |
| Cd      | -0.098                   | -0.089                    |                            |                          |
| La      | -0.091                   | -0.098                    |                            |                          |
| Hf      | -0.096                   | -0.110                    |                            |                          |
| Ta      | -0.092                   | -0.106                    |                            |                          |
| W       | -0.090                   | -0.101                    |                            |                          |
| Re      | -0.098                   | -0.104                    |                            |                          |
| Os      | -0.106                   | -0.106                    |                            |                          |
| Ir      | -0.117                   | -0.112                    |                            |                          |
| Pt      | -0.121                   | -0.112                    |                            |                          |
| Au      | -0.111                   | -0.100                    |                            |                          |
| Hg      | -0.100                   | -0.087                    |                            |                          |

determine the site preference of ternary alloying elements, which is also determined by the formation enthalpies of the intrinsic point defects (VacAl, VacLi, LiAl, AlLi) in binary Li3AlLi alloys [35, 46].

We have also shown the transfer energy as a function of atomic radius of elements in figure 3. It is noted that a general trend that the energy $E_{X\text{Li}}^{\text{X\text{Al}}} \rightarrow \text{Li}$ changes with atomic radius. The elements which have smaller atomic radius than Al are always not preferential to occupy Al-sublattice, however, Zn, Cu, Pt, and Pd do not fall into this behaviour. At the same time, the elements which have larger atomic radius than Li show a site preference on Li sublattice. It is known that the Al and Li sites have different atomic sizes in the metallic lattice, i.e., the atomic radius values are 1.43 Å and 1.52 Å for Al and Li respectively [37]. The Li sites are surrounded by Al atoms and which are smaller than the Li atoms, meaning Li sublattices have larger effective volume than Al sublattices. A similar study of the correlation between solute site occupancy and solute atomic radius has been done in the case of L12-Ni3X (X = Ti, Al, Nb) by the DFT calculations in the Ref. [45], where they concluded that the lowest transfer energy appeared for the solute which had the similar or close atomic radius to the replaced atom. In our study, as shown in figure 3, the lowest $E_{X\text{Li}}^{\text{X\text{Al}}} \rightarrow \text{Li}$ also appears at the values which is at the mid-range of Al and Li atomic radius.

Furthermore, we have also studied the interaction of a solute between its nearest-neighbor (NN) atoms. It is shown in figure 1(a) that the L12-AlLi lattice is a fcc-base structure, meaning each sublattice has 12 1NN atoms of the fcc lattice (see figure 1(a)). The distance between a pair of 1NN atoms is $\sqrt{2} \cdot a_0$ accordind to the symmetrical property of the fcc lattice. However, as we have mentioned previously that the ordered L12 structure of Al3Li consists of two sublattices, i.e., the Al-sublattice (the face centers) and the Li-sublattice (cube corner), as shown in figure 1(a). An Li-sublattice has 12 1NN Al atoms, while a Al-sublattice has 4 1NN Li atoms and 8 1NN Al atoms. Therefore, adding of an alloying element either at Al or Li sublattice produces different effects on the lattice changes of Al3Li. If the change of the lattice spacing is known for different site occupancies, the corresponding experimental data may indicate at which sublattice the alloying element occupies.

We have plotted the 1NN host atom displacements surrounding an impurity in Al3Li as a function of the impurity atomic radius in figure 4. The 1NN host atom displacements have been calculated as the difference between the average of displaced 1NN distances and the ideal 1NN distance. Here $X_{\text{Al}}$ and $X_{\text{Li}}$, represent the
impurities located at Al and Li sublattices, respectively. A general trend can be seen from Figure 4 that the 1NN displacement surrounding an impurity increases as the atomic radius increases along a series. The 1NN displacement is negative when the atomic radius of impurity is smaller than that of host atom (Al or Li), meaning that adding alloying elements is a potential way for controlling and designing the lattice mismatch between the precipitate Al3Li and matrix Al, which could be considered to increase the mechanical properties, e.g., the strength of the Al-Al3Li interface in alloys [4, 47].

4. Conclusion

The density functional theory total energy calculations have been done for studying the site occupancy behaviour of transition metal in L12-Al3Li phase. Our calculated equilibrium lattice parameters and bulk moduli of L12-Al3Li, fcc-Al, and bcc-Li are in good agreement with the available literature data. The intrinsic point defect formation energy and Al3LiX alloy formation energy have been calculated and it is found that a Li antisite defect is preferential to form in L12-Al3Li. The site occupancies of transition metals have been identified by showing a d-valence occupation-dependent trend that early transition metals have a Li sublattice preference and late transition metals have Al sublattice preference. We have also analysed the solute atomic volume effect on the solute site preference and local strain in the L12-Al3Li and shown that smaller solute are not preferential to occupy at Al sublattice and the larger atoms contribute to a significant expansion of the local lattice both on Al sublattice and Li sublattices.

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