Study on the geometric structure and stability of AlnMgn (n = 2–12) clusters using density functional theory

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Abstract
In this study, density functional theory was used to investigate the AlnMgn (n = 2–12) clusters on a microscopic scale. The stable structure of clusters was determined and used as the interaction energies parameter in Wilson equation to deepen the activity prediction of the Wilson equation. The properties of Mg2 and Al2 dimers calculated by using ab initio molecular dynamics were compared with experimental data to verify the reliability of the method. By characterizing the cluster structure, the average binding energy, fragmentation energy, second–order energy difference, vertical ionization potential, vertical electron affinity, chemical hardness, HOMO–LUMO gaps, and distribution of the Al–Mg clusters were determined. With an increase in the cluster size, the symmetry of the Al–Mg clusters decreased, and Al atoms gradually gathered at the center of the cluster, whereas Mg atoms were distributed on the surface of the cluster, which tended to combine with Al atoms. Clusters with even numbers were generally more stable than the adjacent odd–numbered clusters. In particular, the thermodynamic stability of the Al4Mg4 cluster was prominent and was considered as an ideal object to calculate the interaction energies in the activity prediction of Al–Mg alloys.

1. Introduction

With the improvement in production capacity and technical level, Al–Mg alloys have been widely used in aerospace, military industry, and civil fields owing to their excellent properties such as high specific strength, small elastic modulus and good electromagnetic interference resistance. However, the generation of Al–Mg scrap alloys has stimulated considerable interest among researchers. At present, vacuum distillation is one of the effective methods for separating and recovering Al–Mg scrap alloys. Based on thermodynamic research, the effect of separation and recovery is roughly predicted by analyzing the equilibrium vapor pressure of alloying elements [1]. Previous studies have shown that vapor–liquid equilibrium (VLE) composition is also an important theoretical basis for the design of vacuum distillation separation, in which activity is an important thermodynamic parameter. The Wilson equation is used to predict the activity data of alloy components, and reliable data of VLE phase diagrams are obtained to achieve quantitative prediction of the vapor–liquid distribution of alloy components [2, 3].

It is well known that excellent properties of metal clusters are closely related to their atomic structures that can reflect the stability of molten alloys from a microscopic perspective [4–6]. By studying the stable structure of the clusters, the interaction energy prediction of the activity coefficient can be supported by the Wilson equation, and the accuracy of the activity prediction can be further improved using VLE phase diagrams [7, 8].
For accurate prediction of the activity from a microscopic perspective, Yang et al.\(^2\) calculated the interaction energies between pairs of atoms using \textit{ab initio} molecular dynamics (AIMD) and predicted the activity of binary lead–based alloy systems (Pb–Ag, Pb–Cu, and Pb–Sn) by combining Wilson’s equation. Chen et al.\(^10\) used the same method to predict VLE phase diagrams for Pb–Pd and Pb–Pt alloys. The calculated and experimental results were in good agreement. Shi et al.\(^11\) studied the structure, relative stability, and electronic properties of Al\(_n\)L\(_m\) (\(n = 2–12\)) clusters based on first–principles calculations using density functional theory (DFT), and the results showed that a stable Al\(_{12}\)Li\(_3\) cluster is ideal for calculating the Wilson parameters of Al–Li alloys. From the perspective of atomic structure, the binding law between Al and Mg atoms was analyzed, and stable Al\(_n\)Mg\(_m\) clusters that reflect the interaction between Al and Mg pairs of atoms were obtained, providing a reference for the calculation of the Wilson parameters of Al–Mg alloys and the study of their VLE phase diagrams.

In recent years, DFT, which is based on quantum mechanics to simulate relevant electrons, has been widely used in the theoretical study of clusters, owing to its outstanding advantages in accurate prediction of geometric structure and electronic properties\(^12\). Through a series of relevant calculations using DFT, a stable cluster structure can be obtained, and then the structural evolution of Al–Mg alloy systems can be revealed at the atomic level. In fact, the stability of a metal cluster is determined by its composition and the number of valence electrons\(^13, 14\). In the process of studying the cluster stability, it was found that some clusters with special valence electron numbers are more stable\(^15–20\). The electron spherical jellium model (SIM)\(^21\) and the phenomenological shell model (PSM) are used to describe the stability of the cluster structure when the number of valence electrons in the cluster is \(N (N = 8, 18, 20, 34, 40, 58...)\)\(^14, 22\). Chacko et al.\(^21\) calculated the lowest energy structure of the alkali metal Al\(_X\) (\(X = Li, Na, K, Be, Mg\)) cluster based on Born–Oppenheimer molecular dynamics (BOMD), and analyzed its electronic structure and eigenvalue spectrum to determine the validity of the SIM. The results showed that the Al\(_2\)Mg\(_4\) and Al\(_2\)Be\(_4\) clusters exhibit the same jellium model and form a closed shell structure of the 20–electron system. The SIM is considered to be effective with large HOMO–LUMO gaps (HLG) of the Al\(_2\)Mg\(_4\) cluster, as compared to the Al\(_2\)X\(_4\) (\(X = Li, Na, K\)) cluster. Using DFT, Varano et al.\(^23\) studied the properties of Al isomers doped with Mg in the Al\(_3\) cluster, and the results showed that the stability of the Al\(_{13}\) cluster was reduced by Mg atom mixing. Ouyang et al.\(^24\) calculated stable structures of the Al\(_n\) and Al\(_n\)-Mg\(_m\) (\(n = 2–17\)) clusters using DFT, indicating that the clusters have high stability when \(n\) is odd. In the research results of Osorio et al.\(^25\), electron counting rules and the PSM were used to analyze stable structures of the Al\(_n\)Mg\(_m\) (\(x, y = 1–4\)) clusters, and they indicated that the stability of Al\(_n\)Mg stems from the fact that Mg atoms provide electrons to the Al\(_{12}\) substructure and form a polar covalent structure, whereas the stability of the Al\(_2\)Mg\(_2\) and Al\(_2\)Mg\(_4\) clusters is determined by the closed shell structure in the PSM. Zhang et al.\(^26\) systematically studied 55–atom clusters of Al–Mg alloys based on DFT and believed that Al–rich clusters have higher thermodynamic stability and better electronic effects. Based on the genetic algorithm (GA) and DFT, Wang et al.\(^27\) discussed the structure and stability of the Al\(_n\)-Mg\(_m\) (\(n = 4–8, m = 1–3\)) clusters and found that Al–Mg clusters are the same as pure metal clusters of the electronic shell structure. The stability of the cluster depends on the Mg/Al ratio, and a low Mg/Al ratio is superior, which stems from the stronger interaction of the Al–Al bond energy than those of the Al–Mg and Mg–Mg bond energies. Although a large number of Al–Mg clusters have been studied, the small size of equal proportions Al–Mg clusters needs to be further discussed.

Herein, DFT was used to study the stability and electronic properties of the Al\(_n\)Mg\(_m\) (\(n = 2–12\)) clusters, and the binding law of Al–Mg clusters was clarified from the perspective of atomic binding. The stable structure of alloy clusters is determined to provide a theoretical basis for the interaction energies in Wilson equation.

\section{2. Calculation method}

All DFT calculations were performed using the DMol\(^3\) module in the Material Studio software\(^28–30\). The initial structure of Al\(_n\)-Mg\(_m\) cluster was established by adding atoms to the ground state structure of Al\(_n\)-Mg\(_m\) cluster. Then AIMD was used to search and optimize the structure of Al\(_n\)-Mg\(_m\) cluster. Finally, based on DFT calculation, the energy calculation of the optimized structure was carried out to determine the ground state structure of Al\(_n\)-Mg\(_m\) cluster. During the dynamics simulation, the system temperature was set to 300 K, and the total simulation time was set to 100 ps with a time step of 1 fs. The exchange and correlation effects were treated with GGA\(^31–PBE\(^32–34\) as the exchange–correlation functional. The DNP (Double Numerical plus polarization)\(^32\) was adopted as the basis to ensure the calculation accuracy. The convergence criterion of the self–consistent field calculation for the total energy was 10\(^–6\) Ha. For better convergence, a value of 0.005 Ha was considered for smearing. In terms of geometric optimization, the values of the maximum displacement tolerance, energy tolerance, and maximum force tolerance were set to 0.005 \AA, 10\(^–3\) Ha/\AA, and 0.002 Ha/\AA, respectively. Considering the accuracy of the calculation results in this study, the bond lengths, binding energies, and frequencies of Mg\(_2\) and Al\(_2\) were calculated and compared with the relevant experimental data to ensure the reliability of the calculation method above. The relevant values are listed in table 1. As can be seen, the
calculation data are consistent with the experimental data. By comparing with the average binding energies of the Al$_2$Mg$_2$ and Al$_4$Mg$_4$ clusters in a previous report [25], the reliability of the calculation method in this study was further confirmed.

3. Results and discussion

3.1. Cluster geometry

AIMD was used to calculate the structural energy of the Al$_n$Mg$_n$ clusters, and the lowest energy structure was obtained, as illustrated in Figure 1. The Al$_2$Mg$_2$ cluster is described as a symmetric tetrahedral structure with the symmetry group of D$_{2d}$, which is consistent with the Al$_2$Mg$_2$ structure calculated [25] using a gradient-embedded genetic algorithm (GEGA). The original structure of Al$_2$Mg$_2$ is retained in the Al$_3$Mg$_3$ cluster, on which one Mg atom and one Al atom are added to form an octahedral structure with Cs symmetry, which is similar to the structure of the Mg$_6$ cluster [35]. Al atoms are concentrated at the center of the Al$_4$Mg$_4$ cluster, and Mg atoms are distributed at both ends of the cluster, forming an alternating chain structure of fragments with D$_{2d}$ symmetry. When $n = 5$, the cluster symmetry is still significant, being C$_{2v}$, where the Al atom group is the center and the Al and Mg atoms are regularly distributed alternately, forming a twisted double-layer hexagonal ring structure. As the number of atoms in the cluster is increased, the symmetry of the cluster decreases to C$_1$. According to the Jahn–Teller distortion theorem [36], the degeneracy of the Fermi energy level is eliminated in a large-size distorted structure, reducing its overall energy and the symmetry of the cluster structure. When $n = 6$–8, the clusters exhibit a compact spherical structure. As the size is increased further, the Al clusters tend to gather at the center. The spherical structure of the clusters is not satisfied when $n = 9$–11, growing into a long

### Table 1. Calculated and experimental data of the bond lengths (R), binding energies (E$_b$), and frequencies (ω) of Al$_2$ and Mg$_2$.

| Names | Methods | R (Å)  | $E_b$ (eV) | ω (cm$^{-1}$) |
|-------|---------|--------|-----------|--------------|
| Mg$_2$ | Expt. [24] | 3.89   | 0.012     | 51.12        |
|       | GGA–PBE | 3.899  | 0.013     | 48.39        |
| Al$_2$ | Expt. [11] | 2.701  | 1.34 ± 0.06 | 284.2        |
|       | GGA–PBE | 2.679  | 1.44993   | 302.97       |

![Figure 1. Lowest energy structure of the Al$_n$Mg$_n$ ($n = 2$–12) clusters (the corresponding symmetries are in the parentheses).](image)
cage structure. The Al_{12}Mg_{12} cluster is combined in two structures similar to the Al_{6}Mg_{6} cluster, maintaining the approximate structure of the Al_{11}Mg_{11} cluster. At the same time, Mg atoms tend to bond to Al atoms on the cluster surface, and the growth pattern is consistent with that of the Al\textsuperscript{n}Mg\textsuperscript{n} (n = 3–20) clusters of mixed magnesium atoms studied by Xing et al\cite{37}. By referring to the segregation energy of Al–Mg atoms\cite{26}, the distribution trend of Al–Mg atoms is similar to that in this study. Al atoms occupy the central position because of their positive segregation energy, and Mg atoms with negative segregation energy are more inclined to segregate to the surface position.

3.2. Stability of clusters

The stability of the clusters was calculated according to the lowest energy structure. Based on the structural evolution of the Al\textsuperscript{n}Mg\textsuperscript{n} (n = 2–12) clusters, the average binding energy (E\textsubscript{b}), defined by equation (1), was further studied.

\[
E_b = \frac{nE(\text{Al}) + nE(\text{Mg}) - E(\text{Al}_n\text{Mg}_n)}{2n}
\]  
(1)

Where E(Al), E(Mg), and E(Al\textsubscript{n}Mg\textsubscript{n}) are the energies of a single Al atom, a Mg atom, and an Al\textsubscript{n}Mg\textsubscript{n} cluster, respectively. The strength of the binding force between the atoms of the Al–Mg cluster is shown in equation (1), indicating the thermodynamic stability of the cluster. As shown in figure 2, the E\textsubscript{b} of the Al–Mg clusters shows a monotonously increasing trend with an increase in the cluster size, indicating that the stability of the clusters is continuously enhanced. In the range of n = 2–8, the E\textsubscript{b} increases significantly and then slowly, which is the same as the variation trend of the E\textsubscript{b} of Al\textsubscript{n} and Al\textsubscript{n}Mg (n = 3–20) clusters calculated by Xing et al\cite{37}, using.
Particle Swarm Optimization and density functional theory calculations. From the perspective of the surface energy of the cluster [38], at the initial increase stage with the number of atoms, the surface energy of atoms accounts for a small proportion of the total energy of cluster atoms, resulting in the enhanced stability of the cluster. However, the proportion of the surface energy changes smoothly as the cluster size continues to increase, resulting in a slow increase in the subsequent change in the $E_b$. The $E_b$ of the Al$_4$Mg$_4$ and Al$_8$Mg$_8$ clusters increases significantly, indicating that the cluster structure is more stable than the neighboring structure, and the stability of the Al$_4$Mg$_4$ clusters is due to their good symmetry.

In order to illustrate the thermodynamic stability of the clusters further, the relative stability of the Al$_n$Mg$_n$ and adjacent clusters was characterized by the fragmentation energy ($\Delta E$) defined by equation (2):

$$\Delta E(Al_nMg_n) = E(Al_{n-1}Mg_{n-1}) + E(Al_1Mg_1) - E(AlMg)$$  (2)

Where $E(Al_{n-1}Mg_{n-1})$, $E(Al_1Mg_1)$, and $E(Al_nMg_n)$ are the lowest energy values of the Al$_{n-1}$Mg$_{n-1}$, AlMg, and Al$_n$Mg$_n$ clusters, respectively. The required energy is reflected by the value of $\Delta E$ when Al$_n$Mg$_n$ is split into the AlMg and Al$_{n-1}$Mg$_{n-1}$ clusters. Stable clusters stem from high $\Delta E$. As can be seen from figure 3, when $n = 4, 8$, two prominent peaks appear in the $\Delta E$ of the Al$_n$Mg$_n$ clusters, indicating that the corresponding cluster structure requires higher energy than the neighboring structure when cracking, so it is more stable. In a previous report [25], the PSM was used to predict that the stable structure of Al$_4$Mg$_4$ is determined by the closed shell, and the structural stability of the Al$_8$Mg$_8$ cluster is attributed to its typical magic valence electron structure (its electron number is 40, which has the characteristics of magic number).

In relevant studies [11, 39], the second–order energy difference ($\Delta_2E$) was shown to be another important parameter for analyzing the relative stability of cluster structures. The $\Delta_2E$ of the Al$_n$Mg$_n$ ($n = 2–12$) clusters is shown in figure 4, and its definition is equation (3):

$$\Delta_2E(Al_nMg_n) = E(Al_{n-2}Mg_{n-2}) + E(Al_2Mg_2) - E(AlMg)$$  (3)

The value of $\Delta_2E$ reflects the required energy change when the Al$_n$Mg$_n$ cluster is transformed into the Al$_{n-2}$Mg$_{n-2}$ and Al$_2$Mg$_2$ clusters, respectively. Large $\Delta_2E$ leads to the weak ability of the Al$_n$Mg$_n$ cluster to transform into an adjacent structure, which has a stable cluster. The $\Delta_2E$ of the Al$_n$Mg$_n$ clusters can exhibit obvious odd–even oscillations, as shown in figure 4. Except for $n = 10$, the $\Delta_2E$ of the even–numbered clusters is higher than that of the adjacent odd–numbered clusters, indicating that the even–numbered clusters have better thermal stability than the adjacent odd–numbered clusters. The local peak occurs when $n = 4$ and 8, indicating that the Al$_4$Mg$_4$ and Al$_8$Mg$_8$ clusters have better $\Delta_2E$ and stability than the adjacent clusters and that the Al$_4$Mg$_4$ cluster has higher stability.

### 3.3. Electronic properties of clusters

In the cluster study, higher vertical ionization potential (VIP) of the neutral cluster requires more energy to lose electrons into the cations. Correspondingly, lower vertical electron affinity (VEA) of the neutral cluster requires more energy to acquire electrons into anions, so the neutral cluster is more stable [40]. The definitions of the VIP and VEA are shown in equations (4) and (5):

$$VIP = E(Al_nMg_n^+) - E(Al_nMg_n)$$  (4)
In equations (4) and (5), $E(\text{Al}_n\text{Mg}_m^+)$ and $E(\text{Al}_n\text{Mg}_m^-)$ represent the energies with positive charge and negative charge in the ground state structure of $\text{Al}_n\text{Mg}_m$ cluster, respectively. It should be pointed out that the neutral Al-Mg clusters have the same or similar atomic arrangement with the corresponding charged ion clusters [37, 41]. The corresponding electronic properties and change rule of the cluster size are shown in figure 5. The VIP of the Al–Mg cluster decreases, whereas the VEA changes in the opposite trend with the increase in the cluster size, and the odd–even oscillation phenomenon still exists. Owing to the electron–pairing effect [42], the HOMO orbital layer with an even number of valence electron clusters is occupied by two electrons, which leads to clusters with closed electronic shells and to remarkable stability. However, the HOMO orbital layer with an odd number of valence electron clusters makes it easier to obtain an electron by the electron–pairing effect, which leads to clusters with an open shell. In other words, a neutral cluster with an even number of valence electrons has a significantly larger VIP than a neutral cluster with an odd number of valence electrons, and the VEA of the cluster follows the opposite trend. The odd–even oscillation behavior of the clusters indicates that the clusters with an even number of valence electrons will have higher VIP, lower VEA, and higher chemical stability. In terms of the tendency of the $\text{Al}_n\text{Mg}_m$ clusters to become charged ion clusters, the tendency of neutral clusters to become cation clusters decreases with an increase in the cluster size, whereas the tendency to become an anion increases. Similarly, the peaks at $n = 4$ and $8$ indicate that the transformation of the neutral clusters into charged ion clusters is required for a large amount of energy, which is difficult, so they have high chemical stability.

$$\text{VEA} = E(\text{Al}_n\text{Mg}_m^+) - E(\text{Al}_n\text{Mg}_m^-)$$

(5)
Further, the stability of the clusters can be characterized by the chemical hardness ($\eta$), which can be defined by equation (6):

$$\eta = \frac{\text{VIP} - \text{VEA}}{2}$$  \hspace{1cm} (6)

The variation rule of $\eta$ with the cluster size is shown in figure 6. Pearson et al [43] proposed the maximum hardness principle (MHP) based on DFT, indicating that a molecular system with equilibrium stability has the maximum chemical hardness. According to the MHP, the Al$_4$Mg$_4$ cluster is the most stable cluster in this series, and the Al$_8$Mg$_8$ cluster is also stable.

The HOMO–LUMO gaps (HLG) is considered as an index to evaluate the cluster stability, reflecting the ability of electrons to transition from occupied to unoccupied orbitals. The higher the energy gap, the more stable the cluster structure is. The relationship between the HLG changes and the cluster size is shown in figure 7. It can be seen that the sharply increased HLG at $n = 4$ and 8 reach 0.05697 eV and 0.05766 eV, respectively, indicating that the thermodynamic stability of the Al$_4$Mg$_4$ and Al$_8$Mg$_8$ clusters is better than that of their neighboring clusters, which is consistent with the predicted results of $\Delta E_s$, $\Delta^2 E$, and electronic properties.

4. Conclusion

In this study, the AIMD calculation by DFT was used for systematically investigating the Al$_n$Mg$_n$ ($n = 2$–12) clusters. The aim is to determine the stable structure of the alloy clusters for the activity calculation of the interaction energy in Wilson equation. By analyzing the geometric structure, $E_b$, $\Delta E$, $\Delta^2 E$, and a series of laws of the electronic properties of the Al$_n$Mg$_n$ ($n = 2$–12) clusters, the following conclusions are drawn:

1. The stable structure of the Al$_n$Mg$_n$ ($n = 2$–12) clusters was obtained by reliable AIMD calculations, and the distribution law of the Al–Mg cluster was revealed. The symmetry of the cluster decreases with an increase in the cluster size; Al atoms gradually gather at the center of the cluster, and Mg atoms tend to combine with Al atoms and distribute on the surface of the cluster.

2. The $E_b$ and VIP of the clusters increase with the cluster size, and the change trend of the VEA is opposite, showing an obvious odd–even oscillation phenomenon, with local peaks appearing when $n = 4$ and 8.

3. Based on a comprehensive evaluation of the stability and electronic properties of the clusters, it is concluded that the thermodynamic stability of the Al$_4$Mg$_4$ cluster is the most outstanding and can be used as an ideal object for calculating the interaction energies parameters in the activity prediction of Al–Mg alloys.

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