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Analysis of aluminium-magnesium alloy clusters through genetic algorithm

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INTRODUCTION

Metal clusters have attracted a large scientific effort in the past few years due to their potential technological applications at the nanoscale. Mixed metal systems are known to have modified and often desirable properties relative to the pure phases of the individual metal, including improved corrosion resistance, low density and malleability.[1] Metal alloys composed of aluminum and magnesium have been widely recognized to be of importance in industry and aerospace manufacturing.[2]

In this work the structures and properties of Al-Mg alloys are investigated theoretically.

METHODS

A modified genetic algorithm (GA) was employed in the search for the potential energy minimum associated with Al_xMg_y (x+y<=35) clusters using an empirical Gupta many-body potential.[2] The GA initially generates a number of random clusters. The energy of these random clusters are minimized locally and ranked by their energies. The best clusters are then selected as parents and crossed to generate a new population. Mutation is also performed in 15% probability by rotating parts of the cluster by random amounts. Convergence is achieved when no further improvement is reached after a given number of generations. In order to avoid stagnation in a local minimum, the genetic algorithm here employed uses two different evolutionary operators: the operator history (OH) and the annihilator (A), which initiate new GA cycles in the search for different minima.[3, 4]

In order to have a quick way to evaluate the energy, we have employed the analytic Gupta potential. It is based on the second moment approach (SMA) for the tight-binding model, in which the total cohesion energy of a cluster with N atoms, V_{clust} (N), is written as a sum over the atomic contribution (E_i) which are composed of two terms, as:

$$E_i = E_i^{Band} + E_i^{rep} \quad (1)$$

$$E_i^{band} = -\left\{ \sum_{j \neq i}^{N} \xi^2 \exp\left[-2q\left(\frac{r_{ij}}{r^0} - 1 \right) \right] \right\}^{1/2} \quad (2)$$

$$E_i^{rep} = \sum_{j \neq i}^{N} A \exp\left[-p\left(\frac{r_{ij}}{r^0} - 1 \right) \right] \quad (3)$$

The term E_i^{band} is an expression for many bodies and composes the attractive part of the energy, taking into account the character of the metal band connection. Equation 3 is interpreted as a repulsive contribution to ensure the stability of the structure.

The parameters q, p, ξ and A were adjusted in the literature to pure clusters of Al and Mg, which we have employed in the present study. The parameters used are show in table 1. For the Al-Mg bonds, we used an average of such values. [5,6]

Table 1 - Parameters for the Gupta potential for the Al-Mg system.

	Al-Al	Mg-Mg	Al-Mg
r_0 (Å)	2.8637	3.21	3.03685
A (eV)	0.1221	0.198722	0.160411
ξ (eV)	1.316	0.349712	0.832856
p	8.612	15.977780	12.29489
q	2.516	1.684590	2.100295

RESULTS AND DISCUSSION

We have optimized the geometries of Al_xMg_y clusters for several compositions within fixed nuclearities of x+y= 5, 8, 10, 13, 15, 20, 25, 30 and 35 atoms.

Specifically, the 13 atom clusters are considered a magic number[2] (increased stability) since it may form a symmetric icosahedron. Indeed, the literature shows the Al_{13} cluster to be a perfect icosahedron[7], but Mg_{13} is not as symmetric[2].

The most stable structures obtained by our GA calculations for all possible compositions with 13 atom clusters are shown in Fig. 1. As seen, the icosahedral shape is lost for some of them Al_7Mg_6, Al_6Mg_7, Al_5Mg_8, Al_4Mg_9, Al_3Mg_{10} and Al_2Mg_{11}. It is possible to notice the pattern of central aluminum atoms to take pyramidal and bipyramidal geometries, while magnesium does not demonstrate a clear pattern

The structures predicted in this work also show a tendency of aluminum atoms to occupy the center of the alloy clusters, while magnesium is segregated at the surface, as seen in Fig. 1.

The calculation of excess energies (Eq. 4), can provide insights on the preference of alloy formation over the corresponding pure cluster, showed that with about 40% aluminum, the alloy clusters are best stabilized, as seen in the graphic of Fig. 2.

$$E_{excess}(x) = \frac{E_{clust}(x)}{N} - \frac{E^{Mg}{}_{Pure}(x)}{N} - \frac{E^{Al}{}_{pure}(x)}{N} \quad (4)$$

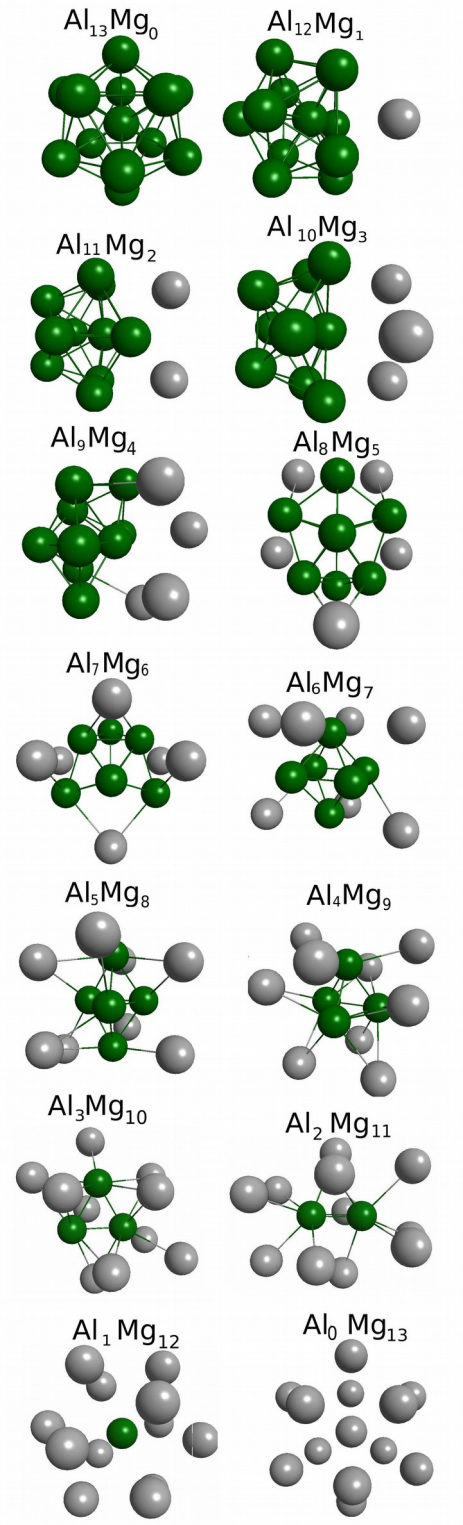

Figure 1. Alloy clusters of 13 atoms with different proportions of Al (green) and Mg (gray) .

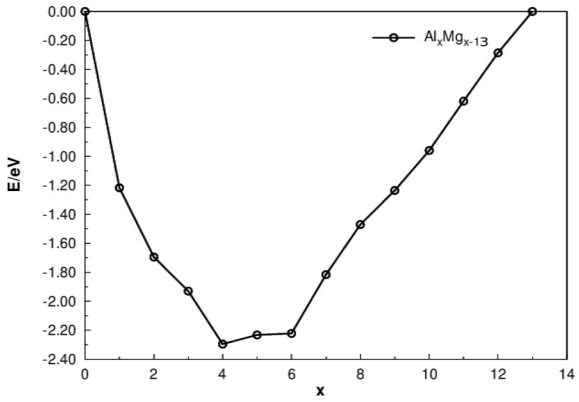

Figure 2. Graphic of excess of energy for cluster with 13 atoms

The calculation of second energy difference shows how much a cluster is stable compared to the neighbor. By calculating the second energy difference (Eq. 5), it is observed that Al_3Mg_{10} and Al_5Mg_8 are particularly stable among the non icosahedral structures, while in the icosahedral ones (more than 8 Al atoms), there is no large peak, showing that they have similar stabilities in Fig. 3.

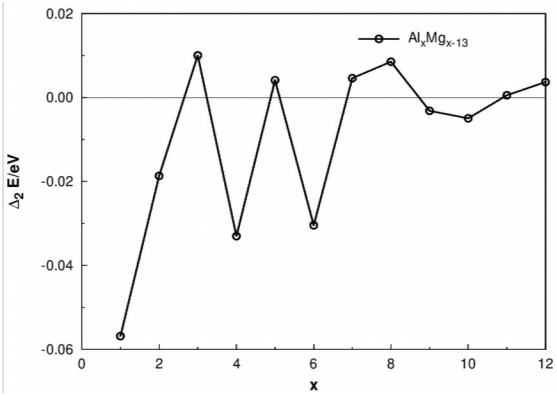

Figure. 3 – Graphic of second energy difference for cluster with 13 atoms

$$\Delta_2 E(x) = \frac{2E_{clust}(x)}{N} - \frac{E_{clust}(x-1)}{N} - \frac{E_{clust}(x+1)}{N} \quad (5)$$

For clusters with 25 atoms, as with others nuclearities, the observations made for 13 atoms are applicable. As a seen in Fig. 4.

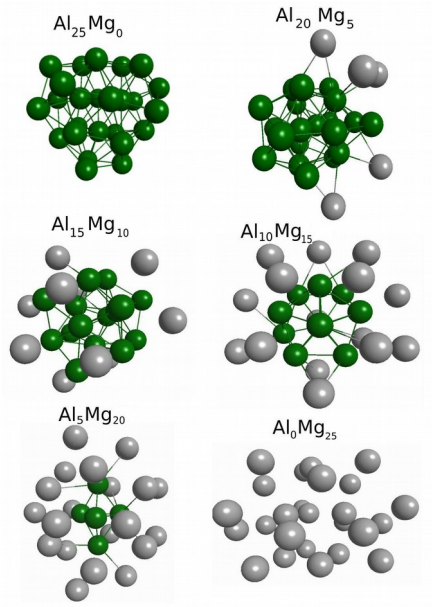

Figure 4. Alloy clusters of 25 atoms with different proportions of Al (green) and Mg (gray).

The central aluminum core tends to show the icosahedral shape whenever possible. Further calculations are being carried out, and confirmation of the structures employing *ab initio* methods is envisaged.

CONCLUSIONS

The modified genetic algorithm coupled with the empirical Gupta potential could predict the general trend of aluminum atoms occupying inner sites, with a ratio of 40%. Additional *ab initio* calculations will be carried out to confirm the results and to obtain new ones.

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