

Theoretical study of aluminium-magnesium alloy clusters through genetic algorithm

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Synopsis. The structures of alloy clusters of Al-Mg up to 55 atoms are explored using a genetic algorithm. The results are investigated using the excess energy concept.

In the past few years clusters have attracted a large scientific effort due to their potential applications at the nanoscience. Mixed metal clusters may also be tuned by composition and can have different properties compared to the pure clusters, including improved corrosion resistance and malleability[1]. Clusters with aluminum and magnesium in composition have been broadly recognized to be of importance in industry [2]. In this work the structures and properties of Al-Mg alloy clusters are investigated theoretically.

A modified genetic algorithm (GA) was employed in the search for the potential energy minimum associated with Al_xMg_y ($x+y \leq 55$) clusters using an empirical Gupta many-body potential, based on the second moment approach (SMA) for the tight-binding model.

Our results show a tendency of aluminum atoms to occupy the center of the alloy clusters, while magnesium is segregated at the surface. The central aluminum core tends to show the icosahedral shape whenever possible. 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[3], but Mg_{13} is not as symmetric. Also it is possible to notice the pattern of central aluminum atoms to take pyramidal and bipyramidal geometries for clusters with 15 to 55 atoms, while magnesium does not demonstrate a clear pattern.

The calculation of excess energies for the system $\text{Al}_x\text{Mg}_{(N-x)}$ (Eq. 1, 2 and 3), can provide insights on the preference of alloy formation over the corresponding pure cluster.

$$E_{\text{excess}} = E_{\text{cluster}} - E_{\alpha} - E_{\beta} \quad (1)$$

$$E_{\alpha} = (N - x) E_{\text{Pure}}^{\text{Mg}}(N) / N \quad (2)$$

$$E_{\beta} = x E_{\text{Pure}}^{\text{Al}}(N) / N \quad (3)$$

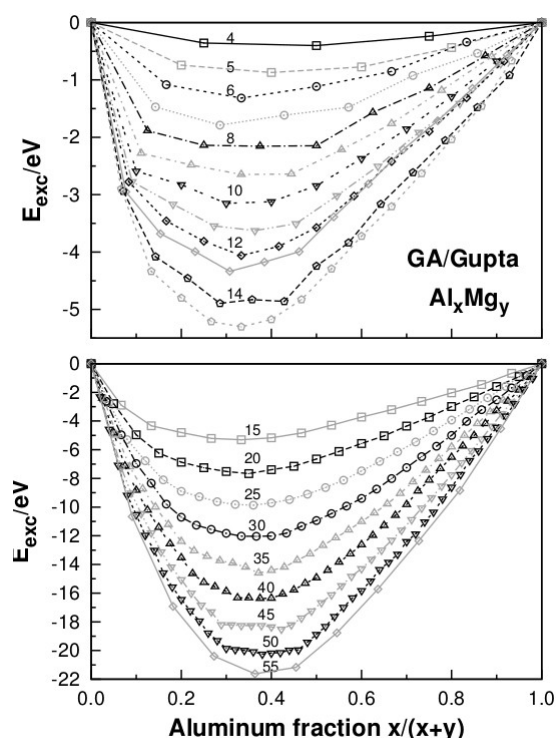


Figure 1. Excess energy as a function of composition. The labels give the total size N

As seen in the graphic of Fig. 1, clusters with ratio of 40% aluminum in composition are the best ones stabilized, according the excess of energy.

Calculations are being carried out for confirmation of the structures employing *ab initio* methods.

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References

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