Development of a Genetic Algorithm for Optimization of Nanoalloys

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Abstract. A genetic algorithm has been developed in order to find the global minimum of platinum-palladium nanoalloy clusters. The effect of biasing the initial population and predating specific clusters has been investigated.

1 Introduction

Clusters are aggregates ranging from a few to many millions of atoms [1]. The desire to fabricate materials with well defined, controllable properties and structures, on the nanometre scale, coupled with the flexibility afforded by intermetallic materials, has engendered considerable interest in bimetallic "nanoalloy" clusters. Our research generally involves using a genetic algorithm (GA) to find the arrangement of atoms corresponding to the global minimum (GM) on the potential energy hypersurface and our standard cluster optimization GA program has been described in a recent review [2].

Here we describe the improvement of our GA for studying nanoalloy clusters, such as those of palladium (Pd) and platinum (Pt) [3,4], using the Gupta many-body potential [5] to describe the Pd–Pd, Pd–Pt and Pt–Pt interactions. In our previous work, we found that certain GM are considerably more difficult to find than others – for example $Pt_{12}Pd_{12}$ [3,4], which was chosen as the test example for developing an improved algorithm. To this end, the standard GA program has been modified to include biasing of the initial population and the use of a "predator" operator to remove certain local minima from the population.

2 Results

In our original GA program, the initial population (gen_0) was chosen at random. In this study, we have used our chemical insight to bias the initial population: by replacing some members of the initial population with selected cluster geometries; and by inserting one or two geometrically favoured clusters into the initial random population. Firstly, particularly unfavorable clusters – the "reverse GM"

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where all Pt and Pd atoms are swapped relative to the GM structure and a cluster where the Pt and Pd atoms are segregated into separate halves of the cluster – were included in gen_0. Although contributing to the diversity of the population, as was expected, this "unfavourable biasing" leads to the GA being less successful at finding the GM than using a completely random gen_0. Secondly, a low energy, "favorable" cluster, was added to 19 randomly generated clusters in gen_0. This particular cluster, which has a potential energy of -105.9919 eV, is the fourth lowest isomer overall, hence it is the third lowest local minimum, LM3. The LM3 structure was selected to "seed" the initial population because it is found (in the generation immediately preceding that in which the GM is found) in 54% of successful GA runs. As the GA is elitist, the LM3 structure is maintained in the population from one genaration to the next. Including LM3 in gen_0, increased the rate of finding the global minimum from 22 to 43%.

We have previously introduced a "predator" operator for removing unwanted individuals or traits from the population [6]. An energy predator can be used to search for low energy minima other than the global minimum, or to enhance the efficiency of the GA by removing specific low energy non-global minima that the GA may be incorrectly converging towards. Since there is a high incidence of convergence of the GA on the sub-optimal structures LM1 and LM2, these structures can be regarded as "traps", which prevent the GA finding the GM. In order to test this hypothesis, predation of these clusters was carried out. With a random gen_0 and predation of LM2, the GM was found 31 times and with predation of LM1 28 times – an increase of 9% and 7%, respectively. With predation of both LM1 and LM2, the GM was found 43 times – an increase of 21%, however when both LM1 and LM2 were predated and LM3 was seeded into gen_0, the GM was found 65 times – an incease of 43%.

In conclusion, the results reported here, together with those from previous studies [2], show that the GA is a powerful technique for finding the GM for nanoalloys, as well as elemental clusters. Biasing the population and predating local minima has produced a more robust algorithm. This strategy can be used to study larger nanoalloy clusters.

References

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