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A Study of the Cu Clusters Using Gray-Coded Genetic Algorithms and Differential Evolution

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Energy minimization studies were carried out for a number of Cu clusters using binary and Gray-coded genetic algorithms along with real coded differential evolution, and their optimized ground state geometries are presented. The potential energy function is constructed using a two-body interaction methodology, involving both attractive and repulsive pair-potential terms. The results obtained through the evolutionary algorithms are compared against those obtained earlier using a Monte Carlo technique.

1. Introduction

Genetic algorithms (GAs) tend to mimic several biological processes in the realm of function optimization.[1-5] Their usage in determining the ground state configuration of various clusters and molecules is becoming increasingly successful and popular.[6-15] In their most common forms, the GAs use a binary representation of variables, and the emulated genetic operators, crossover, and mutation, for example, are made to act on it. As elaborated in our earlier work,[7] this binary representation often suffers from the so-called Hamming Cliff problem. The Hamming distance indicates the number of bits that are different between two binary strings. In a Hamming Cliff situation, a very large perturbation in binary space would cause only a small change in integer space. For example, the decoded value of the binary string 01 111 111 is 127 in the integer space, while the string 10 000 000, which is at a large Hamming distance apart, since all of its corresponding bits are different from the previous one, decodes as 128, the next integer. In such a situation, the usual binary representation is often pushed to the limits of its efficacy, and the GAs tend to become stagnant. The real coded differential evolution (DE),[16] as demonstrated earlier,[7] becomes quite handy in a situation like this. Another option is to use the phenotype operation of creep mutation, where the binary strings are mapped back to the real space, perturbed slightly, and reconverted back to binary. In this study, along with those two procedures, we have experimented with another option, the so-called Gray Coding[1-2] of the binary variables. We applied our methodology on a number of copper clusters and compared the present results with our earlier investigations conducted through Monte Carlo simulation and other methods,[17-18] in which the success of an evolutionary approach became quite apparent.

The details of binary GAs and DE are provided in our earlier papers[3,5-8,12] and are not repeated here. We begin with a brief overview of the Gray Coding technique.

2. The Elements of Gray Coding

Gray coding ingeniously uses the Exclusive OR (XOR) operator between the binary bits. The XOR differs from the more conventional OR operator, as shown in Table 1 using two logical variables, α and β, both of which could be either TRUE or FALSE and thus could be assigned a bit value of either 1 or 0. It is evident from Table 1 that the OR operation returns a TRUE value when any one, or both the operands, α and β, are TRUE. However, in order for an XOR operation to return a TRUE value, one of the operands necessarily has to be TRUE, while the other one needs to remain FALSE.

To convert a binary string, say 10 000 to its Gray equivalent, the first step is to transfer the leftmost bit in the binary, 1 in the present case, unchanged to the same location in the Gray representation. The resultant of an XOR operation between the next bit in the binary and its left-hand side neighbor fills its corresponding position in the Gray string, and the XOR operation continues till all the bit locations are filled up. The binary number 10000 thus translates into 11000 in Gray encoding, and the Gray encoded GAs would use the number as such. The major attraction of the Gray encoding is its unique property that any two adjacent integers, if Gray coded, will have only one corresponding bit different from each other. The Hamming Distance between any two adjacent Gray coded integers is therefore always unity, and this reduces the possibility of getting stranded in a Hamming Cliff, which is quite commonplace in the ordi-

Table 1 Truth Table for OR and XOR Operators

α	β	α OR β	α XOR β
1	1	1	0
0	0	0	0
1	0	1	1
0	1	1	1

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nary binary coded GAs. In this study Gray coding worked quite satisfactorily for the clusters on which it was tried. The details of the energy calculations are provided below.

Table 2 PEF Parameters

Parameter	Value
A_1	110.766008
λ_1	2.09045946
α_1	0.394142248
A_2	–46.1649783
λ_2	1.49853083
α_2	0.207225507
D_{21}	0.436092895
D_{22}	0.245082238

3. The Energy Functional

The potential energy functional (PEF) used in the calculations describes the total interaction energy (Φ) of a system of N particles and is defined as

$$\Phi = D_{21}\phi_{21} + D_{22}\phi_{22} \quad \text{(Eq 1)}$$

where ϕ_{21} and ϕ_{22} are total two-body interaction energies. The parameters D_{21} and D_{22} contain the contribution of many-body interactions other than the pair-interactions and were determined using bulk cohesive energy and bulk stability condition, as detailed elsewhere.[17]

The two-body interaction energy terms were calculated as

$$\phi_{2k} = \sum_{i<j} U_{ij}^{2k} \qquad k = 1,2 \quad \text{(Eq 2)}$$

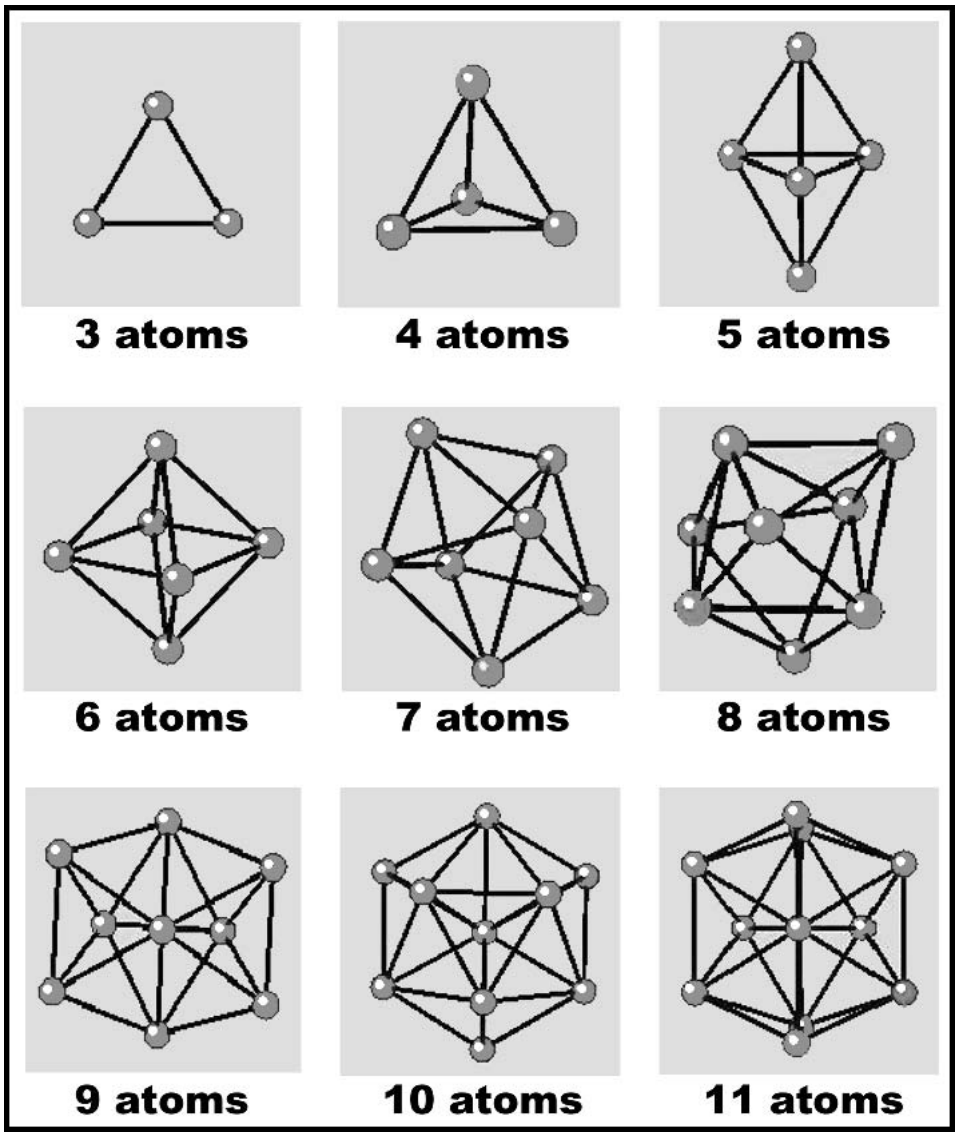

Fig. 1 Ground state configurations of Cu clusters

where $k = 1$ is for repulsive interactions only and $k = 2$ is for attractive interactions only. The explicit form of U_{ij}^{2k} is taken as

$$U_{ij}^{2k} = A_k r_{ij}^{-\lambda_k} e^{-\alpha_k r_{ij}^2} \qquad k = 1,2 \qquad \text{(Eq 3)}$$

where r_{ij} denotes the interatomic distance, and A_k, λ_k, and α_k are the three parameters for two-body interaction, as discussed earlier.[17]

Furthermore, an exact pair potential (this is not exact energy) U_{ij} was defined as

$$U_{ij} = U_{ij}^{21} + U_{ij}^{22} \qquad \text{(Eq 4)}$$

It should be noted here that U_{ij} describes the interaction potential between two atoms only, containing both repulsive and attractive interactions. However, it is also possible to define U_{ij}^{eff}, an effective pair-potential such that

$$U_{ij}^{eff} = D_{21} U_{ij}^{21} + D_{22} U_{ij}^{22} \qquad \text{(Eq 5)}$$

The total interaction energy based upon the effective pair potentials can be also calculated as

$$\Phi = \sum_{i<j} U_{ij}^{eff} \qquad \text{(Eq 6)}$$

The various parameters used for the PEF are shown in Table 2. In these parameters the energy is in eV and the distance is in Å. Further details are provided elsewhere.[17,18]

4. Computational

The calculations reported in this study were performed in a PARAM 10 000 computer located at the campus of Indian Institute of Technology, Kharagpur. This is a 6.4 giga flop parallel machine, scalable up to tera flop range, developed by C-DAC, India, and operates under a UNIX type environment. We have developed our own C code tailor-made for this problem.

The mutation constant[7,16] for the DE runs required

Table 3 Calculated Cluster Energies for the Ground State Configurations

Number of Atoms	Energy, Genetic Algorithm Without Gray Coding, eV	Energy, Genetic Algorithm Using Gray Coding, eV	Energy, Differential Evolution, eV	Energy, Monte Carlo Calculations[18], eV
3	–0.6677	–0.6677	–0.6677	–0.6678
4	–1.3354	…	–1.3355	–1.3352
5	…	…	–2.0220	–2.0215
6	…	…	–2.8529	–2.8524
7	…	–3.6566	–3.6566	–3.6561
8	–4.4283	–4.4286	–4.4286	–4.4280
9	–5.3187	…	–5.3187	–5.3186
10	…	…	–6.2668	–6.2660
11	–7.2205	7.2205	–7.2205	–7.2262

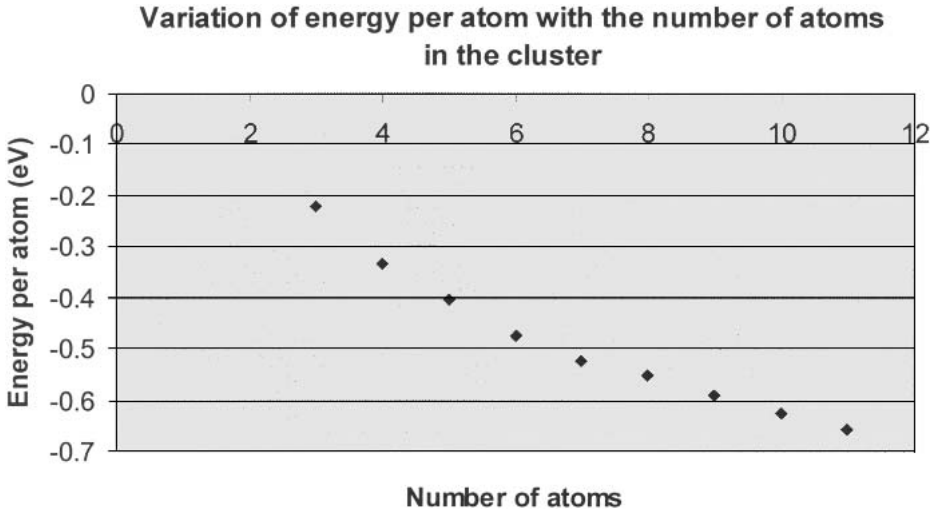

Fig. 2 Variation of energy per atom with cluster size

gradual adjustments between 0.01 and 4.2, while the corresponding crossover probabilities were adjusted in the range of 0.8-0.3. For the binary and Gray coded genetic algorithms both the jump and creep mutation were used, often in tandem. When gray coding was not used, the probabilities for each type of mutation were varied between 0 and 0.005. Along with Gray coding, the bit mutation probability was varied between 0 and 0.001, while the creep mutation probability was adjusted between 0 and 0.003. Only single-point crossover operation was conducted in both the cases. When used with gray coding, the crossover probability was kept within 0.7-0.85. The corresponding range was from 0.6 to 0.8 when Gray coding was not used. The time required for convergence varied from cluster to cluster. We

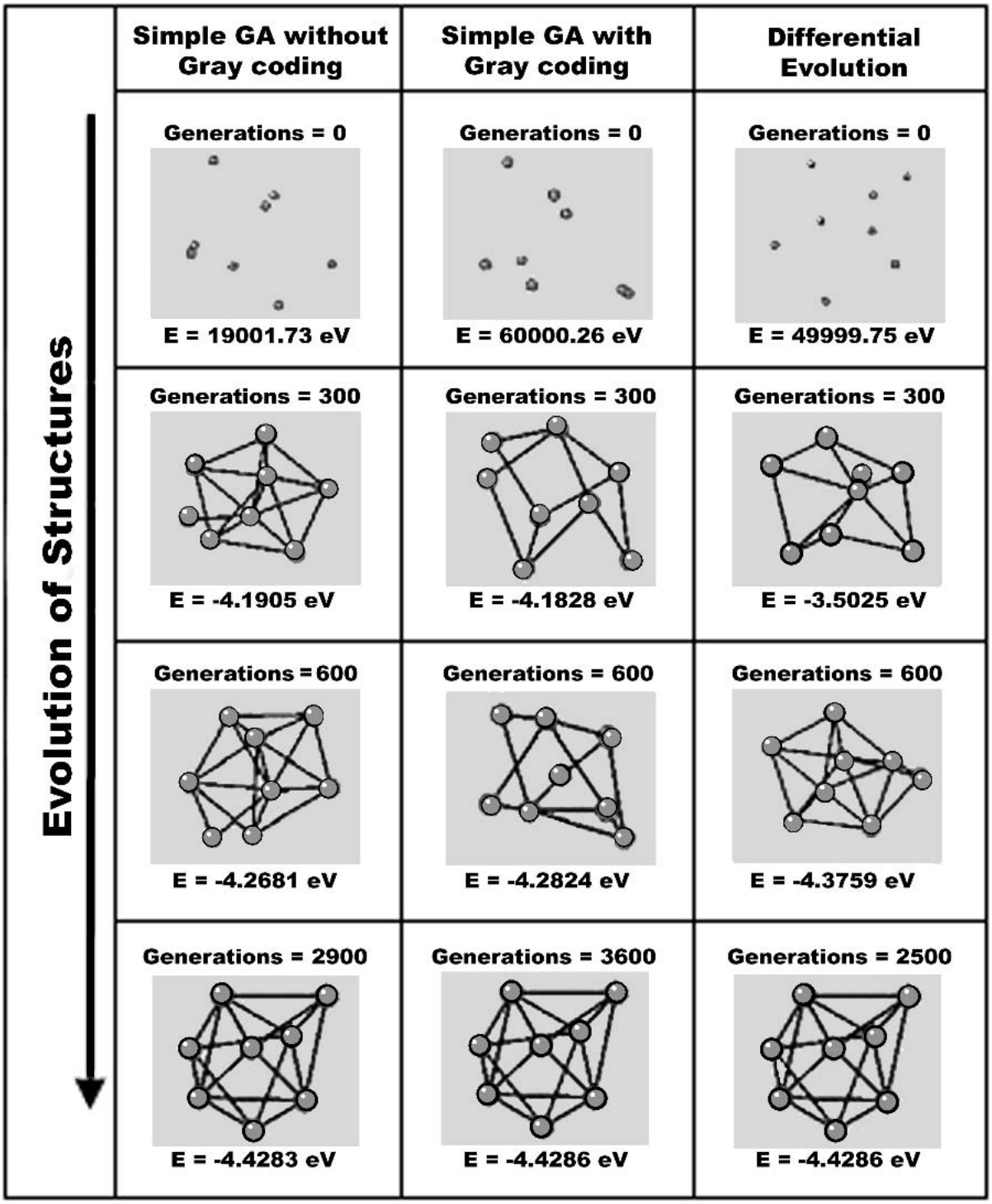

Fig. 3 Evaluation of the ground state structure using various algorithms

usually continued our calculations for several generations after the apparent convergence, with varying crossover and mutation, so that the stability of the observed configuration could be established beyond any reasonable doubts. Thus, for the clusters like Cu_{10} we continued our calculations up to 178 000 generations, while the optimized geometry of Cu_5 was obtained easily within 2000 generations.

5. Results and Discussion

The optimized geometries of the ground state clusters computed in this study are shown in Fig. 1. A 5-fold symmetry was observed in all the clusters containing more than seven atoms. DE was used for computing all the clusters, while the binary and Gray coded genetic algorithms were tried out for some select clusters. The minimized energy values are shown in Table 3, and Fig. 2 shows the variation of energy per atom with the cluster size.

The results are in excellent agreement with the earlier studies[17-18] where a Monte Carlo technique was used in a simulated annealing[19] type of environment. This involves a tedious point-by-point search, by means of a random walk, and GA, in all its variants, performs better than that by efficiently recombining global information in the search space through its crossover operator and continuously performing a local search through mutation.

Among the three evolutionary algorithms used in this study, DE, in general, provided the fastest convergence. However, as it is a greedy scheme, with an explicit bias towards the best offspring, DE sometimes runs into the problem of losing the diversity of the population, which, in turn, leads to a premature convergence. In this study we were able to overcome this problem through a careful adjustment of the mutation constant in the ranges mentioned before.

Each evolutionary algorithm takes it own pathway to converge, as shown in Fig. 3, where each structure denotes the lowest energy configuration at a particular generation for the corresponding algorithm. Unlike one of the Monte Carlo strategies tried out earlier,[18] in which one atom was randomly added to a previously optimized structure, GAs rely heavily upon the randomness of the initial population, and the nature of the intermediate assemblages, thus, may vary from run to run, even for the same variety of the evolutionary technique. It is also worth mentioning at this point that for the system in hand, a large distortion in the lattice is often associated with a small change in the energy; the configurations obtained with and without gray coding after 600 generations (Fig. 3) bear ample evidence of that. This possibly reflects the multi-modal nature of the energy functional. Multi-modality can indeed lead to a false convergence in a local minimum unless adequate precautions are taken. In genetic algorithms, the dual action of crossover and mutation provides an implicit safeguard against this problem by simultaneously performing a global and a local search, as indicated before. However, its efficacy is very sensitive to the proper choice of the genetic parameters, which, as in our previous efforts in this area,[6-9] have required a quite tedious trial and error effort.

6. Concluding Remarks

Several studies in recent years have addressed the cluster and molecular geometry optimization problems associated with GAs.[6-15] The need for designing new materials and the requirements of basic understanding for processes like chemisorption and catalysis, as in the present work, have been the major driving force behind many such research efforts. The nature of genetic algorithms used in those studies, however, varied widely, ranging from a rather simplistic cut and paste to state-of-the-art binary and real coded implementations. The Gray and real coded methodology demonstrated in this study can straighten out many problems associated with such simulations, but possibly not all. For example, we are aware that the strategy that we have been following in our recent works[6-9] cannot prevent multiple occurrences of the same structures with different coordinates, as the atoms are allowed to translate and rotate freely. Furthermore, for problems of this nature, our experience suggests that most genetic algorithms tend to reach a near optimal state rather quickly and then they slow down considerably, sometimes rendering the fine convergence an unacceptably tedious process. However, the time to reach a near optimal region varies from cluster to cluster, and is not always directly correlated to the cluster size. In principle, it may be a better option to use a hybrid scheme that would rely upon a gradient-based method for the final convergence, once the genetic algorithms bring the solution to a near optimal level. All such options need to be meticulously tried out, and for that purpose, calculating the same clusters over again with variant evolutionary techniques, as we have attempted here, appears to be an absolute necessity.

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