

# The Genetic algorithms in optimization of silicon clusters

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**Abstract**— the optimization of molecular structure is a very difficult global optimize problem.As there are many parameters to describe the molecular,it is hard to find the global optimal without an appropriate algorithms.In this paper ,we choose genetic algorithms (GA) to optimize the structure of silicon clusters. Compared to other algorithms,GA has a higher efficiency in finding the global optimal. We make some improvement to the former algorithms.The results prove what we have done is acceptable.

**Key words**-Silicon clusters; genetic algorithms; crossover; mutation; optimization.

## I .INTRODUCTION

### A. Silicon clusters

With the high-pace development of computer technology,a variety of theoretical modeling clusters has risen great interest.What commomly refered to as clusters including atomic clusters and molecular clusters. They are made up of two or more atoms or molecules through a combination of physical and chemical composition of relatively stable aggregates. [1] Stable structure of clusters is an important subject for the common concern of chemists and physicists, because there is a very close connection between the characters of the clusters and its structure. [2] Clusters with special stability of the structure also showed perfect symmetry.

Si nanomaterial has the singular characteristic and the extraordinary special function which many conventional semiconductors are unable to compare favorably with. So Si nanomaterials are one of the hot spots in the field of material science .The various devices produced by semiconductor materials plays an important role in the modern information

society. [3]Thus, studies on cluster structure of semiconductor elements are of great significance.

### B. Genetic algorithms

The Genetic algorithms was first proposed in the 1970s by Professor Holland.[4] and then the theory developed gradually. Genetic algorithms borrow the law of "survival of the fittest" in biological evolution. Through three operators --selection, crossover, and mutation of the individual, process of choosing the fit individuals to elect a high fitness in order to gain the results you want. The genetic algorithm has been applied in many fields. The issues involved generally can be divided into three categories: the classification system in the machine learning, combinatorial optimization problem and complex function optimization. Genetic algorithm has more opportunities to find the global optimal solution than the traditional mathematical optimization method. Deaven and his colleagues improved GA and began to use it in cluster study since 1995.[5] In this paper, we use the a genetic algorithm to optimize silicon clusters with different atom number, and then import coordinates of the atom into Material Studio to simulate the configuration. Compared to the actual structure we build in MS, the algorithm is proved to be basic effective.

## II .CALCULATION DETAILS

### A. Tersoff potential function

The Tersoff function is choosed to calculate the energy of the silicon cluster. The atom in the same system is calculated one by one without repeat.According to the theory of pauling key sequence ,the total energy of the system consists of the interaction between two separate built atom ,the repel interaction between a pair of atoms and the attractive interaction between a pair of atoms with their key sequence multiplied. The key sequence parameters in this potential

function include multi-body part which are related to the environment ,the value of those parameters depends on pairing atoms in the confined environment and the nearest atom.[6] The potential function is given as follows:

$$\Phi = \sum_i^n \sum_{i>j}^n [a_{ij}E_r(r_{ij}) - b_{ij}E_\alpha(r_{ij})] \quad (1)$$

Where

$$E_r(r_{ij}) = A_{ij} \exp(-\lambda_{ij}r_{ij}) \quad (2)$$

$$E_\alpha(r_{ij}) = B_{ij} \exp(-\mu_{ij}r_{ij}) \quad (3)$$

$$a_{ij} = \varepsilon_{ij} (1 + \beta_i^{n_i} \tau_{ij}^{n_i})^{-\frac{1}{2n_i}} \quad (4)$$

$$b_{ij} = \chi_{ij} (1 + \beta_i^{n_i} \xi_{ij}^{n_i})^{-\frac{m_i}{2n_i}} \quad (5)$$

$$\tau_{ij} = \sum_{k \neq i, j} f_c(r_{ik}) \delta_{ik} g(\theta_{ijk}) \quad (6)$$

$$\xi_{ij} = \sum_{k \neq i, j} f_c(r_{ik}) \omega_{ik} g(\theta_{ijk}) \exp[\sigma_{ik}(r_{ij} - r_{ik})] \quad (7)$$

$$g(\theta_{ijk}) = 1 + \frac{c_i^2}{d_i^2} - \frac{c_i^2}{d_i^2 + (h_i - \cos \theta_{ijk})^2} \quad (8)$$

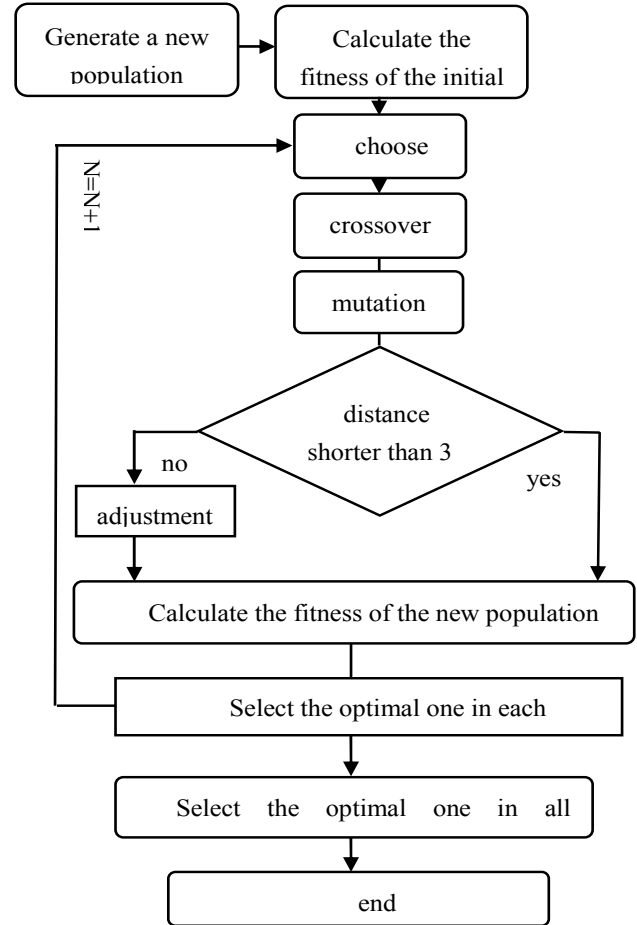
$$f_c(r_{ij}) = \begin{cases} 1 & r_{ij} < R_{ij} \\ \frac{1}{2} \left[ 1 + \cos\left(\pi \frac{r_{ij} - R_{ij}}{S_{ij} - R_{ij}}\right) \right] & R_{ij} < r_{ij} < S_{ij} \\ 0 & S_{ij} < r_{ij} \end{cases} \quad (9)$$

$r_{ij}$  and  $r_{ik}$  are distances between two atoms. Other parameters are given as follows.

Other parameters are given as follows.

Parameter	value	$\sigma/\text{\AA}$	0.0000
A/eV	$1.8308 \times 10^3$	$\beta$	$1.1 \times 10^{-6}$
B/eV	$4.7118 \times 10^2$	n	$7.8734 \times 10^{-1}$
$\lambda/\text{\AA}^{-1}$	2.4799	$c_i$	$1.0039 \times 10^5$
$\mu/\text{\AA}^{-1}$	1.7322	$d_i$	$1.6217 \times 10^1$
R/ $\text{\AA}$	2.7000	$h_i$	$5.9825 \times 10^1$
S/ $\text{\AA}$	3.0000	m	1.0000
$\chi$	1.0000	$\omega$	1.0000
$\varepsilon$	1.0000	$\delta$	0.0000

## B. GA flowchart



### 1) The initial population

Using matlab to generate a population randomly, the numbers of individuals in the population stands for silicon

Table 1 Parameters of Tersoff Function

clusters, Coordinate values decide position of silicon atom in three-dimensional space. By putting the data into the fitness and potential function; we get the fitness of the initial population.

2) *Fitness*

Every individual in the initial population is assigned a fitness value. The clusters with higher fitness own more chances to be chosen so that better character can be passed on to the next generation. In the calculating process, individuals with low higher energy are given higher fitness.[7] We use Exponential function:

$$F_i = \exp(-\alpha\rho_i)$$

Where

$$\rho_i = \frac{V_i - V_{\min}}{V_{\max} - V_{\min}}$$

$V_i$  stands for the energy of the  $i$ th individual,  $V_{\max}$  and  $V_{\min}$  are the highest and the lowest energy of the system.

3) *choose*

we choose Roulette choosing method, so that the clusters with higher fitness are more likely to be chosen.

4) *Crossover*

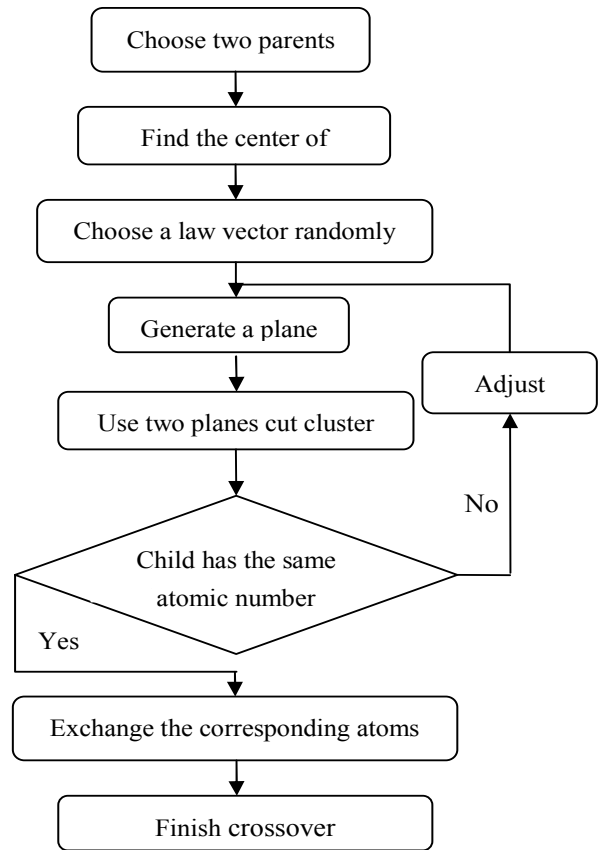
Following are the main steps:

Choose a law vector randomly, and then cut the two parents clusters horizontally via their centers of gravity

Change their upper parts, and slice the fragments, then the new cluster form. If number of atoms in new cluster  $s$  is not equal to that of parents, move the cutting plane according to the law vector produced randomly, until the number of atoms meets the requirement.

The probability of crossover is decided by the fitness of the cluster, that is, the probability is proportional to the fitness.

The flowchart is following:



5) *mutation*

The rate of crossover is much less than that of mutation. Crossover combines the good characters from two parents and passes it on to the child, while mutation generates new characters. The process of making the mutated atoms moving different steps in varied directions is randomized. Keep the small probability of mutation to protect good characters from been obsoleted while new characters are generated in case of local optimum.

6) *improvement for GA*

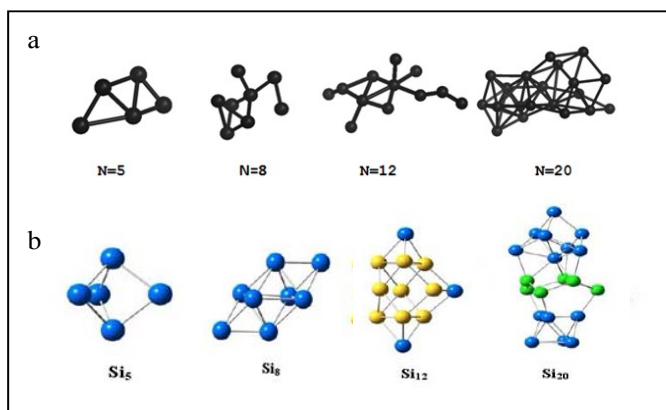
Sometimes, in the process of calculating, the atoms may be isolated (distance from the closest atom is longer than 2~3 Å) in the cluster. Thus, we take some measures to avoid this condition from happening.

When calculating the potential energy of the cluster, if we find isolated atoms in the cluster, except calculating via the equations, we make the cluster's potential energy to have a really high value(1000,000eV) so that it has little chance to get into the next generation. And after the operation of choosing,

mutation and crossover, we will exam all the clusters of the population to find out whether they have isolated atoms. If all of them have isolated atoms, we will adjust these atoms so that they can be closer to the other atoms surrounding them. Besides, the atoms in a cluster are all limited in a relatively small space so that it can be much easier for them to react with the other atoms, thus reducing the quantity of the isolated atoms.

### III.RESULTS AND DISCUSSION

In the progress genetic algorithm, on the basis of Tersoff Potential, we used following parameters: population=N; the rate of crossover=fitness value; the rate of mutation=0.04.The number of the atoms is the variable quantity. Calculations were run in the condition that N=5, 8, 12, 20, and the results are



showed in Fig1.

Figure 1.a)The results of our simulation ;b)The results of Qin[8]

In the course of calculation, the energies are recorded, and that the energy tends to be lower can be concluded.

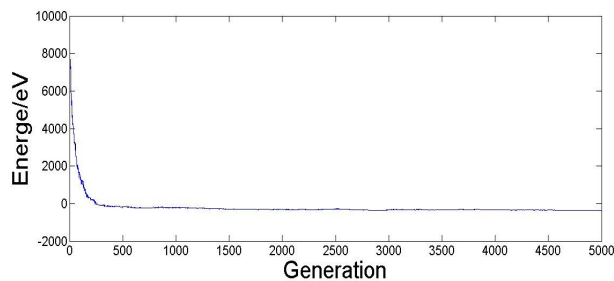


Figure 2.The energy's curve of Si<sub>12</sub>

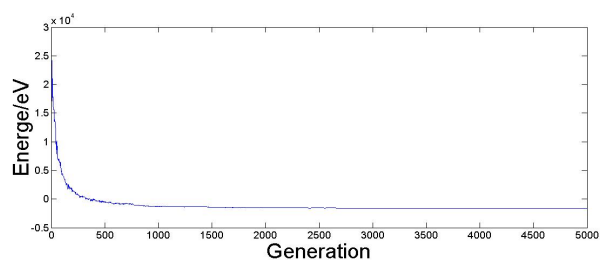


Figure 3.The energy's curve of Si<sub>20</sub>

Meanwhile random Si atoms were also simulated in the Material Explorer by Tersoff potential. Course of compared with those of genetic algorithm, the similar results certify the genetic algorithm. However, when the number N is large, software for molecular simulation, such as Material Explore, Materials Studio, it will take a long time, and the GA method is faster and more convenient relatively.

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