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COMPUTER METHODS IN MATERIALS SCIENCE

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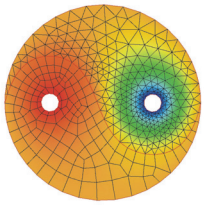

COMPUTATIONAL INTELLIGENCE METHODS IN SEARCHING OF STABLE CONFIGURATIONS OF NANOSTRUCTURES

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Abstract

Application of evolutionary algorithm, artificial immune system and particle swarm optimization in the minimization atomic cluster's total potential energy is presented in this work. These methods of computational intelligence simulate biological processes of the natural environment and organisms such as theory of evolution and biological immune systems and give a strong probability of finding the global optimum. Some examples and discussion on the results of optimization are also presented in this paper.

Key words: nanostructure, intelligence methods, evolutionary algorithms, artificial immune system, particle swarm optimization, modeling

1. INTRODUCTION

This paper deals with computational intelligence methods: evolutionary algorithms, artificial immune systems and the particle swarm optimization applied to the process of minimization of the potential energy of small nanostructures, such as atomic clusters. The atomic clusters are isolated spatial atomic structures which contains up to several thousands of atoms. Ideal clusters have some unique mechanical, optical, magnetic and electronic properties, due to defectless, perfect structure of the atomic clusters. The atomic bindings and potential energy of the cluster can be described using *ab-inito* or DFT computations (Ahlrichs & Elliot, 1999), or empirical atomic potentials (Burczyński et al., 2010; Girifalco & Weizer, 1959; Morse, 1929; Murrell & Mottram, 1990).

One of the most important objectives is to find (for given cluster size) the global minimum of the cluster potential energy, which corresponds to the stable, spatial arrangement of atoms. This is non-trivial, NP-hard problem, because the number of local minima increases almost exponentially with the cluster size. There are many different methods and approaches, applied to deal with this problem. The most popular approaches are random searches, Monte Carlo simulated annealing (Lloyd & Johnston, 1998), basin-hopping (Wales & Doye, 1997) and bio-inspired algorithms e.g. evolutionary algorithms, artificial immune systems and particle swarm optimization. A Genetic Algorithm was applied, probably for the first time to the Morse clusters, by Roberts et. al. (2000) and has became a standard tool in the optimization of the nanostructures (Mrozek et al., 2009; Dugan & Erkoc, 2009). An Adaptive Immune Algorithm was used for optimization of Lennard-Jones clusters by Shao et al. (2004). Zhou et al. performed Particle Swarm Optimization of Ni clus-

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ters (2008). Prediction of the aluminium atoms distribution using a distributed evolutionary algorithm was described by Mrozek et. al. (2005) and further developed in (Burczyński et al. 2010; Mrozek et. al., 2009).

The bio-inspired algorithms simulate biological processes of the natural environment and organisms such as the theory of evolution and the biological immune systems. These approaches, generally, do not need any information about the gradient of the fitness function and give a strong probability of finding the global optimum. The main drawback of these methods is the long time of computations.

The empirical pair-wise and many-body potentials are applied to compute the potential energy and to model interactions between atoms. The two-body Morse potential and the many-body Murrell-Mottram potentials are applied to study spatial configurations of the atomic clusters. The parameters of these potentials are fitted to provide the appropriate properties of a material (equilibrium binding distance, dissociation energy, phonon frequencies etc.). Examples of stable clusters for various numbers of atoms of bulk aluminium are presented.

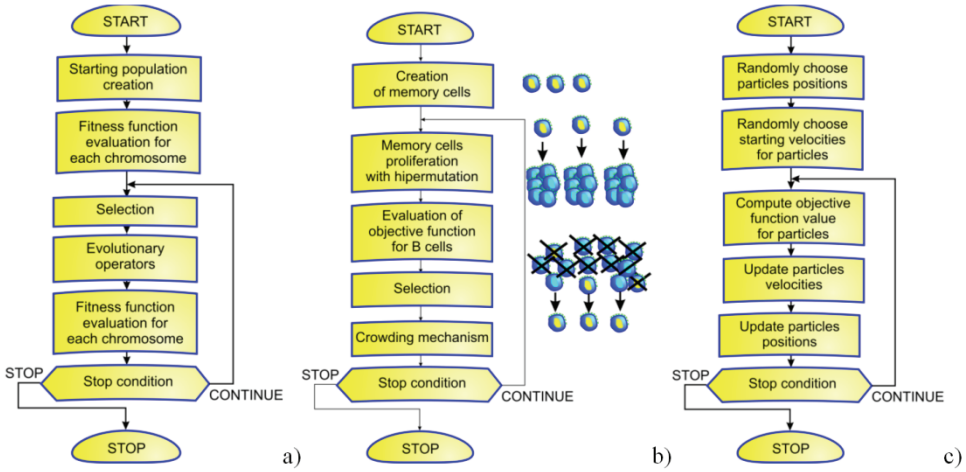

Fig. 1. *The flowcharts of evolutionary algorithm (a), artificial immune system (b) and particle swarm optimization (c).*

2. COMPUTATIONAL INTELLIGENCE METHODS IN MODELING OF ATOMIC CLUSTERS

The heuristic artificial intelligence methods used in modeling of atomic clusters can be divided into two groups. The first one is based on simulation of the certain physical processes, e.g. annealing in metallurgy (Lloyd & Johnston, 1998). The second group of computational intelligence methods is inspired by biological mechanisms in the natural environment and live organisms. The bio-inspired optimization methods of atomic clusters have become very popular in last years (see previous chapter). Most of them give good results for optimization of multimodal functions. This work deals with evolutionary algorithms, the artificial immune system and the particle swarm optimization.

2.1. Evolutionary algorithm (EA)

The genetic and evolutionary algorithms (Michalewicz, 1996) are based on mechanisms taken from biological evolution of species. The selection based on the individual fitness, mutations in chromosomes and individuals crossover are adopted. The simple genetic algorithms operate on binary coded chromosomes. The term evolutionary algorithm is more widely used for different modifications of genetic algorithms (also for algorithms operating on genes containing floating point numbers). The evolutionary algorithms operate on a population of individuals. The individuals contain one chromosome in most cases. The following description concerns the evolutionary algorithm used in numerical examples. The staring population is created randomly. Next the fitness function values are computed for each chromosome. The selection chooses chromosomes for a new parent subpopulation taking into account fitness function values. Evolutionary operators change chromosomes' genes and create chromosomes for the offspring population. The uniform and Gaussian mutations and the simple crossover are randomly chosen to perform chromosome changes. The new chromosomes are evaluated. The algorithm works iteratively till the end optimization condition is fulfilled. The flowchart of evolutionary algorithm is presented in the figure 1a.

2.2. Artificial Immune System (AIS)

This alorithm is developed on the basis of mechanism discovered in biological immune sys-

tems. An immune system contains distributed groups of specialized cells and organs. The main purpose of the immune system is to recognize and destroy pathogens - funguses, viruses, bacteria and improper functioning cells.

The artificial immune systems (AIS) (de Castro & Von Zuben, 2002; de Catro & Timmis, 2003; Wierzchoń, 2001) take only a few elements from the biological immune systems. The most frequently used are the mutation of the B cells, proliferation, memory cells, and recognition by using the B and T cells. The artificial immune systems have been used to optimization problems, classification and also computer viruses recognition. The cloning algorithm Clonalg presented by von Zuben and de Castro uses some mechanisms similar to biological immune systems to global optimization problems. The unknown global optimum is the searched pathogen. The memory cells contain project variables and proliferate during the optimization process. The B cells created from memory cells undergo mutation. The B cells are evaluated and better ones exchange memory cells. In (Wierzchoń, 2001) version of Clonalg the crowding mechanism is used - the diverse between memory cells is forced. A new memory cell is randomly created and substitutes the old one, if two memory cells have similar project variables. The crowding mechanism allows finding not only the global optimum but also other local ones. The presented approach is based on the algorithm presented by Wierzchoń (2001). The mutation operator is changed. The Gaussian mutation is used instead of non-uniform mutation in the presented approach.

The memory cells are created randomly. They proliferate and mutate creating B cells. The number of clones created by each memory cell is determined by the memory cells objective function value. The objective functions for B cells are evaluated. The selection process exchanges some memory cells for better B cells. The selection is performed on the basis of the geometrical distance between each memory cell and B cells (measured by using design variables). The crowding mechanism removes similar memory cells. The similarity is also determined as the geometrical distance between memory cells. The process is iteratively repeated until the stop condition is fulfilled. The stop condition can be expressed as the maximum number of iterations. The flowchart of artificial immune system is shown in the figure 1b.

2.3. Particle Swarm Optimization (PSO)

Swarm optimization is also based on observation done in biology (Chan & Tiwari, 2007; Kennedy et al., 2001). The algorithm has similar behavior as a birds flocking or fish schooling. The individual bird (in the PSO – particle) changes velocity and position taking into account neighbour birds. This social behavior shown by some animals can be very efficient in nature. PSO incorporated some biological elements in the numerical algorithm, such as velocity change of the particle on the base of neighbours. The PSO is an iterative algorithm (figure 1c). The positions of the particles in the search space and starting velocities are defined randomly on the beginning of the algorithm. The changes of particle velocities are due to the velocities of best ever found, best in neighbourhood and previous particle values. The algorithm updates position of all particles in every iteration on the basis of computed velocities.

3. ATOMIC INTERACTIONS – POTENTIAL ENERGY OF THE ATOMIC SYSTEM

The empirical pair-wise and many-body potentials were applied to compute the potential energy and to model interactions between atoms. The two-body Morse potential and the many-body Murrell-Mottram potentials were applied to study spatial configurations of the atomic clusters. The parameters of these potentials are fitted to provide the appropriate properties of a material (equilibrium binding distance, dissociation energy, phonon frequencies etc.).

3.1. Morse potential

This potential is a kind of simple pair-wise potential (Morse, 1929), which depends only on the distances, r_{ij}, between i-th and j-th atom:

$$\Phi^M(r_{ij}) = D_e\left[e^{2\alpha(r_0-r_{ij})} - 2e^{\alpha(r_0-r_{ij})}\right] \qquad (1)$$

where: D_e denotes dissociation energy, r_0 is the equilibrium distance of two atoms (molecules) and α is the scaling parameter, which controls the range of interactions. Short range interactions correspond to high values of α. The potential parameters, fitted to the properties of he various bulk cubic metals are given by Girifalco & Weizer (1959).

3.2. Murrell-Mottram potential

Two and three body interactions are taken into account. For the triad of atoms i, j and k, the general formula can be expressed as (Murrell & Mottram, 1990; Roberts et al., 2000):

$$\Phi^{M-M}\left(r_{ij},r_{ik},r_{jk}\right)=\Phi_2^{M-M}\left(r_{ij}\right)+\Phi_3^{M-M}\left(r_{ij},r_{ik},r_{jk}\right) \quad (2)$$

The two-body part of the Murrell-Mottram potential has the following form:

$$\Phi_2^{M-M}\left(r_{ij}\right)=-D_e\left(1+a_2\rho_{ij}\right)e^{\left(-a_2\rho_{ij}\right)} \quad (3)$$

where $\rho_{ij}=\dfrac{r_{ij}-r_0}{r_0}$.

The three-body term is expressed as:

$$\Phi_3^{M-M}=D_eP_s\left(Q_1,Q_2,Q_3\right)\operatorname{sech}\left(a_3Q_1\right) \quad (4)$$

and the value should not be changed upon interchanging atoms *i*, *j* and *k*. This condition is satisfied when the three-body potential (4) is defined as a function of symmetry coordinates Q_i (i = 1,2,3):

$$\begin{Bmatrix}Q_1\\Q_2\\Q_3\end{Bmatrix}=\begin{bmatrix}\sqrt{1/3} & \sqrt{1/3} & \sqrt{1/3}\\ 0 & \sqrt{1/2} & -\sqrt{1/2}\\ \sqrt{2/3} & -\sqrt{1/6} & -\sqrt{1/6}\end{bmatrix}\begin{Bmatrix}\rho_{ij}\\\rho_{jk}\\\rho_{ki}\end{Bmatrix} \quad (5)$$

For alkali metals (such as aluminium) the following cubic polynomial is applied:

$$P_s\left(Q_1,Q_2,Q_3\right)=c_0+c_1Q_1+c_2Q_1^2+c_2\left(Q_2^2+Q_3^2\right)+ +c_4Q_1^3+c_5Q_1\left(Q_2^2+Q_3^2\right)+c_6\left(Q_3^3-3Q_3Q_2^2\right) \quad (6)$$

The physical meaning of D_e and r_0 is the same as previous, the a_2 and a_3 are scaling parameters. The set of polynomial coefficients c_i (i = 1,2...6) is fitted to specific material properties (Chou & Cohen, 1986).

3.3. Total potential energy of the atomic cluster

The total potential energy of *N*-atom cluster is defined as a sum over all atomic interactions and in the case of the Morse cluster is obtained as:

$$V_{tot}=\sum_{i,j>i}\Phi^M\left(r_{ij}\right) \quad (7)$$

When the Murrell-Mottram structure is considered, the potential energy can be compute as:

$$V_{tot}=\sum_{i,j>i}\Phi_2^{M-M}\left(r_{ij}\right)+\sum_{i,j>i,k>j}\Phi_3^{M-M}\left(r_{ij},r_{ik},r_{jk}\right) \quad (8)$$

The global minimum on the potential energy surface (PES) corresponds to the lowest energy structure, which means the most stable spatial configuration of atoms. The determining global minimum on the atomic PES is generally non trivial, NP-hard problem, because the number of isomers (the structures correspond to the local minima) rises almost exponentially with increasing nulcearity (*N*).

4. METHODOLOGY

The application of the EA, AIS, PSO to determining global minima of PES is similar. Respectively, the chromosomes, memory cells and particles contain the real-valued Cartesian coordinates of each atom in the considered cluster. The total number of project variables is 3*N* (for *N* atom cluster). The initial population is generated randomly and the atoms can move freely in the sphere of radius $r_0\sqrt[3]{N}$.

There are no conditions to avoid penetration between atoms. The fitness function is expressed as the total potential energy of the considered atomic cluster. The formulas (7) and (8) are used directly to compute the fitness function for Morse and Murrell-Mottramm clusters, respectively.

For each *N*-atom cluster, the average binding energy (energy *per* atom) E_B is estimated:

$$E_B\frac{-V_{tot}}{N} \quad (9)$$

The regions of enhanced stability are determined by the second difference in the binding energy (10), which is related to the thermodynamic stability of the atomic cluster and is generally correlated witch experimental mass spectral intensities:

$$D_2\left(N\right)=2E_B\left(N\right)-E_B\left(N+1\right)-E_B\left(N-1\right) \quad (10)$$

The parameters of the Morse potential for bulk aluminium (D_e = 0.2703 eV, r_0 = 3.253 Å, α = 1.1646 Å^{-1}) are taken from (Girifalco & Weizer, 1959). The coefficients of the Murrell-Mottram potential are following: a_2 = 7, a_3 = 8, D_e = 0.9073 eV, r_0 = 2.7568 Å, C_0 = 0.2525, C_1 = -0.4671, C_2 = 4.4903, C_3 = -1.1717, C_4 = 1.6498, C_5 = -5.3579, C_6 = 1.6327 (Lloyd & Johnston, 1998).

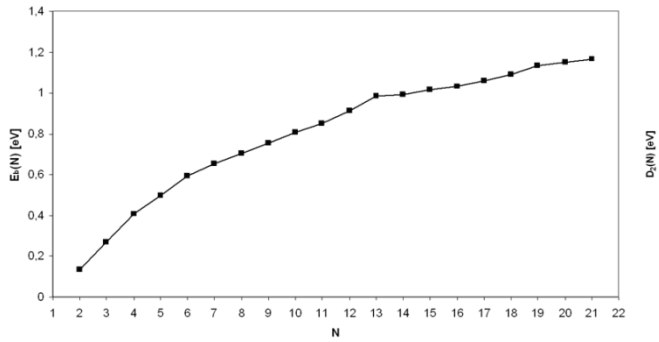

Fig. 2. *Average binding energies and the second differences in the binding energy of the Morse clusters.*

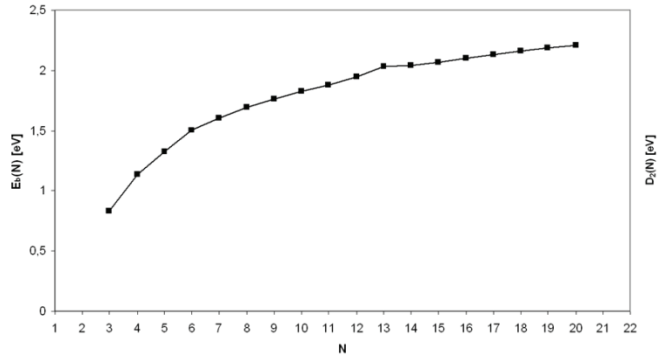

Fig. 3. *Average binding energies and the second differences in the binding energy of the Murrell-Mottram clusters.*

Table 1. *The total number of fitness function evaluations.*

N	EA		AIS		PSO	
	Morse	MM	Morse	MM	Morse	MM
2	3750	X	200	X	600	X
3	6250	12000	300	2368	1350	1350
4	7500	42500	4600	5632	2400	3000
5	21250	100000	6800	7744	5250	6750
6	12500	67500	121200	147825	7200	5250
7	20000	207500	125550	145000	16800	10500
8	58750	205000	486000	232500	26400	28800
9	41250	235000	348096	337500	18900	40500
10	85000	375000	918900	1125000	49500	48000
11	120000	400000	595683	1805625	84150	140250
12	125000	460000	369360	1856250	124200	237600
13	102500	425000	336141	1423125	95550	399750
14	137500	575000	775575	2418750	153300	X
15	167500	660000	1917500	2750625	X	X
16	187500	X	4668750	X	X	X
17	115000	X	2792475	X	X	X
18	295000	X	3027375	X	X	X
19	222500	X	2673000	X	X	X
20	235000	X	2812725	X	X	X

5. RESULTS

The global minima for Morse (N = 2...21) and Murrell-Mottram (N = 3...15) clusters were determined using EA, AIS and PSO. The lowest average binding energies and their second differences, as a function of N, are presented in the figures 2 and 3. The values for Murrell-Mottram structures with nuclearity N = 16...20 (marked *) are taken form (Lloyd & Johnston, 1998).

The peaks in $E_B(N)$ and $D_2(N)$ at N = 4,6,13 and 19 correspond to spatial structures with enhanced stability. The determined stable regions are in good agreement with *jellium* model calculations presented by Chou & Cohen (1986). These clusters have identical shape for both: the Morse and the Murrell-Mottram potentials as shown in the figure 4. The less stable structures are created by modifications of the super stable ones, i.e. additional atoms form next vertexes, glued to the main atomic structure (e.g. N = 21).

Small Morse and Murrell-Mottram aluminium clusters (N = 2...20), in almost all cases, have the same structure. The exceptions are the clusters with the following number of atoms: 9,16,18 and 20. The Murrell-Mottram global minima, in these cases, correspond to the second most stable isomers (local minima) of the Morse potential. It's due to fact, that the PES of the pair-wise interaction model (such as Morse or Lennard-Jones) has significantly more minima than the PES based on the many-body Murrell-Mottram potential. These results are comparable with ones presented in (Lloyd & Johnston, 1998; Shao et al., 2004). The described phenomena, for N = 9 is presented in the figure 5.

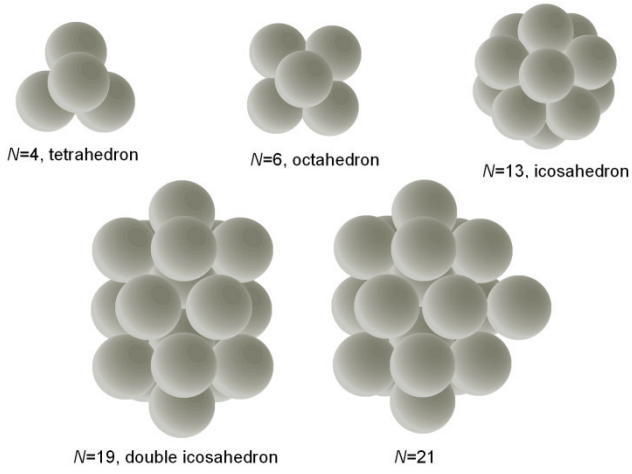

Fig. 4. *The most stable Morse and Murrell-Mottram clusters (except N = 21, see text).*

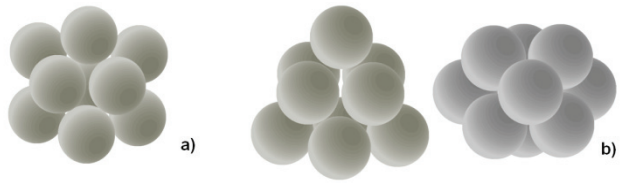

Fig. 5. *Global minimum of Morse cluster (a) and global minimum of Murell-Mottram corresponds to the second stable isomer of the Morse cluster (E_B = 0.748161eV) (b).*

The total number of fitness function evaluations, for each type of the algorithm is presented in table 1.

The behavior and efficiency of the EA and the AIS in atomic cluster modeling are similar. These two algorithms found all the global minima in considered range of *N*. The energy minimization using PSO is generally faster then two others, however the PSO have tremendous tendency to stuck at local minima.

7. CONCLUSIONS

The minimization of the potential energy of the atomic clusters using bio-inspired algorithms was performed. The reason for choosing Morse and Murrell-Mottram potential was available data of energy levels and configurations of atomic structures. All the determined the lowest energy levels and shapes of the atomic structures are in the good agreement with ones presented in bibliography. The Evolutionary Algorithm and Artificial Immune System have no problems with premature convergence and find all the global minima. The main drawback of these algorithms is the long time of the computations. The PSO is generally faster than EA and AIS, but problems with sticking at local minima occurred. It's probably caused by troubles with setting proper values of the PSO parameters.

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METODY INTELIGENCJI OBLICZENIOWEJ W WYZNACZANIU STABILNYCH KONFIGURACJI GEOMETRYCZNYCH NANOSTRUKTUR

Streszczenie

W pracy opisane zostało zastosowanie wybranych metod inteligencji obliczeniowej (algorytmu ewolucyjnego, sztucznego systemu immunologicznego oraz optymalizacji rojem cząstek) do optymalizacji klastrów atomowych. Jako kryterium optymalizacji przyjęto minimalizację całkowitej energii potencjalnej nanostruktury. Do modelowania oddziaływań międzyatomowych użyto potencjałów Morse'a oraz Murrella-Mottrama. W pracy przedstawiono wybrane wyniki optymalizacji oraz ich interpretację.

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