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SEARCHING OF STABLE CONFIGURATIONS OF NANOSTRUCTURES USING COMPUTATIONAL INTELLIGENCE METHODS

POSZUKIWANIE STABILNYCH KONFIGURACJI KLASTRÓW ATOMOWYCH ZA POMOCĄ METOD INTELIGENCJI OBLICZENIOWEJ

Abstract

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. These algorithms simulate biological processes of the natural environment and organisms such as the theory of evolution and the biological immune systems. Mentioned 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.

Keywords: *atomic clusters, Morse Potential, Murrell-Mottram Potential, evolutionary algorithms, artificial immune systems, particle swarm optimization*

Streszczenie

W artykule przedstawiono zastosowanie wybranych metod inteligencji obliczeniowej (algorytmy ewolucyjne, sztuczne systemy immunologiczne, optymalizacja rojem cząstek) do minimalizacji energii potencjalnej klastrów atomowych. Do opisu oddziaływań międzyatomowych użyte zostały potencjały Morsa i Murrella-Mottrama.

Słowa kluczowe: *klastry atomowe, potencjał Morsa, potencjał Murrella-Mottrama, algorytmy ewolucyjne, sztuczne systemy immunologiczne, optymalizacja rojem cząstek*

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1. Introduction

A small nanostructure, called the atomic cluster, is an isolated spatial atomic structure which contains up to several thousands of atoms. The ideal clusters have some unique mechanical, optical, magnetic and electronic properties. It is due to defectless, perfect structure of the atomic clusters. The atomic bondings and potential energy of the cluster can be described using *ab-inito* computations, density functional theory [1] or empirical atomic potentials (see chapter 4). 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 [10, 17]. This is a non-trivial, NP-hard problem, because the number of local minima increases almost exponentially [20] with the cluster size. There are many different methods and approaches, applied to deal with this problem. Lloyd and Johnson [10] adopted the Random Searches and Monte Carlo Simulated Annealing to study atomic clusters. Doye and Wales applied Basin Hopping Monte Carlo Algorithm to the Morse (with different range parameters) and Lennard-Jones [19] clusters. The Genetic Algorithm was applied for the first time to the Morse potential by Roberts, Johnson et. al [17]. Prediction of the aluminium atoms distribution using Distributed Evolutionary Algorithm was described by Mrozek et. al [14]. An Adaptive Immune Algorithm was used for optimization of Lennard-Jones clusters by Shao, Cheng and Chai [18]. Zhou performed Particle Swarm Optimization of Ni clusters [23].

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 [10]. The second group of computational intelligence methods is inspired by biological mechanisms in natural environment and live organisms. The bio--inspired optimization methods of atomic clusters have become very popular in last years [13, 17, 18, 23]. 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

The genetic and evolutionary algorithms (EA) [11] 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 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 Fig. 1a.

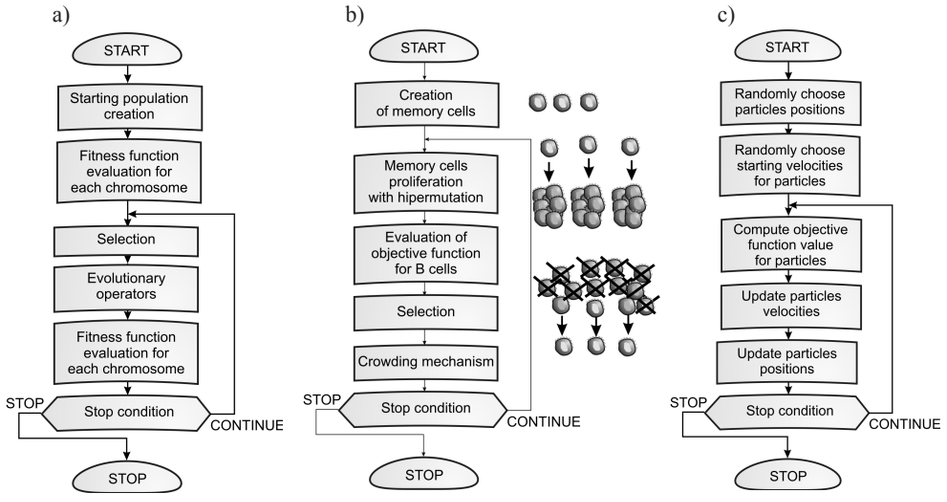

Fig. 1. The flowcharts of evolutionary algorithm (a), artificial immune system (b) and particle swarm optimization (c)

Rys. 1. Schemat blokowy algorytmu ewolucyjnego (a), sztucznego systemu immunologicznego (b) optymalizacji rojem cząstek (c)

2.2. Artificial Immune System

The artificial immune systems (AIS) are developed on the basis of mechanism discovered in biological immune systems. An immune system is a complex system which 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) [2, 3, 21, 22] 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 [22] 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 in [22]. 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 Fig. 1b.

2.3. Particle Swarm Optimization

The particle swarm optimization (PSO) algorithm is also based on observation done in biology [4, 8, 9]. 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 (Fig. 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 bonding distance, dissociation energy, phonon frequencies etc.).

3.1. Morse potential

The Morse potential is a kind of simple pair-wise potential [7,12], which depends only on the distances, r_{ij}, between i-th and j-th atom.

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

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 the various bulk cubic metals are included in [7].

3.2. Murrel-Mottram (MM) potential

This kind of potential takes into account 2–3 body interactions [15, 16]. For the triad of atoms *i*, *j* and *k*, the general formula can be expressed as

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

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

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

and the relative atomic distance can be written as

$$\rho_{ij} = \frac{r_{ij} - r_0}{r_0} \tag{4}$$

The three-body term is expressed as

$$\Phi_3^{M-M} = D_e P_s\left(Q_1, Q_2, Q_3\right) F_D\left(a_3, Q_1\right) \tag{5}$$

and the value shouldn't be changed upon interchanging atoms *i*, *j* and *k*. This condition is satisfied when the three-body potential (5) is defined as a function of symmetry coordinates Q_i (i = 1, 2, 3)

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

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

$$\begin{aligned} P_s\left(Q_1, Q_2, Q_3\right) = {} & c_0 + c_1 Q_1 + c_2 Q_1^2 + c_2\left(Q_2^2 + Q_3^2\right) + \\ & + c_4 Q_1^3 + c_5 Q_1\left(Q_2^2 + Q_3^2\right) + c_6\left(Q_3^3 - 3Q_3 Q_2^2\right) \end{aligned} \tag{7}$$

and the damping function F_D is given by

$$F_D\left(a_3, Q_1\right) = \operatorname{sech}\left(a_3 Q_1\right) \tag{8}$$

The physical meaning of the 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 [6].

3.3. The potential energy of the atomic cluster

The total potential energy of *N*-atom cluster (so-called Potential Energy Surface, PES), described using is defined as a sum over all atomic interactions.

The total potential energy of the Morse cluster

$$V_{\text{tot}} = \sum_{i,j>i} \Phi^{M}\left(r_{ij}\right) \tag{9}$$

The total potential energy of Murrell-Mottram structure

$$V_{\text{tot}} = \sum_{i,j>i} \Phi_2^{M-M}(r_{ij}) + \sum_{i,j>i,k>j} \Phi_3^{M-M}\left(r_{ij}, r_{ik}, r_{jk}\right) \tag{10}$$

The global minimum on the PES (the lowest energy structure) corresponds to 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*) [10, 18, 20].

4. Methodology

The application of the EA, AIS, PSO to determining global minima of PES is quite 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 lie in the cube of side dimension *C*:

$$C = r_0 N^{\frac{1}{3}} \tag{11}$$

The fitness function is expressed as the total potential energy of the considered atomic cluster. The formulas (9) and (10) 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

$$E_B \frac{-V_{\text{tot}}}{N} \tag{12}$$

The regions of enhanced stability are determined by the second difference in the binding energy (13), which is related to the thermodynamic stability of the atomic cluster [10] and is generally correlated witch experimental mass spectral intensities.

$$D_2(N) = 2E_B(N) - E_B(N+1) - E_B(N-1) \tag{13}$$

The comparison of the bio-inspired algorithms with respect to number of fitness function evaluations (for given *N*-atom cluster and potential type) is performed.

The parameters of the Morse potential for bulk aluminium are as follow: $D_e = 0.2703$eV, $r_0 = 3.253$Å, $\alpha = 1.1646$ Å^{-1} [7]. The coefficients of the Murrell-Mottram potential are presented in Tab. 1.

Table 1
Parameters of the Murrell-Mottram potential [6]

Parameter	Value
a_2	7
a_3	8
D_e [eV]	0.9073
r_0 [Å]	2.7568
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

5. Results

The global minima for Morse (N = 2...21) and Murrell-Mottram (N = 3...15) clusters were determined using EA and AIS. The lowest energy levels for each cluster are shown in the Tab. 2. The values for Murrell-Mottram structures with nuclearity N = 16...20 (marked with *) are taken form [10].

The lowest average binding energies and their second differences, as a function of N, are presented in the following Fig. 2, 3, 4 and 5, respectively for Morse and Murrell-Mottram clusters.

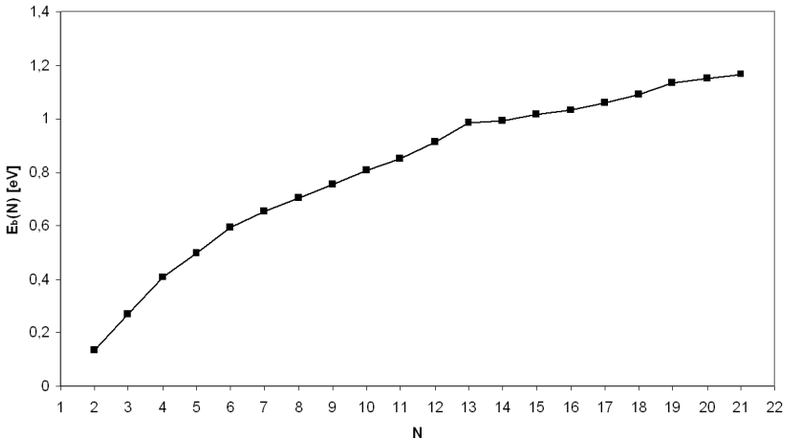

Fig. 2. Average binding energies of the Morse Clusters

Rys. 2. Średnia energia wiązania (potencjał Morsa)

Table 2

Global minima for Morse and Murrell-Mottram clusters

N	E_B [eV]	
	Morse	Murrell-Mottram
2	0.13515	–
3	0.2703	0.8317
4	0.40545	1.13783
5	0.49642	1.3247
6	0.59286	1.5039
7	0.65393	1.6046
8	0.70494	1.6923
9	0.75344	1.764
10	0.80528	1.8282
11	0.85051	1.8805
12	0.91256	1.9482
13	0.98672	2.0313
14	0.99274	2.0375
15	1.01499	2.0719
16	1.03278	2.1045*
17	1.06	2.1354*
18	1.0933	2.1618*
19	1.13553	2.189*
20	1.15096	2.20718*
21	1.1651	–

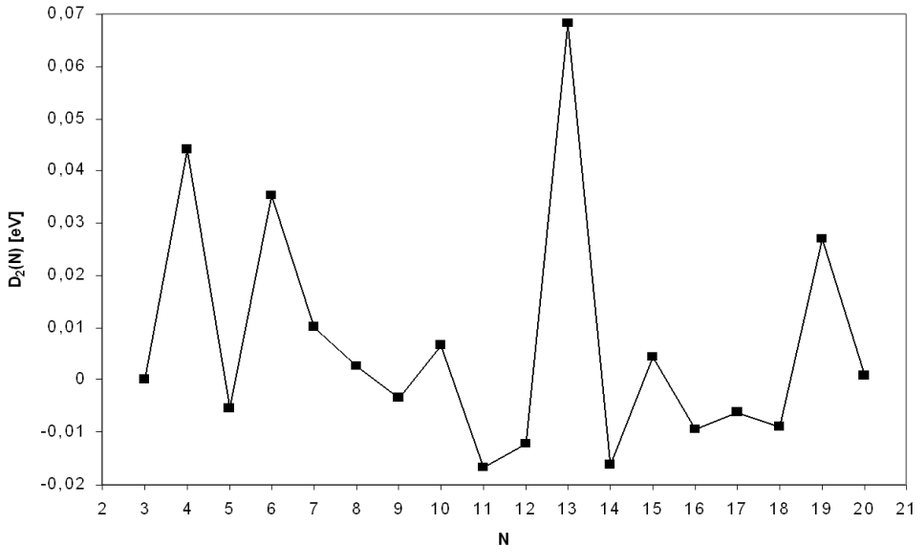

Fig. 3. Second difference in the binding energy of the Morse Clusters

Rys. 3. Iloraz róznicowy energii wiązania (potencjał Morsa)

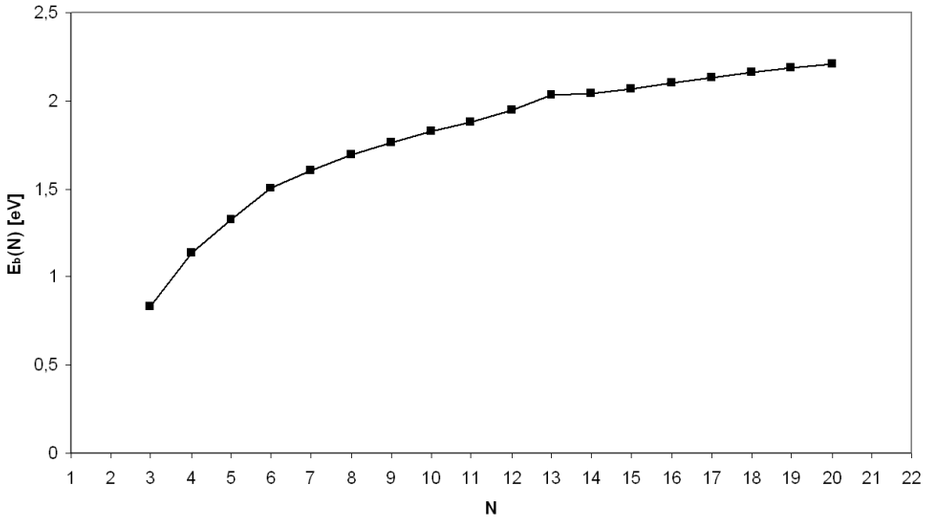

Fig. 4. Average binding energies of the Murrell-Mottram Clusters

Rys. 4. Średnia energia wiązania (potencja Murrela-Mottrama)

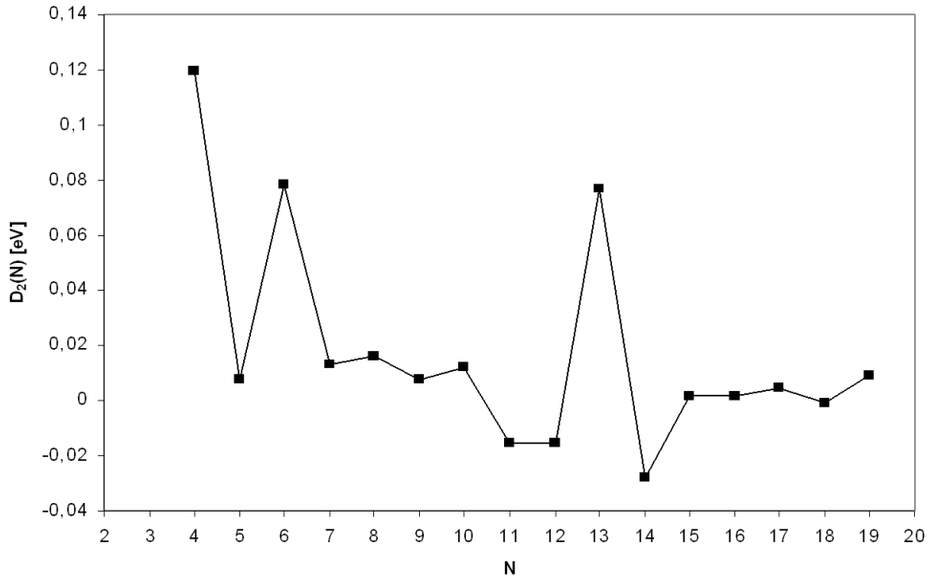

Fig. 5. Second difference in the binding energy of the Murrell-Mottram clusters

Rys. 5. Iloraz róznicowy energii wiązania (potencja Murrela-Mottrama)

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 in [5]. These clusters have identical shape for both: the Morse and the Murrell-Mottram potentials as shown in the Fig. 6.

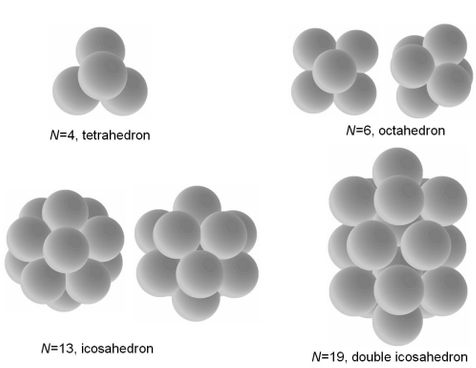

Fig. 6. The most stable Morse and Murrell-Mottram clusters

Rys. 6. Układy atomów o podwyższonej stabilności (dla potencjałów Morsa i Mirrella-Mottrama)

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, 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 pairwise interaction model (such as More or Lennard-Jones) has significantly more minima

than the PES based on the many-body Murrel-Mottram potential. These results are comparable with ones presented in [10, 18]. The described phenomena, for $N = 9$ is presented in the Fig. 7.

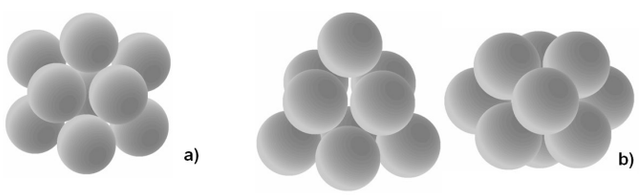

Fig. 7a) global minimum of Morse cluster, b) global minimum of Murell-Mottram corresponds to the second stable isomer of the Morse cluster ($E_B = 0.748161$eV)

Rys. 7a) Klaster dziewięcioatomowy: a) minimum globalne (dla pot. Murrella-Mottrama) posiadające identyczny kształt jak drugi izomer klastra z potencjałem Morsa

The total number of fitness function evaluations, for each type of the algorithm is presented in the Tab. 3.

Table 3

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	12 000	300	2368	1350	1350
4	7500	42 500	4600	5632	2400	3000
5	21 250	100 000	6800	7744	5250	6750
6	12 500	67 500	121 200	147 825	7200	5250
7	20 000	207 500	125 550	145 000	16 800	10 500
8	58 750	205 000	486 000	232 500	26 400	28 800
9	41 250	235 000	348 096	337 500	18 900	40 500
10	85 000	375 000	918 900	1 125 000	49 500	48 000
11	120 000	400 000	595 683	1 805 625	84 150	140 250
12	125 000	460 000	369 360	1 856 250	124 200	237 600
13	102 500	425 000	336 141	1 423 125	95 550	399 750
14	137 500	575 000	775 575	2 418 750	153 300	X
15	167 500	660 000	1 917 500	2 750 625	X	X
16	187 500	X	4 668 750	X	X	X
17	115 000	X	2 792 475	X	X	X
18	295 000	X	3 027 375	X	X	X
19	222 500	X	2 673 000	X	X	X
20	235 000	X	2 812 725	X	X	X

15	167 500	660 000	1 917 500	2 750 625	X	X
16	187 500	X	4 668 750	X	X	X
17	115 000	X	2 792 475	X	X	X
18	295 000	X	3 027 375	X	X	X
19	222 500	X	2 673 000	X	X	X
20	235 000	X	2 812 725	X	X	X

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.

6. Conclusions

The minimization of the potential energy of the atomic clusters using bio-inspired algorithms was performed. All the determined the lowest energy levels and shapes of the atomic structures are in good agreement with ones presented in bibliography (see chapter 2). 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. The reason for choosing Morse and Murrell-Mottram potential was available data of energy levels and configurations of atomic structures

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