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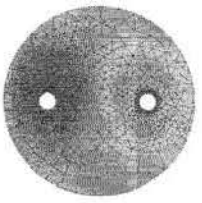
AKAPIT

COMPUTER METHODS IN MATERIALS SCIENCE

Informatyka w Technologii Materiałów

Vol. 15, 2015, No. 1



HYBRID PARALLEL EVOLUTIONARY ALGORITHM IN OPTIMIZATION OF 2D GRAPEHENE-LIKE MATERIALS

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Abstract

Development and application of the hybrid parallel evolutionary-conjugated gradient algorithm for searching for new, stable atomic arrangements of the two-dimensional graphene-like carbon lattices was described in this paper. The main goal of the optimization is to find stable arrangements of carbon atoms under imposed conditions (e.g. density, shape and size of the unit cell). Such configurations correspond to the minimal values of the total potential energy of the atomic system. Thus, the fitness function is formulated as the total potential energy of the atoms. Interactions between carbon atoms are modeled using Adaptive Intermolecular Reactive Bond Order potential. The parallel approach used in computations allows significant reduction of computation time. Validation of the achieved results and example of the model of new 2D material obtained using presented method were presented in this paper. The numerical scalability tests of the algorithm were performed on the IBM BlueGene/Q supercomputer.

Key words: nano-scale modeling, carbon materials, AIREBO potential, evolutionary algorithm, conjugate gradient minimization, parallel computing

1. INTRODUCTION

Carbon has many allotropes: the ones occurring naturally such as diamond, graphite and amorphous phase, as well as numerous synthetic structures like graphene, nanotubes and their derivatives. This phenomenon is caused by existence of carbon atoms in various hybridization states i.e. atoms of carbon with different electronic configurations, which determine types of bondings, angles between them and spatial arrangement of neighboring atoms.

In the recent years, graphene and similar two-dimensional materials are the subjects of particular interest of researchers (Cranford & Buehler, 2011; Enyashin & Ivanovskii, 2011; Narita et al., 2000; Peng et al., 2012; Scarpa et al., 2009) because of unique electronic, thermal and mechanical properties of such structures. Additionally, two-dimensional graphene-like materials can be used to create another, more complex class of nanostructures, like nanotubes.

Two-dimensional graphene-like materials can be considered as periodic, flat atomic networks, made of stable configurations of carbon atoms in certain hybridization states. It can be observed (figure 1), that each flat carbon network consists of certain parts like benzene rings (or other polygonal elements) and acetylenic linkages of different length connected and replicated periodically in each crystallographic direction. Thus, depend on arrangement of the considered structure, rectangular or triclinic unit cell of given size and atomic density can be identified in the each type of the flat periodic network. An overview of such structures (like graphyne

ISSN 1641-8581

and supergraphene), along with detailed description and investigation of their structural and electronic properties using thight-binding method can be found in the work by Enyashin and Ivanovskii (2011). The stress-strain relations and mechanical properties were obtained by Mrozek and Burczynski (2013).

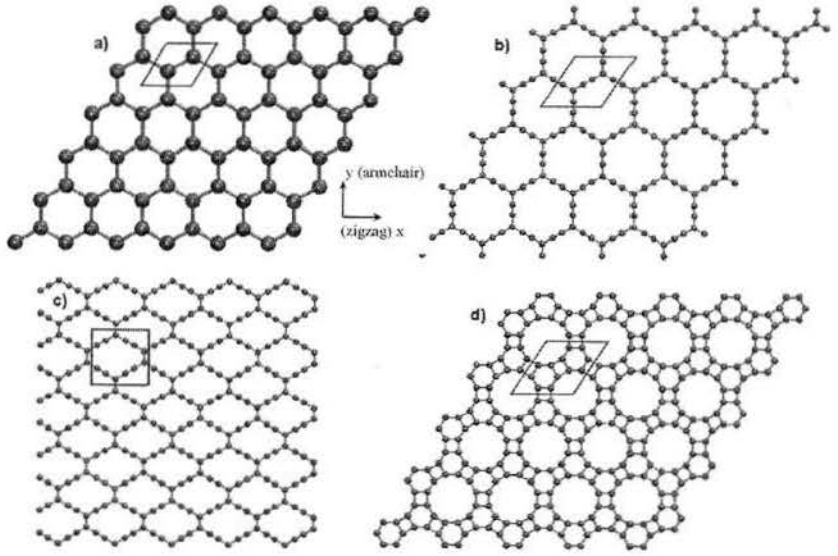

Fig. 1. Two-dimensional, periodic carbon networks: grapheme (a), supergraphene (b), structures made from distorted hexagons (c) and dodecagons (d).

Many examples of theoretically-predicted, two dimensional graphene-like materials, their periodic, modular structure suggest that potentially another, similar stable constructions can be built. In the combination with unique properties of the two-dimensional graphene-like materials, these facts became an inspiration to develop the method for finding new types of stable flat carbon networks. Such algorithm was proposed by authors and presented in this paper, along with validation of the achieved results and numerical examples.

Since the stable configurations of atoms correspond to the global (or local – in the case of isomers) minima on the Potential Energy Surface (PES), such a task can be considered as an optimization problem. However, searching for the global minimum on the PES is a non-trivial, NP-hard problem, because the number of local minima increases almost exponentially with the number of atoms in the considered structure.

Full quantum ab-initio methods, due to high costs of computations, are usually applied to the relatively small atomic systems. On the other hand, classical optimization methods (e.g. gradient-based ones) have problems with more complex, multimodal functions and reveal tendencies to stuck in local minima. That is why many various heuristic and artificial intelligence-based approaches have been recently applied to deal with similar problem of minimization of the potential energy of the atomic clusters (small, isolated atomic systems). Historically, the first group of the methods is based on searching of the PES, combined with simulation of the certain physical processes, e.g. Random Searches and Monte Carlo (MC) Simulated Annealing (Lloyd & Johnson, 1998) and Basin Hopping Monte Carlo (Wales & Doye, 1997). The second group of computational intelligence methods is inspired by biological mechanisms, present in natural environment and live organisms. The bio-inspired optimization methods of atomic structures, such as Genetic Algorithm (Roberts et al., 2000), Artificial Immune System (AIS) (Shao et al., 2004), and Particle Swarm Optimization (PSO) (Zhou et al., 2008) have become very popular in last years. Both of them give high probability of finding global minimum on the PES, however effectiveness is ransomed by long time of computations.

Authors of this paper successfully implemented set of bio-inspired algorithms: Distributed Evolutionary Algorithm (EA) (Mrozek et al., 2005), AIS and PSO (Mrozek et al., 2010) for investigation of small aluminium clusters with pair-wise Morse and Murrell-Mottram potentials.

Searching for new two-dimensional, graphene-like structures can be performed in the same manner, however needs more sophisticated interatomic interaction model, so called bond-order potential, should be applied. The bond-order potential is able to handle various hybridization states of carbon atoms, allowing creation of bondings with proper, neighborhood-dependent geometry. Additionally, in opposite to the isolated for environment atomic clusters, new algorithm should impose periodicity of the created structure.

Proposed and presented in this work hybrid algorithm combines Parallel Evolutionary Algorithm, prepared by the authors, and conjugated-gradient optimization, built-in LAMMPS software package (Lammps, 2014) which assists forming of the new atomic configuration. Behavior and potential energy of carbon atoms is determined using Adaptive Intermolecular Reactive Bond Order (AIREBO) potential, as developed by Stuart et al. (2000). Presented

algorithm has modular construction, thus each component can be replaced with functional equivalent (e.g. EA with AIS, gradient optimization with molecular dynamics, etc.) or adapted to use on new computer architectures. It should be noted that routines built-in LAMMPS program are effectively parallelized and can be used on multiprocessor computers (using MPI), as well as on GPUs (via CUDA). Proposed method can be extended to optimization of the three-dimensional molecular structures and may be considered as an alternative approach to existing ones such as the *ab-initio*/PSO algorithm called CALYPSO (Wang et al., 2010).

Presented work, is a continuation of author's investigations and modeling of atomic systems (Mrozek & Burczynski, 2013) and developed version of approach applied to the minimization of energy of atomic clusters (Mrozek et al., 2010). In the following chapters of this paper, proposed algorithm was described in detail, along with necessary validation of the results and numerical example.

The parallel version of algorithms for IBM BlueGene/Q supercomputer were implemented. The results of scalability tests for up to 512 cores are presented in the paper.

2. HYBRID EVOLUTIONARY-GRADIENT OPTIMIZATION METHOD

Proposed method incorporates two optimization techniques: the heuristic Evolutionary Algorithm (EA) and classical Conjugated Gradient (CG) routine. The EA (Michalewicz, 1996) mimics the mechanisms well-known from biological evolution of species, i.e. EA process the population of individuals. In this application, like in most practical cases, the individuals contain only one chromosome with vectors of genes (so-called design variables). The floating point representation of genes is used in optimization algorithm (Kuś & Burczyński, 2008). The genes (g1,...,gm) are the real-valued Cartesian coordinates of each atom. The range of coordinates is constrained by dimensions of the unit cell of newly created atomic lattice. Thus, the total number of design variables (genes) equals 2m, where 2 is the dimension of the problem and m denotes the number of atoms. Such construction is schematically presented (for three dimensional case) in figure 2.

In the initial population, each individual represents certain, constant number of atoms with randomly generated coordinates placed in the area of the unit cell with periodic boundaries. Dimensions and type (rectangular or triclinic) of the unit cell, as well as number of atoms, are the part of set of the parameters of the simulation. Such approach allows regulation of atomic density of created structure. It should be noted, that periodicity of the atomic structure significantly reduces number of design variables.

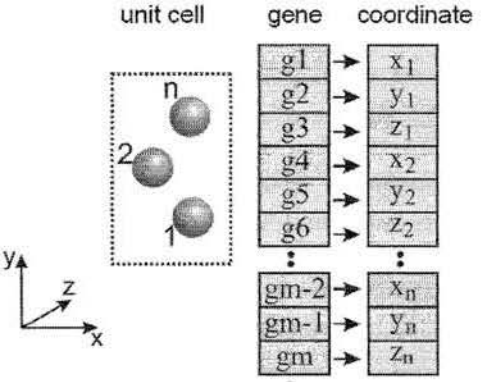

Fig. 2. Construction of the chromosome.

The fitness function is formulated as the total potential energy of the considered atomic system, i.e. sum over all potential energies of particular atomic interactions given by equation (1). Choosing the proper interaction model is crucial for this kind of task. In the presented case, potential energy, as well as neighborhood-dependent behavior of the carbon atoms is determined using Adaptive Intermolecular Reactive Bond Order (AIREBO) potential (Stuart et al., 2000), an extended REBO (E^{REBO}) model proposed by Brenner et al. (2002) with additional torsion ($E^{TORSION}$) and long range terms (E^{LJ}):

$$FF = \sum_i \sum_{j \neq i} \left(E_{ij}^{REBO} + E_{ij}^{LJ} + \sum_{k \neq i,j} \sum_{l \neq i,j,k} E_{kijl}^{TORSION} \right) \quad (1)$$

Application of AIREBO potential has a drawback, because this kind of model treats the long range interactions in the simplified way, using Lennard-Jones-like function (E^{LJ} term in equation 1) for computation of interactions of this type. Other, more accurate, approach of modeling carbon-carbon interactions can be applied: e.g. ReaxFF model, based on the first-principles calculations, developed by Chenoweth et al. (2008) or second generation Long-range Carbon Bond Order potential (LCBOPII) (Los et al., 2005). However, the AIREBO potential is fitted to handle different spatial configurations and hybridizations types of carbon atoms and is computationally more effective than the ReaxFF approach, which requires additional equilibration of the atomic charge every certain number of iterations (Rappe & Goddard, 1991; Nakano, 1997). Additionally, application of the AIREBO potential to the examination of mechanical

properties of various two dimensional graphene-like materials has been already performed by Mrozek and Burczynski, (2013) yields good agreement with results obtained by other researchers.

It should be noted, that the way of generation initial positions of the atoms may results in very small distances between them, or even overlapped atoms. Such configurations have high potential energies and are very unstable. Similar phenomenon may occur after mutation and crossover operations, preformed by EA. That is why initial and offspring populations have to be equilibrated, i.e. potential energy has to be minimized by correction of the positions of the atoms, before the first run of the EA. The coordinates of atoms are transferred to the LAMMPS program and the equilibration process is performed using potential energy minimization routine based on the Polak-Ribiere CG algorithm (Press et al., 2007). The minimized functional was defined in the same way as the fitness function (1), used in EA. Such approach, combined with bond order potential, ensures that structure is not only properly equilibrated, but additionally spatial configurations of atoms conform the rules characteristic for the molecular geometry of flat carbon networks. The periodicity of newly-created structure is also guaranteed by this routine, as well as proper boundary conditions, imposed on the unit cell.

After the conjugated-gradient minimization, the total potential energy (i.e. fitness function) is computed for each individual in the population. This part of algorithm is also handled by the LAMMPS.

The CG optimization is the most time-consuming part of the algorithm. To overcome this problem, authors decided to parallelize proposed algorithm and make it suitable for running on the multiprocessor computers (Kuś & Burczyński, 2008). Thus, the population is scattered into certain number of parts using MPI library. In the next step, each part is further processed in parallel way using dedicated instance of LAMMPS running on separate node of the computer.

Such minimized atomic structures, along with estimated values of fitness function are gathered together and imported to EA. The EA performs selection and invokes evolutionary operators like mutation and crossover. The selection chooses chromosomes for a new parent subpopulation taking into account values of the fitness function. Evolutionary operators change chromosome's genes and create new chromosomes for the offspring population. The uniform and Gaussian mutations, the simple crossover and ranking selection were implemented in presented algorithm (Kuś & Burczyński, 2008).

The main hybrid evolutionary-gradient algorithm works in iterative way: the offspring population is scattered into parts again, exported to the conjugated-gradient minimizer built-in LAMMPS. In the subsequent step all the data are gathered and exported to the EA, which perform selection of individuals and other evolution operations. These steps are repeated until the stop condition is not satisfied. The stop condition can be formulated as given maximum number of iterations or lack of improvement of the fitness functions during certain time interval. The flowchart of the Hybrid Parallel Evolutionary Algorithm is presented in figure 3.

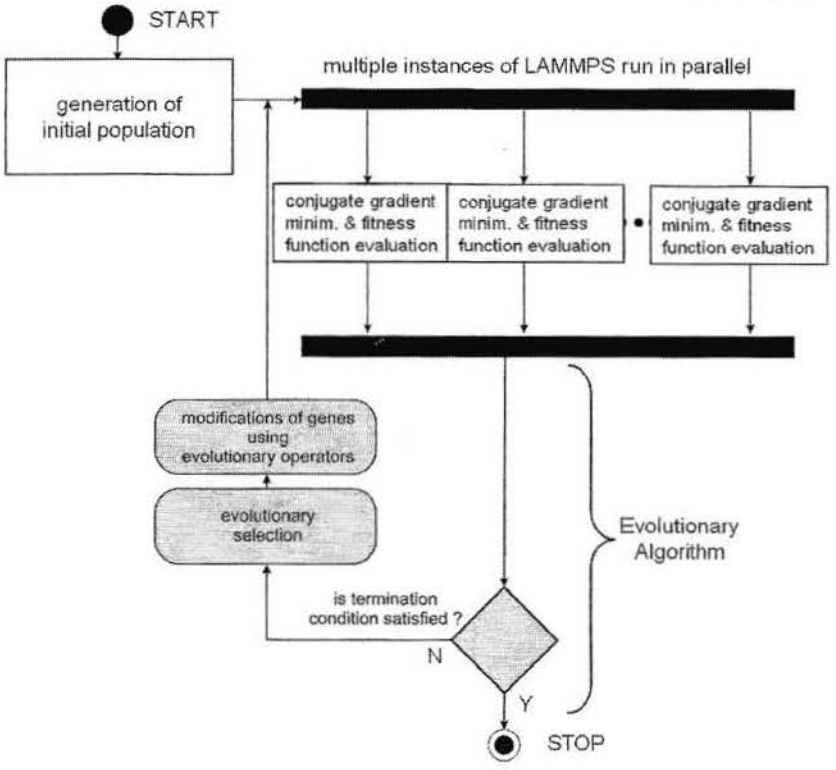

Fig. 3. Block diagram of hybrid parallel evolutionary optimization algorithm.

Algorithm in the form presented in figure 3 is dedicated for optimization rather small atomic systems (up to tens of atoms). However, since the computational routines built-in LAMMPS software package, including CG

energy minimization, are parallelized itself, it is possible to adapt described method to work effectively even with large, three dimensional structures. It can be done by the additional domain decomposition of each atomic system (individual) and running CG in parallel on the cores of each computational node. Parallelization in LAMMPS can be performed in classical manner, using MPI or OpenMP libraries, as well on GPUs, using CUDA. Such massive-parallel allows application of presented method to run effectively on supercomputers or new computer architectures.

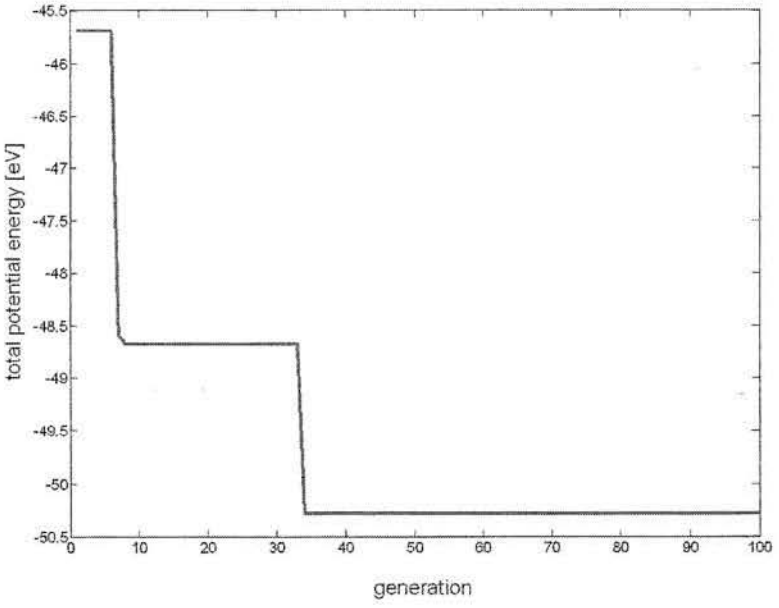

Fig. 4. Progress of minimization of total potential energy.

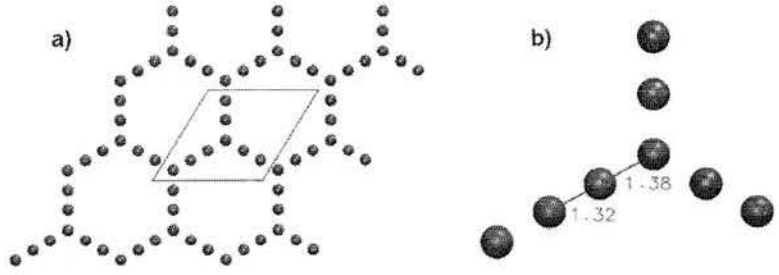

Fig. 5. Supergraphene – as found by optimization algorithm: structure (a), unit cell and bond lengths (b).

3. VALIDATION AND RESULTS

In the first step authors tried to find arrangements of carbon atoms which are already known from literature. Such approach was applied to verify the results, obtained with use of proposed algorithm. Two examples of known 2D graphene-like materials: supergraphene and network made of distorted hexagons, were selected for testing purposes (Enyashin & Ivanovskii, 2011). It should be noted, that presented configuration of the unit cells (shown in figure 1b and 1c, respectively) is non-unique and represents only one of the possible variants. It is an important fact, since proposed algorithm works on unit cells with given shape and atomic density. The results of validation, as well as examples of the obtained new carbon-based structures were presented and described in the following chapter. In the all of presented cases the population consists of 100 individuals. The probabilities of mutation and crossover operations were equal to 10%. Supergraphene (figure 1b) has a honeycomb structure, similar to graphene, where regular carbon-carbon bonds were replaced with acetylenic linkages, thus contains sp^2 and sp^1 hybridized atoms. Progress of energy minimization in function of iterations of evolutionary algorithm was presented in figure 4. The final structure of the supergraphene (figure 5a) was obtained in 34th generation. Triclinic unit cell (10Å×6Å), along with bond lengths, was shown in figure 5b. For comparison, the bond lengths computed using tight binding method (Enyashin & Ivanovskii, 2011) equals to 1.248Å between sp^1- sp^1 atoms and 1.402Å in the case of sp^1- sp^2 bonds. Analogical distances, time-averaged during run of classical Molecular Dynamics (MD) with the same AIREBO potential, were equal to 1.33Å and 1.39Å, respectively (Mrozek & Burczynski, 2013).

The second structure, used for testing purposes, is a combination of supergraphene and standard graphene lattices (figure 1c). This structure is built of distorted hexagons i.e. vertical acetylenic linkages of supergraphene were replaced with double carbon-carbon bonds. This structure also contains sp^2 and sp^1 hybridized atoms. The orthogonal unit cell was found with use of proposed algorithm in 5th iteration (figure 6). Resultant lattice and corresponding unit cell were shown in the figure 7a and 7b, respectively. Obtained unit cell has dimensions of 5Å×5Å and contains only 6 atoms instead of the one presented in paper by Enyashin and Ivanovskii, (2011): 7.03Å×6.91Å and 36 atoms, (see figure 1c).

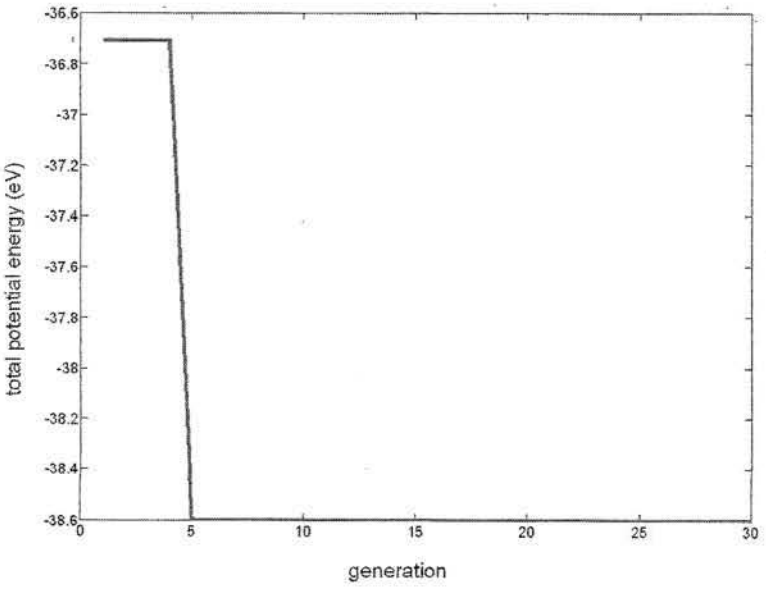

Fig. 6. Progress of minimization of total potential energy.

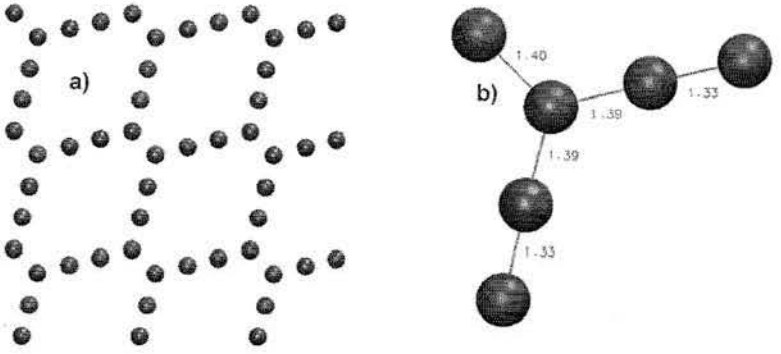

Fig. 7. Lattice from figure 1c – as found by optimization algorithm: structure (a), unit cell and bond lengths (b).

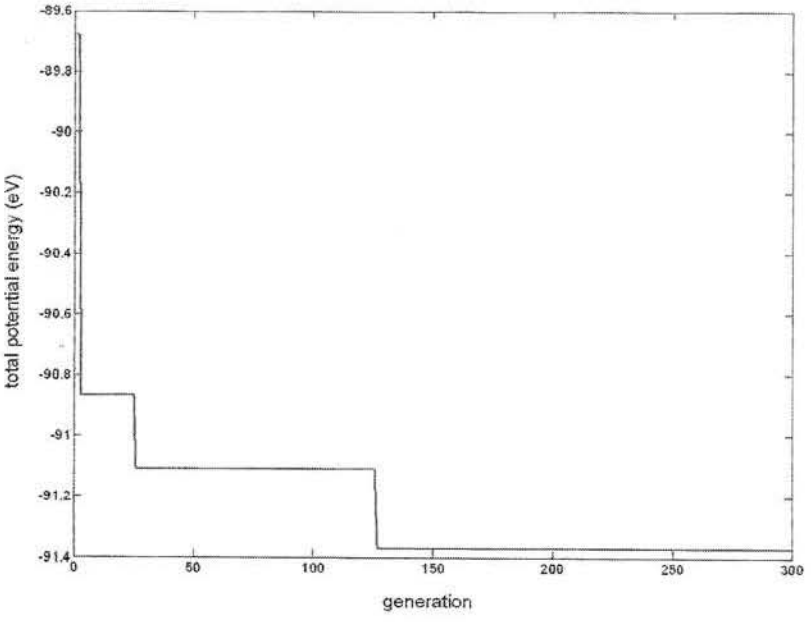

Fig. 8. Progress of minimization of total potential energy.

Again, similar difference between bond lengths, obtained using various computational methods and models occurred. The interatomic distances, revealed during optimization were presented in figure 7b. The tight binding computations, performed by Enyashin and Ivanovskii (2011) predicted distances of 1.237Å between sp^1-sp^1 atoms. Distances between sp^1- sp^2 and sp^2- sp^2 atoms equals to 1.413Å and 1.422Å, respectively.

Since test cases yields promising results, hybrid optimization algorithm was applied to search for the new stable configurations of given number of carbon atoms in unit cell of given size and periodic boundaries. In the following example 14 carbon atoms placed in the 7Å×6Å rectangular unit cell have undergone the process of minimization of total potential energy. The rest of the algorithm's parameters remained unchanged.

The progress of optimization was shown in figure 8. The final arrangement of the atoms was obtained in 127th generation. The result – a flat polycyclic network made of dodecagons of sp^2 hybridized carbon atoms was presented in figure 9a. More detailed view on unit cell, along with atom's potential energies and bond lengths, was shown in figure 9b.

The scalability of parallel algorithm was tested on IBM BlueGene/Q supercomputer located at ICM Warsaw. The supercomputer is build from 16 core one chip IBM PowerPC A2 1.6 GHz nodes connected by using 5D torus 40Gb low latency network. Each of the nodes has 16GB RAM, if all cores are used the 1GB per core is available. The number of atoms in unit cell is low and the memory consumption is low, and the 1GB per core is sufficient in discussed problem. The tests were performed for 1, 8, 16, 32, 64, 128, 256 and 512 cores. The lowest possible numbers of nodes were chosen (1 node for 1, 8, 16, 2 nodes for 32, 4 nodes for 64, 8 nodes for

128, 16 nodes for 256 and 32 nodes for 512 cores). The number of chromosomes in evolutionary algorithm was 512, the gradient minimization and objective function was computed using single core. The work was divided evenly between cores, ex. for 128 cores test case, each of the 128 nodes performs gradient minimization for 4 chromosomes. The MPI was used in parallelization of evolutionary algorithm. The speedup of the computations were computed and presented in figure 10. The maximum speedup was about 167 for 512 cores. The wall time was measured from start of the program till the end of all computations (including creation of objects etc.). The performance of the algorithm is not close to the linear and optimization of the code is planned in the future.

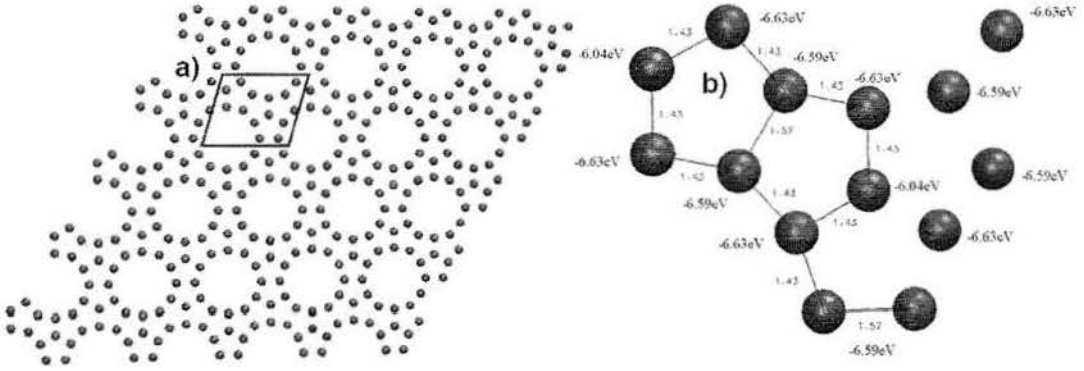

Fig. 9. New carbon network found by optimization algorithm: structure (a), unit cell (b).

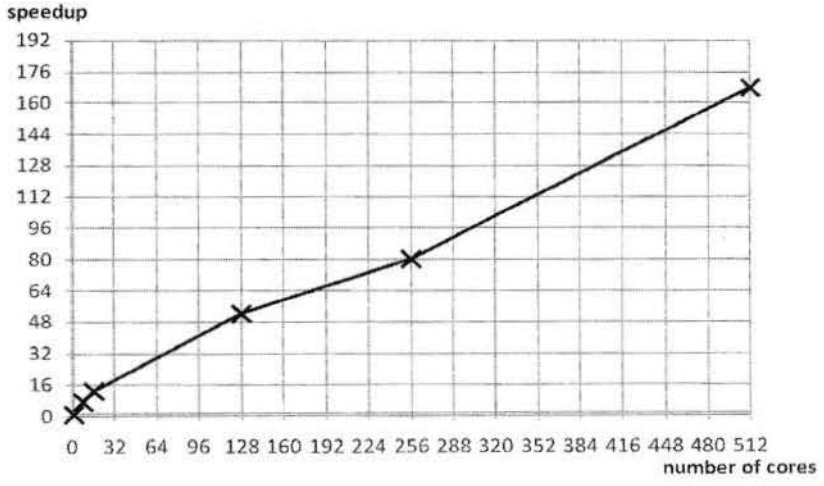

Fig. 10. The scalability of optimization algorithm.

4. CONCLUSIONS

The hybrid parallel evolutionary algorithm, applied to searching for the new two-dimensional graphene-like materials was described and obtained results were presented in this paper. Proposed method was able to find already-known structures like supergraphene, as well as new, stable one. The final form and properties of optimized structures depends on the assumed size, type and atomic density of the unit cell. Thus, the considered optimization problem can be reformulated, even using multi-criteria approach, and applied to searching for molecular structure with predefined material properties (e.g. stiffness tensor). Every component of the presented algorithm can be replaced with functional equivalent (e.g. optimization method, atomic potential), additionally proposed approach is ready to use in the optimization of the three-dimensional molecular structures. The parallel approach used in the most time consuming parts of algorithm such as conjugated gradient minimization and evaluation of the fitness function significantly reduces the time of optimization. The scalability of the algorithm for up to 512 cores on IBM BlueGene/Q was tested and presented in the paper. Analysis of the times of computations yields great scalability of implemented algorithm. Obtained results and possible applications of described method make it a potential tool for molecular optimization, not only for the flat, carbon systems.

ACKNOWLEDGEMENT

Calculations were performed at the Interdisciplinary Centre for Modelling Mathematical and Computational Modelling at the University of Warsaw under the grant G56-1.

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POSZUKIWANIE NOWYCH, PŁASKICH MATERIAŁÓW GRAFENOPODOBNYCH PRZY UŻYCIU HYBRYDOWEGO ALGORYTMU OPTYMALIZACJI

Streszczenie

W artykule przedstawiona została metoda optymalizacji płaskich sieci zbudowanych z atomów węgla. Proponowane podejście bazuje na połączeniu równoległego algorytmu ewolucyjnego z metodą gradientu sprzężonego. Funkcją celu jest wartość energii potencjalnej całego układu atomów. Głównym zadaniem algorytmu jest znalezienie stabilnych położeń atomów w komórce elementarnej - odpowiadających minimum energii potencjalnej całego układu. Algorytm ewolucyjny został zrównoleglony (podział populacji na części), ponadto wspomagający go algorytm gradientowy (wbudowany w program LAMMPS) może również być uruchomiony w wersji sekwencyjnej, jak i równoległej. Jako model oddziaływań między atomami węgla zastosowano potencjał AIREBO, uwzględniający różne stany hybrydyzacji atomów węgla. W pracy zaprezentowano wyniki optymalizacji obejmujące poszukiwania znanych materiałów literatury płaskich materiałów grafenopodobnych, jak i nowych konfiguracji. Ponadto, dla nowych struktur wyznaczono parametry mechaniczne.

Received: November 13, 2014
Received in a revised form: December 12, 2014
Accepted: December 17, 2014