Generation of graphene-like atoms structures by means of memetic algorithms

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ABSTRACT

The optimization of new graphene-like structures allows to obtain new stable structures with unique material properties. The goal of the paper is to describe an algorithm which can be used to solve optimization problem and define optimization objectives and constraints on design variables. Carbon has many allotropes such as diamond, graphite and amorphous phase, as well as numerous synthetic structures like graphene and nanotubes. 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. Two dimensional graphene-like materials can be considered as periodic, flat atomic networks, made of stable configurations of carbon atoms in certain hybridization states. Depend on arrangement of the considered structure, rectangular or triclinic unit cell of given size and atomic density can be identified. 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. 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.

The memetic algorithms [1] are based on combining evolutionary, global, population based algorithm with local improvements methods for some individuals or chromosomes. The memetic algorithms are sometimes named hybrid algorithms or hybrid evolutionary algorithms because they are kind of hybrid of global and local optimization techniques [2]. The global evolutionary algorithm coupled with local conjugate gradient algorithm is used in the paper. The driving part of the optimization is the evolutionary algorithm with evolving population of problems potential solutions. The typical operators like mutation and crossover are used without modifications. The selection are also preserved. The gradient algorithm modifies the genes of all chromosomes before computing fitness functions. The modification leads to modification of evolutionary algorithm process of optimum search. The evolutionary operators moves chromosomes to the new areas of attraction and the gradient based algorithm moves chromosome to the local optimum value. The proposed approach works well for highly multimodal fitness function for which is hard to close to local optimum using typical evolutionary algorithm.

The full paper will contain detailed description of memetic algorithm build on top of evolutionary algorithm and conjugate gradient method provided for atomic structures by LAMMPS package[3]. The examples of optimized structures will be shown. The paper is extended work presented in [4].

References

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