Creation of new graphene-like materials by means of the hybrid parallel evolutionary algorithm

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ABSTRACT

The application of a hybrid algorithm for creating new, stable atomic arrangements of the two-dimensional graphene-like carbon lattices is presented. The hybrid algorithm combines the Parallel Evolutionary Algorithm, prepared by the authors, and the conjugated-gradient method, built-in LAMMPS software package, which assists forming of a new atomic configuration. The main aim is to find stable arrangements of carbon atoms under imposed conditions. It means that optimal density, shape and size of the unit cell are searched. Optimal configurations correspond to the minimal values of the total potential energy of the carbon atomic system. The fitness function is formulated as the total potential energy of atoms. Interactions between carbon atoms are modeled using the Adaptive Intermolecular Reactive Bond Order (AIREBO) potential [3]. The computational parallel approach presented in the paper allows significant reduction of computation time. Validation of the obtained results and examples of models of a new 2D material are presented. The numerical scalability tests of the algorithm are performed on the IBM BlueGene/Q supercomputer. Presented hybrid 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). Presented work, is a continuation of author's investigations on modeling of atomic systems [1] and developed version of the approach applied to the minimization of energy of atomic clusters [2].

REFERENCES

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