INTELLIGENT DESIGN OF NEW 2D NANO-MATERIALS

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<u>*Summary*</u> New stable atomic arrangements in 2D nanostructures based on carbon (C) and as well as on molybdenum (Mo) using a memetic algorithm and the density functional theory (DFT) are presented. The semiconducting carbon allotrope as graphene-like material and the Single-Layered Molybdenum Disulfide (SLMoS$_2$) heterostructures with desired mechanical properties are created.

INTRODUCTION

2D materials play important role in modern materials science. Apart from materials based on carbon, e.g. graphene, there is possible to create new 2D materials based on molybdenum. New graphen-like materials X and Y created by hybrid intelligent approach [1, 2] represent the first class of materials. One of the most prominent 2D material based on molybdenum is the molybdenum disulfide (MoS$_2$), which reveals polymorphism at the nanolevel.

Optimal design technique enabling to obtain new 2D semiconducting carbon allotrope as graphene-like material and SLMoS$_2$ heterostructures with desired mechanical properties is presented. The proposed method is based on the memetic global optimization of the potential energy of the nanostructure. The behaviour and energy of the atoms is determined by the AEROBO potential in the case of graphene and the REAX-FF potential in the case of molybdenum. Examples of such semiconducting carbon allotrope and periodic SLMoS$_2$ 2H/1T heterostructure are presented with corresponding mechanical properties.

INTELLIGENT DESIGN BASED ON MEMETIC COMPUTING

The memetic algorithm, proposed and presented in this work, combines the parallel **E**volutionary **A**lgorithm (EA) prepared by the authors, and the classical **C**onjugated-**G**radient (CG) minimization of the total potential energy of the optimized atomic system. Since the processed structure is considered as a discrete atomic model, the behavior and the potential energy of carbon atoms are determined using the **A**daptive **I**ntermolecular **R**eactive **E**mpirical **B**ond **O**rder (AIREBO) in the case nanostructures based on carbon and REAAX-FF in the case of nanostructures based on molybdenum.

A chromosome represents design variables in the form of real-valued Cartesian coordinates of each atom in the considered unit cell of the newly created atomic lattice. Each chromosome represents a certain spatial arrangement of atoms. In the initial population, atoms have randomly generated coordinates and are placed in the area of the unit cell with periodic boundaries. Dimensions, the rectangular or triclinic type of the unit cell, as well as the number of atoms, are part of a set of parameters of the simulation. Such an approach enables controlling the value of atomic density of the newly-created structure. The periodicity of the atomic structure significantly reduces the number of design variables.

The fitness function is formulated as the total potential energy of the considered atomic system, i.e., the total sum of all potential energies of particular atomic interactions.

The periodicity of the newly-created structure is also achieved in this step by proper boundary conditions, imposed on the unit cell. After the CG minimization of the potential energy, the objective function is computed for each individual in the population. The CG optimization is the most time-consuming part of the algorithm. To overcome this problem, the authors decided to parallelize the proposed algorithm and make it suitable for running on multiprocessor computers. Thus, the population is scattered into certain number of parts using the MPI library. In the next step, each part is further processed in the parallel way.

DESIGNING OF NEW 2D SEMICONDUCTING CARBON ALLOTROPE

A new, single-atom thick semiconducting 2D-graphene-like material, called Anisotropic-Cyclicgraphene, is generated by the two stage searching strategy linking molecular and *ab initio* approaches. The candidate is derived from the memetic based algorithm and molecular simulations and next is profoundly analysed using the first-principles density functional theory from the structural, mechanical, phonon, and electronic properties point of view.

The structure of the 2D-graphene-like material is considered as a discrete atomic model, with imposed periodic boundaries. The behavior of such a system is investigated using one of the molecular methods. The potential energy of carbon atoms, the forces acting between them and the overall behavior is determined by the AIREBO potential, especially developed for hydrocarbons.

The goal is to discover an atomic structure with stable configuration, predefined number of atoms and elastic material properties. The elastic properties are computed based on the molecular analysis of a structure with applied small strains.   The atomic structures with orthotropic elastic material properties are taken into account. The objective function depends on the norm of differences between of prescribed and computed elastic properties [3].

First-principles calculations with the use of the density functional theory (DFT) within the pseudopotential, plane-wave

approximation (PP-PW) are made using the Cambridge Serial Total Energy Package (CASTEP). For structural, mechanical and phonon calculations the modified Perdew-Burke-Ernzerhof generalized gradient approximation for solids is applied as an exchange-correlation functional whereas for band structure computations the hybrid exchange-correlation functional HSE06.

The material derived from the first stage is then profoundly analyzed using the first-principles density functional theory from the structural, mechanical, phonon and electronic properties point of view. The proposed Anisotropic-Cyclicgraphene is mechanically, dynamically and thermally stable and can be semiconducting-like with a direct band gap of 0.829 eV [4].

DESIGNING OF NEW 2D MATERIALS BASED ON MOLYBDENUM

One of the most prominent 2D material based on molybdenum is the Single-Layered Molybdenum Disulfide ($SLMoS_2$), which reveals polymorphism at the nanolevel.

The 2H phase has semiconducting properties and approx. Young's modulus equals to 130 N/m, while the 1T polymorph reveals metallic or ferroelectric properties and two times lower stiffness [2]. Both phases of MoS_2 can exist simultaneously [3].

Intelligent designing $SLMoS_2$ heterostructures (a 2H lattice with Δ-shape 1T inclusion) with desired mechanical properties is presented. The memetic optimization approach enabling to obtain MoS_2 heterostructures with desired mechanical properties is applied. The behaviour and energy of the atoms is determined by the REAX-FF potential [5]. Examples of such periodic $SLMoS_2$ 2H/1T heterostructures are presented in the paper with corresponding mechanical properties.

CONCLUSIONS

The presented approach is applied to design of 2D nano-materials based on carbon as well as molybdenum.

The process of designing nano-material based carbon consists of two stages. In the first molecular stage the optimization problem is solved using the memetic algorithm. The second stage based on the first-principles density functional theory is used to examine results from the previous step. The proposed polymorph of graphene is mechanically, dynamically, and thermally stable and can be semiconducting with a direct band gap of 0.829 eV.

The intelligent optimization technique is also applied to obtain nano-structures based on molybdenum – $SLMoS_2$ heterostructures with desired mechanical properties.

Some results in this paper are unique and we trust will be verified by other works. The synthesis of the proposed structure is a separate task and goes beyond the area of this work.

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