CMM-SolMech 2022 conference

S08 Nanomaterials and nanocomposites, their properties and applications

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DESIGN OF NANOSTRUCTURES BASED ON MOLYBDENUM

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2D materials play important role in modern material science. Apart from graphene [2] based on carbon there is possible to create new 2D materials based on molybdenum. One of the most prominent 2D material is the Molybdenum Disulfide (MoS2), 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 [3]. Both phases of MoS2 can exist simultaneously [4]. This paper presents an optimization approach enabling to obtain MoS2 heterostructures with desired mechanical properties. The proposed memetic approach combines the global optimization, based on the bio-inspired algorithms (e.g. evolutionary algorithm) with the local conjugated-gradient minimization of the potential energy of the nanostructure [2]. The behavior and energy of the atoms is determined by the REAX-FF potential [1,3].
Memetic optimization of MoS2 with presence of defects in the form of missing S atoms or the substitution of Mo atoms in place of S is also considered. The MoS2 structure is modelled with the use of LAMMPS software and the Stillinger-Weber interatomic potential is used

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