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OPTIMAL DESIGN OF MECHANICAL PROPERTIES OF MoS2 NANOSTRUCTURES

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The paper describes optimal design 2D nanomaterial – molybdenum disulfide MoS_2. The optimization problem is defined as a minimization of difference of actual and predefined mechanical properties of the structure. The predefined properties of material stiffness matrix are given by the user and the actual properties depend on results of the direct problem.

The optimization procedure based on intelligent computing [1] introduces modifications to the atomic structure by eliminating part of the atoms and creating voids. The shapes of the voids are defined using design variables and predefined shapes.

The atomic structure is periodic and only part of the structure is modelled [3]. The objective function is computed on the base of mechanical properties obtained using molecular statics analysis. The LAMMPS software [2] is used for direct problems solving.

The paper contains numerical examples showing the resulting atomic MoS2 structures for chosen prescribed mechanical properties. The differences between expected and best found results were discussed.

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