BIOINSPIRED OPTIMIZATION OF MECHANICAL PROPERTIES OF TWO-PHASE SINGLE-LAYERED MoS_2 STRUCTURES

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So-called two-dimensional (2D) materials play important role in modern material science, development of the optoelectronic devices and even combined, micro-electromechanical systems (sensors, actuators). One of the most prominent 2D material (apart from graphene) 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 [3]. As described by [1] both phases of $SLMoS_2$ can exist simultaneously. This paper presents optimization technique which allows to obtain $SLMoS_2$ heterostructures (a 2H lattice with Δ-shape 1T inclusion) with desired mechanical properties. Proposed method combines the global optimization, based on the bio-inspired algorithms (evolutionary, artificial immune system, etc.) 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 [3]. Two examples of such periodic $SLMoS_2$ 2H/1T heterostructures are shown in Figure 1 with corresponding mechanical properties.

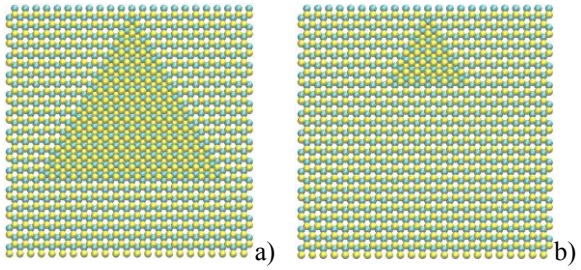

Figure 1. Two 72x72Å $SLMoS_2$ heterostructures with diffrent amout of 1T phase. Young's moduli under 1% strain: a) 122 N/m - isotropic, b) 143/130 N/m (zigzag/armchair direction).

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