Modelling of molybdenum-based 2D materials

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Abstract

The flat, two dimensional materials play important role in the research and industrial applications in the last 15 years. The new materials with flat atomic structures are discovered every month. The focus of the paper is on the modelling of the single layer molybdenum disulphide based material. The numerical simulations and mechanical material properties are described and discussed.

Keywords: molybdenum, two dimensional materials, molecular modelling, MoS_2

1. Introduction

The two dimensional (2D) materials are important for creation of modern composites, sensors, electronic and optical devices. The most of the research up to now is focused on graphene based materials. The last years bring a large range of 2D materials with different mechanical, thermal, electric and optic properties [2,4,5,8]. Some of the material can be produced nowadays, some exists only as a numerical models. The authors discovered 2D structures of materials based on the carbon in previous research [7]. The paper focuses on modelling flat material, based on molybdenum disulphide.

2. Numerical modelling of MoS_2 sheet

Several approaches of modelling molybdenum disulfide (MoS_2) materials have been recently developed. The most accurate *ab-inito* calculations have the highest computational cost, thus are restricted to simulate rather small atomic systems. Simulations of the phenomena which occur in larger scales (e.g. order of micrometers) require different, simpler but less time-consuming approaches like Molecular Dynamic (MD) method, equipped with proper interaction model, called atomic potential.

In the work, the atomic potential energy and interactions between Mo and S atoms are described using Stillinger-Weber potential [1]:

$$\Phi(1,...,N)=\sum_{i<j}V_2(i,j)+\sum_{i<j<k}V_3(i,j,k) \tag{1}$$

which combines two- (2) and three-body interactions (3), respectively:

$$V_2=\varepsilon A\left(B\sigma^{p}r_{ij}^{-p}-\sigma^{q}r_{ij}^{-q}\right)e^{\left[\sigma\left(r_{ij}-a\sigma\right)^{-1}\right]} \tag{2}$$

$$V_3=\varepsilon\lambda e^{\left[\gamma\sigma\left(r_{ij}-a\sigma\right)^{-1}+\gamma\sigma\left(r_{jk}-a\sigma\right)^{-1}\right]}\left(\cos\theta_{jik}-\cos\theta_0\right)^2 \tag{3}$$

The term V_2 depends on linear distances (r_{ij}) between pair of atoms *i* and *j*, while V_3 additionally takes into account angular configuration between particular triad of atoms *j*-*i*-*k*. The values of the set of parameters, visible in equations (2) and (3) are taken form [1] and were fitted to mimic properties (i.e. lattice constants, phonon spectrum, thermal and mechanical properties) of Single-Layer MoS_2 ($SLMoS_2$) materials.

The model of two dimensional, periodic structure of the $SLMoS_2$ used in computations is presented in Fig. 1.

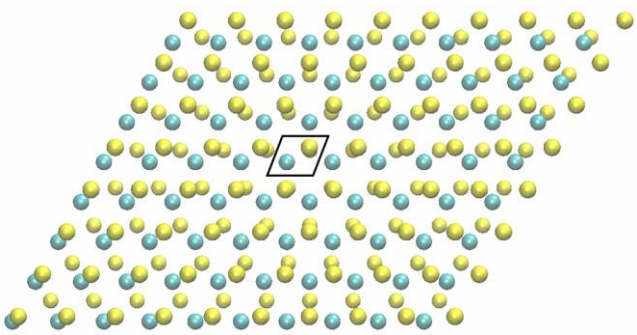

Figure 1: The structure of the two dimensional sheet of Single-Layer MoS_2

Although, similar to the graphene, the single-layer MoS_2 is considered as a 2D material, actually is made from three layers of atoms: the one, central layer of Mo atoms is coated by two layers of S atoms. The triclinic unit cell, marked in the Fig. 1, contains one Mo atom and two S atoms and in the resultant lattice each Mo atom has six S nearest-neighbours.

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The computational model were created and solved with use of presented potential (1) and LAMMPS software [3].

3. Mechanical properties of MoS_2 sheet

The several Molecular Dynamic based simulations of the tensile tests were performed in the wide range of temperatures (10K-300K) using atomic models of various sizes. One of the results is shown in Fig 2. The investigated atomic model of $SLMoS_2$ contains 2400 atoms, has triclinic unit cell and dimensions of 125Å x 55Å. Periodic boundaries were imposed in the two dimensions. Temperature of the simulation was set to 10K to keep the amount of kinetic energy (thus fluctuations of the atoms) at low level. Such test conditions were validated and described in detail by the authors in [6].

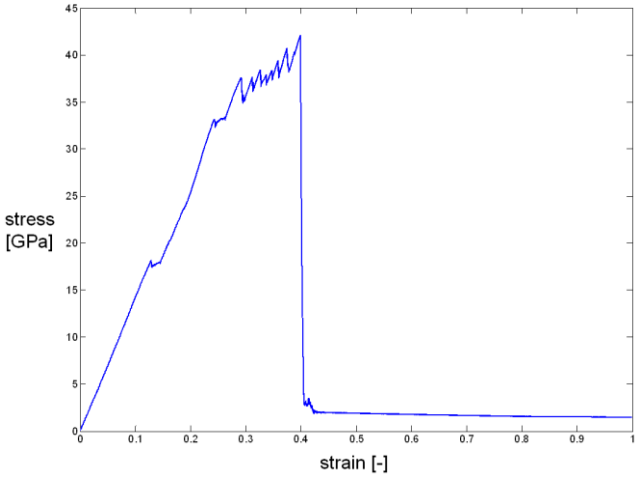

Figure 2: The results of tensile test for $SLMoS_2$

The resultant stress-strain characteristic (in the zigzag direction) is presented in the Fig. 2. The SLMoS2 reveals linear behaviour in small strain range. The average Young modulus is equal to 85.3 N/m (140GPa, assuming 6.09Å thickness of the layer). The values of the Young moduli reported in literature vary between 90-240N/m and depend on applied method, model and test conditions [1].

4. Conclusions

The molecular analysis of $SLMoS_2$ was presented in the paper. The influence of the size of the atomic model was taken into account. The results, obtained using molecular statics (simulations at 0K) and dynamics (set of simulations preformed at finite temperatures from 10K to 300K) are comparable with the results found in literature. The presented model can be used in future research for discovery new atomic structures of two dimensional materials.

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