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The influence of defects on mechanical properties in molybdenum disulfide flat material

Wacław Kuś[1,2], Mohammed Javeed Akhter[2], Adam Mrozek[3], Tadeusz Burczyński[2]

[1] Silesian University of Technology, Gliwice, Poland
[2] Institute of Fundamental Technological Research Polish Academy of Science, Warszawa, Poland
[3] AGH University of Science and Technology, Cracow, Poland
Emails of the all authors: waclaw.kus@polsl.pl, mjakhter@ippt.pan.pl, amrozek@agh.edu.pl, tburczynski@ippt.pan.pl

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1. Introduction

The paper is devoted to computationally derivation of mechanical properties of two dimensional structures based on molybdenum disulfide. The two dimensional materials have been a focus of attention for scientists. The carbon based materials are the most frequently analyzed. The number of discovered flat materials is growing rapidly. The molybdenum disulfide is a flat material with known mechanical properties [3,4]. The paper takes into account not only ideal flat structure, but also material containing defects. The main defects in MoS2 are due to missing sulphur atoms in structure, the influence of these defects on mechanical properties are presented in the paper. It is found that the increase of defects concentration leads to the noticeable decrease in the stiffness,

2. The mechanical properties evaluation

The mechanical properties of atomic structures can be obtained with use of molecular static method[1]. The molecular statics takes into account positions of atoms and forces between them. The interatomic forces are defined on the base of atomic potentials and are in most cases nonlinear functions of distances between atoms. The potentials can be defined as a function of two, three or more atoms interactions. The interatomic potentials are created on the basis of results of ab initio analyses. The Stilinger Webber [5] interatomic potential is used in the paper. The molecular static analyses were performed with use LAMPS software [2]. The mechanical properties can be obtained by disturbing stable position of atomic structure [3,4].

3. Numerical results

The influence of defect on mechanical properties of MoS2 was analysed with use of flat structure with 338 Mo atoms. The defect where the sulphur atoms are missing from the structure are considered. The perfect structure without defects is shown in Fig. 1a,b. The structure contains one Mo layer and two S layers. The perfect structure was modified by removing part of the sulphur atoms. The percentage of removed sulphur atoms is a parameter of the modified structure. The removed sulphur atoms were chosen randomly. The example of structures with 5% and 25% of removed atoms are shown in Fig. 1c,d. The mechanical properties of the structures with defects are presented in Table 1. The mechanical properties are shown as a stiffness in two directions and shear stiffness.

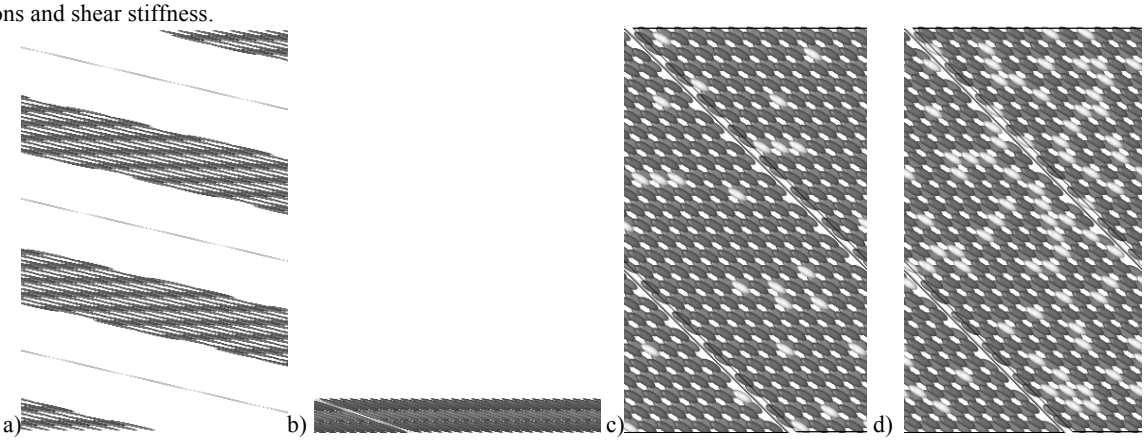

Figure 1. The MoS2 structures: a) perfect - view from top, b) side view, c) with 5% missing sulfur atoms, d) with 25% missing sulfur atoms (light gray color in c) and d) means removed atoms)

Table 1. Mechanical properties of the structures.

Structure	C_{11} [N/m]	C_{22} [N/m]	C_{12} [N/m]
without defects	149.0	150.0	52.0
0.1% defects	148.8	149.5	52.0
1% defects	145.9	146.7	50.9
2% defects	141.7	141.5	49.1
5% defects	130.1	126.9	43.9
10% defects	116.8	110.5	38.1
15% defects	102.5	89.9	30.9
20% defects	80.5	79.7	21.1
25% defects	68.5	64.2	18.6

In Table 1, we show the intrinsic engineering constants of MoS2 structure versus the defect percentage at 0 K, compared with those of the perfect MoS2 sheet. C_{11}, C_{22} and C_{12} denote the elements of stiffness matrix. The perfect structure MoS_2 can be treated as isotropic 2D elastic materials due to the symmetric geometry, the defects have small influence on difference between stiffness in two directions.

The results shows high influence of defects on mechanical properties. The 5% missing sulphurs lead to above 10% change in stiffness of the structure. The influence is even higher when the ratio of defects grows. The obtained results show importance of analysing of flat structures taking into account possibility of defects and their influence on the mechanical properties.

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