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A Comparative Investigation of the Mechanical Properties of Single and Bi Layer MoS_2 Structures: Influences of Defect, Strain Rate and Temperature

Ahmet Emin ŞENTÜRK*[1]

Abstract

In this paper, the mechanical properties of single and bi layer molybdenum disulfide (MoS_2) structures are investigated using uniaxial tensile molecular dynamics (MD) simulation. According to the results of MD simulations, these structures show superior mechanical properties (failure strain, ultimate tensile strength and Young's modulus) for various applications of nanodevice. The mechanical properties of single and bi layer MoS_2 structures are studied at four different temperatures between 300 K and 900 K and different strain rates from 10^7 s^{-1} to 10^9 s^{-1}. As temperature increases up to 900 K, the mechanical properties of single and bi layer MoS_2 structures gradually decrease, due to the high temprerature's weakening effect. Also, changing of temperatures shows more effect on the bi layer MoS_2 structure than single layer MoS_2 structure. Furthermore, MD results show that the mechanical properties of single and bi layer MoS_2 structures demonstrate increasing trend when the strain rate increases. Different strain rates indicate similar effects on the mechanical properties of single and bi layer MoS_2 structures. On the other hand, the mechanical properties of these structures are adversely affected by structural defects. Accordingly, the influences of two different S atom types vacancy defect on the mechanical properties of single and bi layer MoS_2 structures are examined. When the vacancy defect concentrations in MoS_2 structures increase, the mechanical properties of these structures decrease significantly. In addition, S atom bi vacancy defects type exerts more effect on the mechanical properties of single and bi layer MoS_2 structures than S atom single vacancy defect type do by increasing concentration. Additionally, vacancy defects indicate more influence on the bi layer MoS_2 structure than single layer MoS_2 structure. Finally, the results of this study make them excellent candidate for nano-mechanical systems.

Keywords: molecular dynamics, MoS_2 structure, mechanical properties.

1. INTRODUCTION

The discovery of 2D nanomaterials, many investigations have been conducted for the applications in nanodevice. Due to 2D transition metal dichalcogenides' (TMDs) electronic, mechanical, thermal, structural properties and many potential applications [1-5], they have gained increasing attention, recently. For example, molybdenum disulfide (MoS_2), a 2D semiconductor, is promising member of TMDs family with hexagonal lattice structure. Different from graphene, because of its considerable band gap, MoS_2 is proposed as an excellent potential candidate in flexible electronics and optoelectronic devices [6, 7], piezoelectronics [8],

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high-performance field-effect transistors [3], and valleytronics, [9, 10]. MoS_2 can be further manipulated via changing its stacking order [11], number of layer [12], or by application of mechanical strain [13, 14]. MoS_2 is consisting of S_{upper}–Mo–S_{lower} triple thickness layers. During synthesizing or processing, in reality, structural defects, such as, Stone-Wales and vacancy, are unavoidably observed in MoS_2. Structural defect affects the physical, mechanical and chemical properties of MoS_2. Only vacancy defect was examined in this investigation.

The mechanical properties of 2D nanostructures have examined by several researchers using molecular dynamics (MD) simulations, in recent years [15, 16]. The published knowledges regarding the mechanical properties of single and bi layers MoS_2 structures are still limited, despite of the earlier experimental realization of these structures. Comprehensive computational estimates of the mechanical properties of single and bi layers MoS_2 structures are examined, in this investigation. Additionally, understanding the effects of vacancy defect on the mechanical properties of MoS_2 structure are crucial issue. Mamun et al. [17] investigated the effects of different types of vacancy defects, such as, single and bi-vacancy, on thermal properties of single layer MoS_2 structure. They indicated that thermal property of single layer MoS_2 structure is significantly reduced with increasing defect concentrations. However, the effects of vacancy defect on the mechanical properties of MoS_2 structure get less attention from authors. Thus, the influences of single and bi vacancy defects on the single and bi layers MoS_2 structures are studied. In this work, because of problems in experimental characterizations of 2D nanomaterials, MD simulation was used as an alternative of experimental studies.

2. SIMULATION METHODS AND PHYSICAL MODELS

In this investigation, the VNL package [18] was used for visualization, while all MD simulations of MoS_2 structure were conducted by using LAMMPS [19], which is the publicly available simulation code. The physical model of the atomistic structure of MoS_2 was illustrated in Figure 1. Single and bi layer MoS_2 structures consisting of 7500 and 15000 atoms, respectively, were built with almost 13.6 nm in width and 15.8 nm in length.

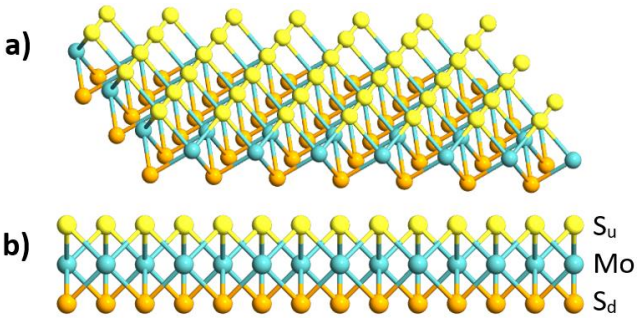


Figure 1 Physical model of the non-defective single layer MoS_2 structure: Mo represents a molybdenum atom and S_d and S_u represent S atom in the lower and upper layer, a) top and b) side views

To compute the mechanical properties of single and bi layer MoS_2 structures, uniaxial tensile test was conducted at room temperature (300 K) for loading condition. Integration scheme of velocity Verlet was used in the calculation to solve the motion-equations with a time step of 0.5 fs. For defining the interatomic interactions of single and bi layer MoS_2 structures, the correctness of force field is so important. There are several potential for use in MD simulations, such as Stillinger-Weber (SW), Tersoff and Brenner. The Tersoff and Brenner bond-order potentials have had particular success for carbon-based materials. Beside these potentials, the SW potential is another successful empirical potential for covalently bonded systems. The SW potential has a simpler form and fewer parameters than the Brenner potential, so it is much faster. One of the practical advantage of the SW potential is that it has been implemented in almost all available MD simulation packages. For these structures, the SW potential is chosen. This potential is simple and contains all possible atomic interactions of S and Mo [20, 21]. Therefore, it is used to describe the interatomic interactions of these structures. Additionally, this potential provides an accurate prediction for the structural parameters of MoS_2. The form of SW potential can be written as,

$$E = \sum_i \sum_{j>i} \emptyset_2(r_{ij}) + \sum_i \sum_{j\neq i} \sum_{k>j} \emptyset_3(r_{ij}, r_{ik}, \theta_{ijk}) \quad (1)$$

The two-body interaction potential $\emptyset_2$ takes the following form.

$$\emptyset_2(r_{ij}) = A_{ij}\left(\frac{B_{ij}}{r_{ij}^4} - 1\right) \times exp\left[\frac{\rho_{ij}}{r_{ij} - r_{ij}^{max}}\right] \quad (2)$$

The three-body interaction potential $\emptyset_3$ in Equation (1) is modeled as;

$$\emptyset_3(r_{ij}, r_{ik}, \theta_{ijk}) = K_{ijk} exp\left[\frac{\rho_{ij}}{r_{ij} - r_{ij}^{max}} + \frac{\rho_{ik}}{r_{ik} - r_{ik}^{max}}\right] \times \left(cos\theta_{ijk} - cos\theta_{0,ijk}\right)^2 \quad (3)$$

$\emptyset_2$ and $\emptyset_3$ represents the two body (bond stretching) and three body (bond bending) interactions. The pair separations are described by r_{ij} and r_{ik}. The angle between the separation vectors centering on atom-i is denoted by θ_{ijk}. The potential parameters are A, B, K, ρ, along with r^{max} cutoff radii and equilibrium angles and they rely upon on the atoms interacting with each other. Periodic boundary conditions (PBCs) are used to the in-plane directions (x and y directions), in order to minimize edge effects. Single and bi layer MoS_2 structures are uniaxially stretched at strain rate of 10^9 s^{-1}. Virial stresses are computed at each strain's level to acquire a stress–strain response. The Young's modulus (YM) of MoS_2 structure was computed at low level of the strain (up to 0.05) of the linear region. The stress (σ), strain (ε) and YM (E) of single and bi layer MoS_2 structures can be written as:

$$\varepsilon = \frac{l - l_0}{l_0} \quad (4)$$

$$\sigma = \frac{1}{At}\frac{\partial U}{\partial \varepsilon} \quad (5)$$

$$E = \frac{1}{At}\frac{\partial^2 U}{\partial^2 \varepsilon} \quad (6)$$

here, the thickness, surface area and strain energy of single and bi layer MoS_2 structures are expressed by t, A and U, respectively. The final and initial lengths of these structures are denoted by l and l_0, respectively.

3. RESULTS AND DISCUSSION

Firstly, to understand the energetic stability of the MoS_2 structure, per-atom cohesive energy was computed as:

$$E_{coh} = \left(\sum_i E_i - E_t\right)/n \quad (7)$$

here n, E_t and E_i denote the total number of atoms in the cell, total energy per cell and the energy of the i-th isolated atom, respectively. MD results indicated that the cohesive energy of MoS_2 structure is negative, -10.41 eV. This result indicate that MoS_2 structure is energetically stable.

3.1. Mechanical Properties

In this section, the MD simulations system was employed to investigate the effects of various temperatures, structural defects and different strain rates on mechanical properties of single and bi layers MoS_2 structures. Firstly, the computed uniaxial stress–strain response for considered single layer MoS_2 structure was showed in Figure

2. The YM, ultimate tensile strength (UTS) and failure strain (FS) of single layer MoS_2 structure were acquired at low strain levels (up to 0.05). At 300 K, the acquired YM, UTS and FS values of single layer MoS_2 structure are 0.202 TPa, 42.7 GPa and 0.155, respectively. These results are in agreement with the previous study [22] on the single layer MoS_2 structure. Also, the mechanical properties of bi layer MoS_2 structure were studied. The YM, UTS and FS of bi layer MoS_2 structure are 0.191 TPa, 40.3 GPa and 0.149, respectively. These results revealed that these structures have outstandingly high mechanical properties.

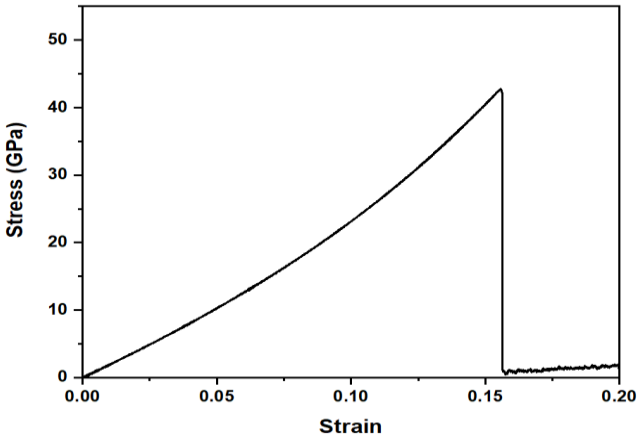
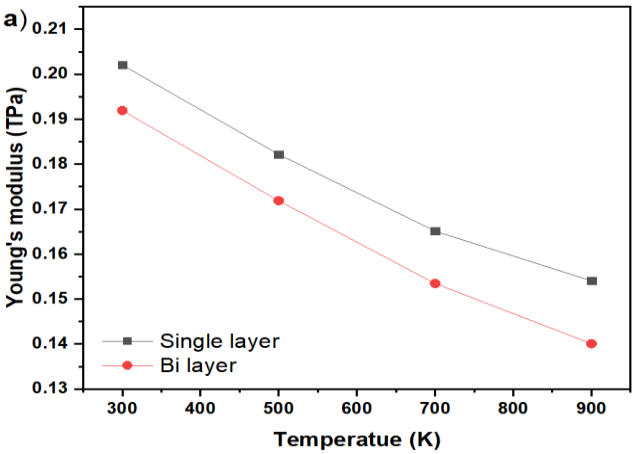


Figure 2 Stress-strain curve of pristine MoS_2 structure at room temperature

3.1.1. Temperature Effects

In this part of this study, the effects of various temperatures on the mechanical properties of single and bi layer MoS_2 structures were examined. Using MD simulations for single and bi layer MoS_2 structures at 300 K, 500 K, 700 K and 900 K, the UTS, FS and YM values of single and bi layer MoS_2 structures are presented in Figure 3. According to these results, by rising the temperatures up to 900 K, the UTS, FS and YM of single and bi layer MoS_2 structures gradually reduce. With increasing temperature, these structures become softer and less stiff. The atomic thermal vibrations get more dramatically robust and the vibrational amplitudes seem to be more tremendous while the temperature is growing up. This growing prompts the interatomic distance expands. When the distances of neighbors atoms increase, the interaction energy of atoms decrease by increasing temperature. Therefore, the UTS of single and bi layer MoS_2 structures reduces. Also, by increasing temperature, the strain energy reduces because of the rising kinetic energy. Hence, high temperatures affect the FS adversely. As temperature is increased, the binding energy between atoms reduces. Thus, the YM values of single and bi layer MoS_2 structures decrease.

According to Figure 3, when the temperature rises from 300 K to 900 K, the maximum variations in the YM of single and bi layer MoS_2 structures are around 23.7% and 27%, respectively. The UTS of single and bi layer MoS_2 structures are 66.3% and 68.3% lower than those at room temperature, respectively, when the temperature is increased to 900K. Similar to other properties, the FS reduction of single and bi layer MoS_2 structures are computed around 55.1% and 59.2%, respectively, as the temperatures rise from 300 K to 900 K. The difference between monolayer and multilayer MoS_2 can be lies in the presence of the van der Waals interlayer interaction. The interlayer van der Waals interaction between adjacent layers is not that strong. Therefore, it cannot boost the mechanical properties for multilayer MoS_2 significantly. As a result, changing of temperatures shows more effect on the bi layer MoS_2 structure than single layer MoS_2 structure. It is important to note that, the van der Waals interaction can be strengthened by various methods such as, chemical functionalization and surface roughness modification.



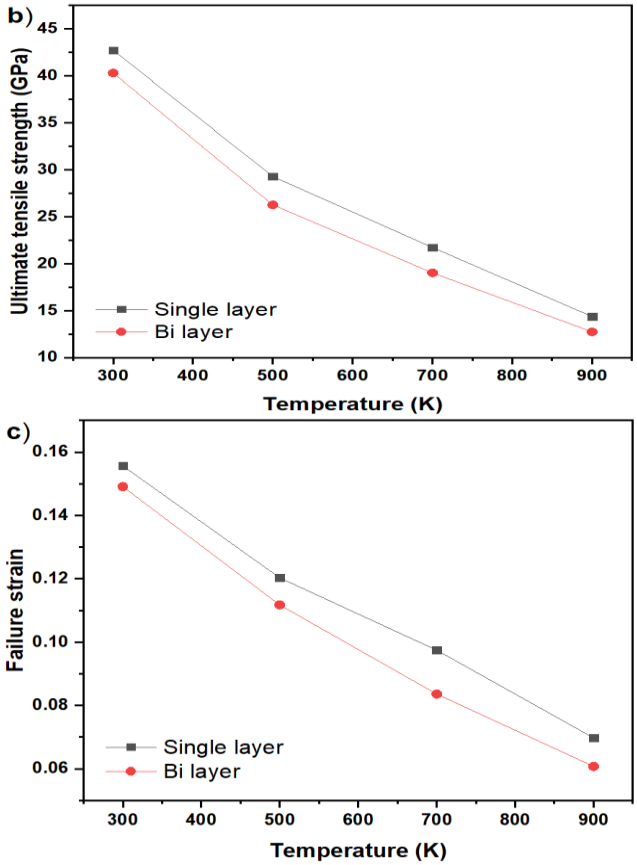


Figure 3 a) Young's modulus b) ultimate tensile strength and c) failure strain of MoS_2 structure as a function of different temperatures

3.1.2. Strain Rate Effects

The effects of different strain rates on the mechanical properties of single and bi layer MoS_2 structures were studied. In Figure 4, the UTS, FS and YM of single and bi layer MoS_2 structures were shown as a function of different strain rate. It can be seen in Figure 4, as the strain rate rises from 10^7 s^{-1} to 10^9 s^{-1}, the YM, UTS and FS of single and bi layer MoS_2 structures show an increasing trend. Additionaly, it can be said that the strain rates influence on the mechanical properties of single and bi layer MoS_2 structures indicate similar behavior. As observed in Figure 4, as the strain rate reduces from 10^9 s^{-1} to 10^7 s^{-1}, the maximum differences in the UTS, FS and YM of single layer MoS_2 structure are around 13.1%, 22.4% and 25.6%, respectively, at 300 K. Additionally, as shown in Figure 4, the UTS, FS and YM reduction of bi layer MoS_2 structure are almost 14.6%, 21.4% and 24.5%, respectively, when the strain rate is decreased to 10^7 s^{-1}, at room temperatue. Also, various strain rates show similar influences on the UTS, FS and YM of single and bi layer MoS_2 structures.

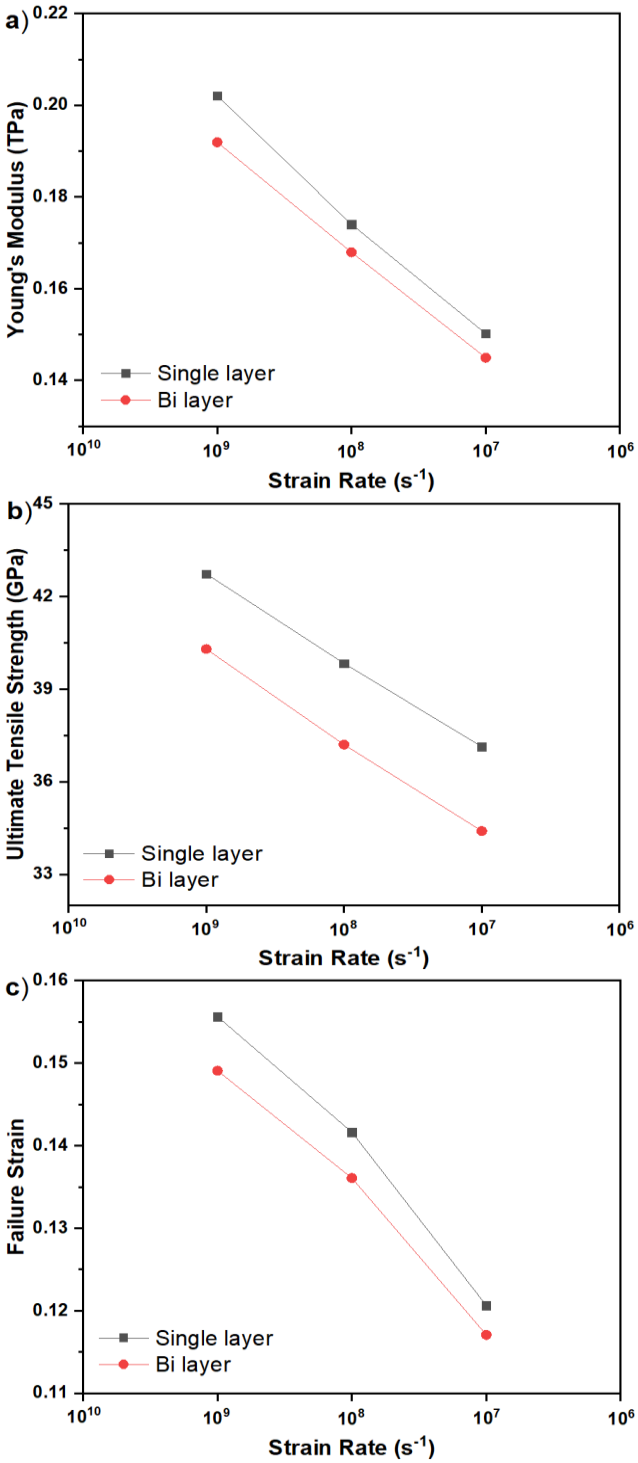


Figure 4 a) Young's modulus b) ultimate tensile strength and c) failure strain of MoS_2 structure as a function of different strain rates

3.1.3. Defect Effects

The influences of two different S atom types vacancy defect (point and bi vacancy) on the

mechanical properties of single and bi layer MoS_2 structures were investigated, in this part. It is important to note that experimentally introduce S atom defects into the MoS_2 structures is found to be easier than defects caused by Mo atom defects [23]. Therefore, only S atom vacancy defect was examined, in this study. The atomic structures of the defective MoS_2 with point and bi vacancy defects are shown in Figure 5.

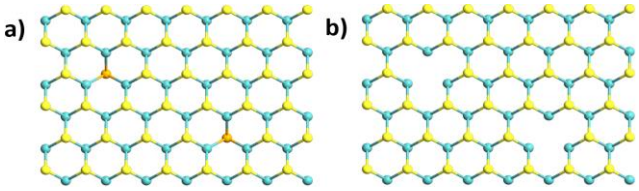


Figure 5 The atomic structure of the defective MoS_2 structures with a) point and b) bi vacancies

As observed in Figure 6, due to the S atom point and bi vacancy defects in the single and bi layer MoS_2 structures at 300 K, the mechanical properties of these structures decrease. Additionally, in Figure 6, the effects of eight various concentrations of S atom vacancy defects on the UTS, FS and YM of single and bi layer MoS_2 structures were investigated. As the point and bi vacancy defects concentration increases up to to 4%, the mechanical properties of single and bi layer MoS_2 structures containing vacancy defects gradually reduce, in Figure 6. The MD simulation results in Fig. indicated that the type of S atom bi vacancy defect exerts more influence on the FS, UTS and YM than other do with increasing concentrations because type of S atom bi vacancy defect occurs a hole in the structure. For single layer MoS_2 structure, the maximum variations in the YM, UTS and FS between the pristine MoS_2 structure and that one with S atom bi vacancy defect type are about 27.9%, 78.3% and 64.1%, respectively, in Figure 6. Furthermore, as shown in Figure 6, the variations of the YM, UTS and FS between the pristine MoS_2 structure and that one with S atom single vacancy defect type are changed between 22.9%, 72.9% and 58.8%, respectively. Also, for bi layer MoS_2 structure, the maximum variations in the YM, UTS and FS between the pristine bi layer MoS_2 structure and that one with S atom bi vacancy defect type are almost 25%, 82% and 65.1%, respectively, in Figure 6. In addition, the differences of the YM, UTS and FS between the pristine bi layer MoS_2 structure and that one with S atom single vacancy defect type are changed between 20%, 77.3% and 60.4%, respectively. For both single and bi layer MoS_2 structures, vacancy defect type's changing indicates more influence on the FS and UTS than YM does by rising defect concentration.

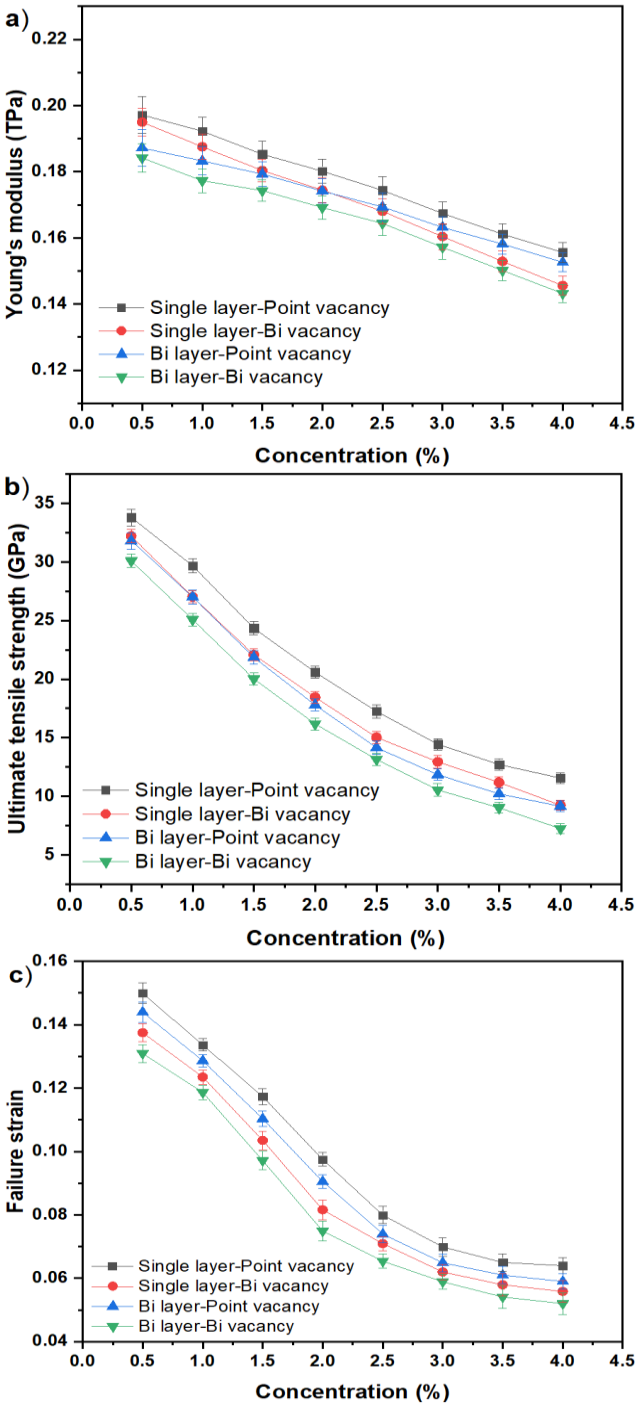


Figure 6 a) Young's modulus b) ultimate tensile strength and c) failure strain of single and bi layer MoS_2 structures as a function of the concentration of point and bi S atoms vacancy defects

4. CONCLUSIONS

In this study, via utilizing MD simulations, the mechanical properties (FS, UTS and YM) of single and bi layer MoS_2 structures are investigated. Also, the influences of various strain rates, vacancy defects and temperatures on the single and bi layer MoS_2 structures are studied. MD simulation results indicated that single and bi layer MoS_2 structures have ultra high mechanical properties. The influences of four various temperatures from 300 K to 900 K on the mechanical properties of single and bi layer MoS_2 structures are examined. As the atomic bonds become weaker at higher temperatures, the lower FS, UTS and YM values occur. In addition, bi layer MoS_2 structure has lower mechanical properties than single layer MoS_2 structure, at high temperature. It is also demonstrated that the existence of point and bi vacancy defects in single and bi layer MoS_2 structures reduce the mechanical properties of these structures remarkably by increasing concentrations of defects. Furthermore, S atom bi vacancy defect type exerts more effect on the mechanical properties of single and bi layer MoS_2 structures than S atom single vacancy defect type do with increasing concentrations. The effects of various strain rates from from 10^7 s^{-1} to 10^9 s^{-1} on the FS, UTS and YM of single and bi layer MoS_2 structures are studied. The FS, UTS and YM of single and bi layer MoS_2 structures indicate increasing trend, as the strain rate increases. Single and bi layer MoS_2 structures, along with superior electronic properties, exhibit ultra high mechanical properties which make it a promising candidate for nano-mechanical system.

Conflict of Interest

No conflict of interest or common interest has been declared by the authors.

Ethics Committee Approval

This study does not require ethics committee permission or any special permission.

Research and Publication Ethics

The author of the paper declare that he complies with the scientific, ethical and quotation rules of SAUJS in all processes of the paper and that he does not make any falsification on the data collected. In addition, he declares that Sakarya University Journal of Science and its editorial board have no responsibility for any ethical violations that may be encountered, and that this study has not been evaluated in any academic publication environment other than Sakarya University Journal of Science.

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