Effect of point defects and nanopores on the fracture behaviors in single-layer MoS₂ nanosheets

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Abstract
Point defects and nanopores are inevitable and particularly noticeable in single-layer (SL) MoS₂. Molecular dynamics (MD) simulations have been done to comprehensively study the influences of point defects and nanopores on tensile deformation behaviors of SLMoS₂ nanosheets, and the dependences of fracture properties on defect type and concentration, pore size, temperature and strain rate are discussed. The formation energy of S vacancy (V_S) is the lowest one, but that of V_MoS₆ is the highest one, corresponding to the highest and lowest fracture stress, respectively. The local stress concentration around point defects and nanopores might lead to the early bond breaking and subsequent nucleation of cracks and brittle fracture upon tensile loading. A modified Griffith criterion is proposed to describe the defect concentration and pore size dependent fracture stress and strain. These findings provide us an important guideline for the structural design of 2D materials in future applications.

1. Introduction
Structural defects usually cause dramatic deterioration of the mechanical properties of the materials [1−4], which becomes more pronounced in the recently developed two-dimensional (2D) materials [5], slight bond breaking in 2D materials might result in destructive fracture. Therefore, atomic-scale defects will strongly affect the mechanical behaviors of 2D materials and, it is important to understand the fracture mechanisms and deformation behaviors at atomistic level [6−8].

Single-layer MoS₂ (SLMoS₂), as a typical 2D materials, has a direct band gap of 1.8 eV and promising applications in next-generation field-effect transistors, optoelectronics, energy harvesting devices and flexible electronics nano-devices [9, 10]. Large-area SLMoS₂ nanosheets have been fabricated by mechanical exfoliation (ME), chemical vapor deposition (CVD) and physical vapor deposition (PVD), and point defects, grain boundaries and nano-pores are often observed [11, 12], in particular, point defects [13, 14]. Furthermore, point defects can also be generated by irradiation [15]. Experimentally, 6 types of point defects have been observed in SLMoS₂, including monosulfur vacancy (V_s), disulfur vacancy (V₂s), vacancy complex of Mo and nearby three sulfur (V_MoS₃), vacancy complex of Mo nearby three disulfur pairs (V_MoS₆), and antisite defects with a Mo atom substituting a S₂ column (MoSₓ) or a S₂ column substituting a Mo atom (S₂Mo) [16]. Based on the density functional theory (DFT), the SLMoS₂ with the V_s defect has the lowest formation energy, so that the V_s defects are frequently observed in CVD and ME samples. The MoS₂ and S₂Mo defects are found in PVD samples and, V_MoS₃ and V_MoS₆ defects in swift heavy ion and electron-beam irradiation samples [17, 18]. Moreover, for 2D MoS₂ nanosheets, the sonication treatment will induce defect-rich samples, including vacancies, nano-ripples, and nanopores [19, 20]. The V_s defect distribution in CVD SLMoS₂ was visualized by using dark-field optical microscopy and the measured defect density is about 2 \( \times 10^{10} \) cm\(^{-2}\) [21]. Similarly, the concentration of V_s defect in CVD and ME SLMoS₂ could be up to 1.2 \( \pm 0.4 \) \( \times 10^{13} \) cm\(^{-2}\), and the concentration of MoS₂ defect in
PVD samples even reached to 2.8 $\pm$ 0.3 $\times 10^{13}$ cm$^{-2}$ [22]. Song et al [23] probed a few V$_S$ defects at a time in CVD grown single-layer MoS$_2$ by combining noise–current analysis with atomic force microscopy, suggesting the defect density is on the on the order $10^{11}$ cm$^{-2}$. The V$_S$ defects could also diffuse and are agglomerated into nanopores in SLMoS$_2$ under electron irradiation [24, 25], and the nanopore membranes could greatly improve the water desalination filter technology and DNA sequencing [26, 27]. Such inevitable defects play crucial roles not only in tuning electrical properties but also in reducing mechanical properties of 2D materials. It has been demonstrated that SLMoS$_2$ can sustain a theoretical elastic strain of over 10% that is one order of magnitude larger than that of conventional materials. Unfortunately, the experimental strain limit is much lower than 10%, for instance, 1% biaxial strain by Yang et al [28], 2.5% uniform local strain by Castellanos-Gomez et al [29] and 0.32% uniaxial tensile strain by John et al [30]. The main reason is the unavoidable high-density defects, such as point defects and nano-pores, inducing earlier fracture. A comprehensive understanding on the mechanical properties of defective SLMoS$_2$ nanosheets as well as fracture behaviors is needed for better further design of nano-devices.

Compared with bulk materials, it is a challenge to quantitatively study the fracture behaviors of 2D materials. Recently, atomic force microscopy (AFM) nano-indentation, pressurized bubble loading combining with Raman spectra, and in situ tensile tests in transmission electron microscopy (TEM) have been employed to measure the elastic modulus, interlayer and interfacial shear stress, tensile strength of 2D materials [31–35]. However, it is still difficult to observe and characterize the defects and structural evolution straightforward. In comparison, large-scale molecular dynamics (MD) simulations and theoretical research appear as feasible method studying the mechanical properties and fracture behaviors of defective 2D materials at atomic scale [36–39]. The previous MD simulations by Zhang et al [40] suggested that the fracture and tensile strength was flaw size independent if the nanocrystalline graphene below a critical flaw size. Further, it was also found by Yin et al that the crack would likely to extended along zigzag direction in graphene [41]. Based on MD simulation results, a geometrical factor to modify the Griffith criterion was proposed. The modified Griffith criterion was well matched with MD results in single-layer black phosphorus (SLBP), SLMoS$_2$, and SL/BLMoSe$_2$ and it is still valid even when the crack length is changed from hundreds of nanometers to several nanometers [42, 43].

Recently, the effects of defect types on the mechanical behaviors of SLMoS$_2$ are investigated by using reactive MD simulation [44]. However, the fracture behavior and mechanism in SLMoS$_2$ nanosheets containing point defects and nanopores remains unclear. In this work, MD simulation is performed to study the fracture behaviors of defective SLMoS$_2$ nanosheets under tensile loading, as well as the influences of point defect types, concentration, pore size, temperature and strain rate.

2. Simulation model and method

In this work, LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) is used to conduct the MD simulations [45]. Stillinger-Webber (SW) potential developed by Jiang et al [46] is adopted to describe the interatomic interactions, bond breaking and reforming in SLMoS$_2$. The simulated elastic properties, deformation behavior, thermal conductivity, and phonon spectrum based on the SW potential show good agreement with the DFT and experimental results [47].

In SLMoS$_2$, the Mo monolayer is sandwiched by two S layers and the Mo and S atoms are covalently bonded with each other. Based on the lattice constant of 2H-MoS$_2$ ($a = 3.16$ Å), the initial model of SLMoS$_2$ nanosheet is established. Figure 1(a) shows the schematic presentation of 50 $\times$ 50 nm$^2$ SLMoS$_2$ nanosheet with one central point defect or one nanopore. Figure 1(b) shows the atomic structures of different point defects in the center of 50 $\times$ 50 nm$^2$ SLMoS$_2$ nanosheet, defined as V$_S$-SLMoS$_2$, V$_{MoS_2}$-SLMoS$_2$, Mo$_{S_2}$-SLMoS$_2$, V$_{MoS_2}$-SLMoS$_2$, V$_{MoS_6}$-SLMoS$_2$, and S$_2$Mo$_6$-SLMoS$_2$. Figure 1(c) shows the atomic configurations of hexagonal nanopore with zigzag edges, and the width of nanopore is defined as 2R, referred as NP-SLMoS$_2$.

The initial SLMoS$_2$ nanosheets are relaxed in the NPT (number of atoms N, pressure P, and temperature T are constant) ensemble at $T = 10$ K and $P = 0$ Pa for 2 ns and the nanosheets are thermally equilibrated using the Nosé-Hoover thermostat [48, 49]. The periodic boundary conditions (PBCs) are applied in all directions and a vacuum region 30 Å in width along all directions is added to avoid the interactions of atoms near the opposite edges, which is totally the same as free boundary conditions. Hence, the zigzag or armchair edge of SLMoS$_2$ can be distinguished according to the atomic arrangement. After fully relaxed, the axial tensile loading is applied to SLMoS$_2$ nanosheets along zigzag and armchair direction. The atomic stress is calculated using the virial definition and a thickness of 0.61 nm is used to calculate the volume of the system [41, 50]. For comparison, the temperature in the range of 10 K to 400 K and the strain rate in the range of $1 \times 10^{-2}$ s$^{-1}$ to $10^{3}$ s$^{-1}$ is considered. The atomistic structures and stress distribution are visualized by the OVITO package [51].
3. Results and discussion

In order to reveal the formation mechanism of point defects, the formation energy of point defects $E_f$ is calculated by \( E_f = E_{\text{defect}} - E_{\text{bulk}} - \sum_i n_i \mu_i \) \(^{(1)}\), in which $E_{\text{defect}}$ and $E_{\text{bulk}}$ are the total energies of the SLMoS$_2$ nanosheet with and without point defect, respectively, $n_i$ is the number of deleted atoms and $\mu_i$ is their chemical potential, for Mo or S atom. In this study, the chemical potential of Mo and S are in a thermal equilibrium with MoS$_2$, \( \mu_{\text{Mo}} = \mu_{\text{MoS}_2} \) and \( \mu_{\text{S}} = \mu_{\text{S}} \), respectively. Hence, the accessible range of $\mu_{\text{Mo}}$ and $\mu_{\text{S}}$ values is limited by the lowest-energy phases of these elements, based on DFT calculations, the upper and lower bounds for the chemical potential are 0 and $-1.4$ eV, respectively. Figure 2\(^{(a)}\) shows the calculated defect formation energies. In the whole range of S chemical potential (from $-1.4$ to 0 eV), V$_S$ has the lowest formation energy, from 0.55 to 1.99 eV, while V$_{\text{MoS}_6}$ displays the highest formation energy, from 9.69 to 14.03 eV, respectively. Zhou et al \(^{[16]}\) showed the formation energy of V$_S$ is in the range from 1.8 to 2.3 eV, and the formation energy of V$_{\text{MoS}_6}$ is in the range from 11.16 to 16.53 eV. Komsa et al \(^{[18]}\) also calculated the formation energy of V$_S$ from 1.53 to 2.3 eV, and the formation energy of V$_{\text{MoS}_6}$ of 10.92 eV, respectively. Experimentally, V$_S$ has been frequently observed in SLMoS$_2$ fabricated by CVD, but other defects (V$_{\text{MoS}_3}$, V$_{\text{MoS}_6}$) were observed upon electron irradiation \(^{[24, 25]}\).

Figure 2\(^{(b)}\) plots the stress-strain curves of defect-free and defective SLMoS$_2$ nanosheet under tensile loading along zigzag and armchair directions. The peaks on the stress-strain curves correspond to the fracture stress and strain. As shown in figures 2\(^{(c)}\) and \(^{(d)}\), the point defects strongly weaken the mechanical properties of SLMoS$_2$ nanosheets. The fracture stress of defect-free SLMoS$_2$ nanosheet is 18.06 GPa and 20.03 GPa along zigzag and armchair directions, respectively, but it is reduced down to 16.45 GPa by 8.9% and 17.66 GPa by 11.8% for V$_S$-SLMoS$_2$, even down to 14.68 GPa by 18.7% and 13.85 GPa by 30.8% for V$_{\text{MoS}_6}$-SLMoS$_2$. The fracture strain of defect-free SLMoS$_2$ nanosheet is 16.11% and 17.13% along zigzag and armchair directions, respectively, and is reduced down to 13.52% by 16.07% and 13.36% by 22% for V$_S$-SLMoS$_2$, and down to 11.3% by 29.8% and 9.49% by 44.6% for V$_{\text{MoS}_6}$-SLMoS$_2$. Moreover, the fracture stress and strain of V$_S$-SLMoS$_2$ are the highest, while that of V$_{\text{MoS}_6}$-SLMoS$_2$ are the lowest. In fact, the fracture stress and strain are close related to the formation energy of point defects, that is, the lower formation energy of defects commonly leads to the larger fracture stress and strain. The formation energy of V$_S$ is the lowest, inducing the smallest lattice distortion and stress concentration. Hence, the crack is more difficult to nucleate around V$_S$. However, for the higher formation energy defect, i.e., V$_{\text{MoS}_6}$, the larger lattice distortion and stress concentration is observed, resulting the easier crack nucleation.

Figure 3 displays the atomic configuration evolution when fracture occurs in defective SLMoS$_2$ nanosheet, and the atomic configurations around point defects are shown in the inserts. As shown in figure 3\(^{(a)}\), the stress concentration appears near the V$_S$ defect at the strain of 13.5% and, which causes the breaking of S-Mo bonds at the strain of 13.52%, then a crack nucleates and propagates perpendicular to the loading direction. The fracture edges are misty, hackly and exhibit single path when the tensile loaded along zigzag direction. However, the crack branching emerges after the crack nucleation if the tensile loading is along armchair direction. Experimentally, Wang et al \(^{[52]}\) mainly present in situ TEM to study the crack propagation in a freestanding...
CVD single-layer MoS$_2$, suggesting that crack propagation is mostly in the zigzag direction and S atoms are very important in sustaining large crack tip. The results are showing remarkable agreement with our MD results.

In order to reveal the influence of defect concentrations, temperature, and strain rate on the mechanical properties of SLMoS$_2$ nanosheets, an exampled of VS-SLMoS$_2$ nanosheet, the randomly distributed VS point defects are introduced. The VS defects density is in the range from 0.021% to 2.22%, by randomly deleting the upper S atoms. It is worth noting that the defects density ($\rho$) is calculated as $\rho = N_V / N_{total}$, where $N_V$ is the number of VS defects and $N_{total}$ is the total number of SLMoS$_2$ nanosheet. Hence, as compared with previous experimental results [21–23], the corresponding defects density is in the range from $7.6 \times 10^{-5}$ nm$^2$ to $8 \times 10^{-3}$ nm$^2$, which is reasonable. Figure 4(a) plots the stress-strain curves of VS-SLMoS$_2$ nanosheet with different defect concentrations. As shown in figure 4(b), as the Vs defect concentration is increased from 0.021% to 2.22%, the fracture stress of VS-SLMoS$_2$ nanosheet is gradually reduced from 16.38 GPa to 11.89 GPa by 27.4% and from 15.93 GPa to 12.4 GPa by 22.2%, when tensile loaded along zigzag and armchair directions, respectively. The fracture strain is decreased from 13.37% to 9.39% by 29.7%, from 11.48% to 8.87% by 22.7%, respectively. Hasanian et al [38] demonstrated that the increase of defect contents from 0.1% to 2% significantly reduced the tensile fracture strength and strain of MoS$_2$ by using reactive MD simulation, showing remarkable agreement with our results. Further, combining the MD results, continuum fracture mechanics and Griffith criterion, the fracture stress and strain can be given [36],

\[
\sigma_f = \sigma_0 \left(1 - \frac{E(1 - 2v)}{2\pi \rho^2} \right)^{\frac{1}{2}} 
\]

\[
\varepsilon_f = \varepsilon_0 \left(1 - \frac{E(1 - 2v)}{2\pi \rho^2} \right)^{\frac{1}{2}} 
\]

in which $\sigma_f$ and $\varepsilon_f$ are the fracture stress and strain, $\rho$ is the defect concentration in percentage, $\sigma_0$ and $\varepsilon_0$ are the fracture stress and strain of SLMoS$_2$ nanosheet containing only one VS point defect, the elastic modulus $E$ is 165.7 GPa and 167 GPa along zigzag and armchair directions, respectively, and the Poisson’s ratio $v$ is 0.267. The results based on equations (3) and (4) are plotted in figure 4(b), of which the relationship between fracture stress, strain and defect concentration are well predicted.

For a given defect concentration of 0.021%, the tensile loading along zigzag direction is applied to VS-SLMoS$_2$ nanosheets at the temperature in the range of 10 K–400 K and with the strain rate in the range of $1 \times 10^2$ s$^{-1}$ to $10^3$ s$^{-1}$. The corresponding stress-strain curves are plotted in figure S1 (available online at Figure 2. (a) The formation energies of different defects and the reported results for comparison. (b) The stress-strain curves of the SLMoS$_2$ nanosheets containing different point defects, (c) fracture stress and (d) fracture strain.}


As shown in figure 4(c), the fracture stress and strain are reduced from 16.26 GPa to 10.41 GPa by 35.9% and from 13.37% to 8.18% by 38.8%, respectively. More thermal vibration modes and thus fragile covalent bonds will be activated at higher temperature, which leads to lowered fracture stress and strain. The fracture stress of SLSMoS$_2$ nanosheet as a function of temperature and strain rate can be given by

$$\sigma_f(\dot{\varepsilon}, T) = \frac{U_0}{\gamma} + \frac{k}{\gamma} \ln \left( \frac{\gamma E \dot{\varepsilon} \tau_0}{n_i k T} \right) T$$

in which $E$ is the elastic modulus, $U_0$ is the bond dissociation energy of S-Mo bond, $\tau_0$ is the period of atomic vibration, $n_i$ is the number of sites available for state transition, $\gamma$ is the activation volume, and $k$ is Boltzmann’s constant. For a given strain rate, the fracture stress is reduced with elevating temperature. As the strain rate increases, the fracture stress and strain increase slowly because of the insignificant strain rate sensitivity at lower temperature. At a given temperature, the relation between the fracture stress and strain rate can be rewritten as

$$\ln \sigma_f(\dot{\varepsilon}) = \ln C + m \ln \dot{\varepsilon}$$

in which $m$ is the strain rate sensitivity. The log-log plot between fracture stress, fracture strain and strain rate are shown in figure 4(d), the value of $m$ is obtained from the slope of linear fitting. In fact, the atoms could respond to the thermal fluctuation and stress relaxation timely at a lower strain rate. The value of $m$ is 0.0028 at 10 K, and it is much lower than the value of other 2D materials at room temperature.

Figures 5(a) and (b) show the statistical distributions of Mo–S bond lengths in V$_5$-SLMoS$_2$ nanosheets with lower (0.021%) and higher (2.22%) defect concentration under tensile loading along zigzag direction, respectively. As the tensile strain increases, the Mo–S bond length is elongated from 2.38 Å to 2.48 Å and from...
Figure 4. (a) The stress-strain curves of VS-SLMoS$_2$ nanosheets with different defect concentrations and (c) the fracture stress and strain as a function of defect concentration. The fracture stress and strain as a function of (c) temperature and (d) strain rate.

Figure 5. Statistical distributions of S-Mo bond lengths in VS-SLMoS$_2$ nanosheets with the defect concentrations of (a) 0.021%, (b) 2.22% under tensile loading along zigzag direction and (c) for different defect concentrations at the fracture strain. The typical atomic configuration evolution for the defect concentrations of (d) 0.021% and (e) 2.22%, respectively. The top, middle and bottom panels are colored by the out-of-plane displacement, the shear strain per atom and the stress per atom, respectively.
2.38 Å to 2.44 Å for the defect concentrations of 0.021% and 2.22%, respectively. Figure 5(c) shows the bond length distributions at the fracture strain, and figures 5(d) and (e) show the typical atomic configurations during fracture process for the defect concentrations of 0.021% and 2.22%, respectively. The top, middle and bottom panels are colored by the out-of-plane displacement, the shear strain per atom and the stress per atom, respectively. The stress concentration and local strain around the Vs defects cause the breaking of S-Mo bonds much earlier and thus a crack around the defects. The crack propagates rapidly perpendicular to the loading direction. In particular, for the higher defect concentration, point defects induce remarkable stress concentration, thus resulting in the earlier breaking of Mo-S bonds. As indicated in figure 5(e), the stress might promote the diffusion of Vs defects and the formation of Vs lines.

Furthermore, V_{MoS_3} and V_{MoS_6} point defects might merge into a nanopore during ion irradiation process. The tensile loading on the NP-SLMoS_2 nanosheet is also simulated to study the influences of nanopores. Figure 6(a) displays the stress-strain curves of NP-SLMoS_2 nanosheets with the pore size of 3–8.5 nm and, figure 6(b) shows the fracture stress and strain. The modified Griffith criterion is adopted to describe the brittle fracture of NP-SLMoS_2 nanosheet [34, 36],

\begin{align}
\sigma_f &= \frac{\alpha}{F(\phi)} \sqrt{\frac{E\omega}{\pi R}} \\
\varepsilon_f &= \frac{\alpha}{F(\phi)E} \sqrt{\frac{E\omega}{\pi R}}
\end{align}

in which E is the elastic modulus of 165 GPa and 167 GPa for zigzag and armchair direction, respectively, R is the half width of nanopore, \(\omega\) is the edge energy of 1.94 J m\(^{-2}\) and 1.84 J m\(^{-2}\) for armchair and zigzag edges, respectively, \(\alpha\) is the geometrical correction and \(F(\phi)\) is a geometrical factor [43]. The theoretical results are displayed as the blue lines in figure 7(b), and are in excellent agreement with the MD results. Figures 6(c) and (d) show the temperature and strain rate effect on the mechanical properties of NP-SLMoS_2 nanosheet with a pore width of 3 nm. The corresponding stress–strain curves are plotted in figure S2. As the temperature increases from 10 K to 400 K, the fracture stress and strain decrease (figure 6(c)), similar to the results of Vs-SLMoS_2 nanosheet. As shown in figure 6(d), the fracture stress and strain are increased as the strain rate is increased from \(1 \times 10^7\) s\(^{-1}\) to \(10^9\) s\(^{-1}\) at 10 K. For the same tensile conditions, the strain rate sensitivity (SRS, m) of NP-SLMoS_2 nanosheet is

![Figure 6](image-url)
10 times higher than that of Vs-SLMoS2 nanosheet, similar to the findings that larger defects own higher strain rate sensitivity in bulk metals [55].

For a given pore width of 8.5 nm, figures 7(a) and (b) show the atomic configuration evolution of NP-SLMoS2 nanosheet upon tensile loading along zigzag and armchair direction, respectively. The out-of-plane displacement, shear strain and stress distribution per atom are exhibited, and the atomistic details are marked in the inserts. As seen in figure 7(a), stress concentration near the sharp corners of a hexagonal pore leads to the breaking of surrounding S-Mo bonds and the nucleation of two fresh cracks at the tensile strain of 5.1%. Subsequently, the cracks propagate rapidly from the pore edges to the nanosheet edges, nearly perpendicular to the tensile direction, as the tensile strain is up to 5.4%. Similar events are observed when tensile loading along armchair direction, as shown in figure 7(b). More interestingly, the newly formed cracks are misty, hackly for the former case, but almost atomically flat with zigzag edges for later case, which has been verified in our previous work [43].

4. Conclusion

In summary, MD simulations are performed to study the effect of point defects and nanopores on the fracture properties of single-layer MoS2 nanosheet. The effect of point defect type and concentration, pore size, temperature and strain rate are systematically discussed. It is found that the lower formation energy of Vs defects corresponds to the higher fracture stress, compared with other defects. The local stress concentration around point defects and nanopores might cause the early breaching of S-Mo bonds upon tensile loading, and thus the nucleation of cracks and brittle fracture. A modified Griffith criterion is adopted to describe the defect concentration and pore size dependent fracture stress and strain. The findings provide us an important guideline for the structural design of 2D materials in future applications.

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Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.
Conflicts of interest

The authors declare no competing financial interest.

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