The buckling of single-layer MoS$_2$ under uniaxial compression

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Abstract

Molecular dynamics simulations are performed to investigate the buckling of single-layer MoS$_2$ under uniaxial compression. The strain rate is found to have an important effect on the critical buckling strain, where higher strain rate leads to larger critical strain. The critical strain is almost temperature-independent for $T < 50$ K, and it increases with increasing temperature for $T > 50$ K owing to the thermal vibration assisted healing mechanism on the buckling deformation. The length-dependence of the critical strain from our simulations is in good agreement with the prediction of the Euler buckling theory.

Keywords: molybdenum disulphide, buckling, uniaxial compression

1. Introduction

Molybdenum disulphide (MoS$_2$) is a semiconductor with a bulk bandgap above 1.2 eV [1], which can be further manipulated by changing its thickness [2], or through application of mechanical strain [3–6]. This finite bandgap is a key reason for the excitement surrounding MoS$_2$ as compared to graphene as graphene has a zero bandgap [7–9]. Because of its direct bandgap and also its well-known properties as a lubricant, MoS$_2$ has attracted considerable attention in recent years [10, 11]. For example, Radisavljevic et al [12] demonstrated the application of single-layer MoS$_2$ (SLMoS$_2$) as a good transistor. The strain and the electronic noise effects were found to be important for the SLMoS$_2$ transistor [5, 13–15].

Besides the electronic properties, several recent works have addressed the thermal and mechanical properties of SLMoS$_2$ [16–25]. Recently, we have parametrized the Stillinger–Weber potential for SLMoS$_2$ [26]. Based on this Stillinger–Weber potential, we derived an analytic formula for the elastic bending modulus of the SLMoS$_2$, where the importance of the finite thickness effect was revealed [27]. We have also shown that the MoS$_2$ resonator has a much higher quality factor than the graphene resonator [28].

As an important mechanical phenomenon, the buckling of graphene has attracted lots of attention in recent years [29–40]. Compared to graphene, the bending modulus of SLMoS$_2$ is higher by a factor of seven due to its finite thickness [27], yet the in-plane bending stiffness in SLMoS$_2$ is smaller than graphene by a factor of five [26]. As a result, the SLMoS$_2$ should be more difficult to buckle than graphene, according to the Euler buckling theory, which says that the buckling critical strain is proportional to the bending modulus to in-plane stiffness ratio [41]. This advantage would be of some benefit for the application of SLMoS$_2$ in some mechanical devices, where the avoidance of buckling is desirable. However, the study of buckling of SLMoS$_2$ is still lacking, and is thus the focus of the present work.

In this paper, we study the buckling of the SLMoS$_2$ under uniaxial compression via molecular dynamics (MD) simulations. We find that the critical buckling strain increases linearly with the increase of the strain rate, and this strain rate effect becomes more important for longer SLMoS$_2$. The critical strain is almost temperature-independent in low-temperature regions, but it increases considerably with increasing temperature for temperatures above 50 K because the buckling deformation is repaired by the thermal vibration at higher temperatures. We show that the critical strain depends on the length ($L$) as $\epsilon_c \propto 40.6/L^2$, which is in good agreement with...
After some simple algebra, we get the general strain energy corresponding to a general mode \((m, n)\) as

\[
V_s = \frac{1}{2} \int \int \left[ N_x \left( \frac{\partial w}{\partial x} \right)^2 + N_y \left( \frac{\partial w}{\partial y} \right)^2 + 2N_{xy} \frac{\partial w}{\partial x} \frac{\partial w}{\partial y} \right] \, dx \, dy
\]

\[
= \frac{\pi^2}{8} L_x L_y N_x m^2 \frac{\alpha_{mn}^2}{L_x^2} \text{,} \tag{2}
\]

where \(N_x\) is the force in the \(x\) direction. The bending energy corresponding to the mode \((m, n)\) is

\[
V_D = \frac{D}{2} \int \int \left\{ \left( \frac{\partial^2 w}{\partial x^2} \right)^2 + \frac{1}{2} \left( \frac{\partial^2 w}{\partial y^2} \right)^2 - 2(1 - \nu) \left( \frac{\partial^2 w}{\partial x \partial y} \right)^2 \right\} \, dx \, dy
\]

\[
= \frac{\pi^4 L_x L_y}{8} D a_{mn}^2 \left( \frac{m}{L_x} \right)^2 + \left( \frac{n}{L_y} \right)^2 \text{.} \tag{3}
\]

where \(\nu\) is the Poisson ratio and \(D\) is the bending modulus.

Within the configuration just before buckling, the strain energy is at its maximum and there is no bending energy. After buckling, this maximum strain energy is fully converted into the bending energy; i.e. \(V_s = V_D\). From this equation, we get the critical force for buckling

\[
N_x = -\frac{\pi^2 D}{L_y} \left( \frac{m L_y}{L_x} + \frac{n^2 L_x}{m L_y} \right)^2.
\]

Recall that \(N_x = C_{11} \epsilon\) with \(C_{11}\) as the in-plane stiffness, so we get the critical strain for buckling,

\[
\epsilon_c = -\frac{\pi^2 D}{C_{11} L_y^2} \left( \frac{m L_y}{L_x} + \frac{n^2 L_x}{m L_y} \right)^2. \tag{4}
\]

Obviously, the minimum value of \(\epsilon_c\) is chosen at \((m, n) = (2, 0)\); i.e. the buckling happens by deforming the SLMoS\(_2\) into the shape of the first lowest-frequency normal mode shown in the top panel of figure 1. We note that the choice of \(m = 2\) instead of \(m = 1\) here is the result of the constraint from the periodic boundary condition applied in the \(x\) direction. The Stillinger-Weber potential gives a bending modulus [27] \(D = 9.61 \text{ eV}\) and the in-plane tension stiffness [26] \(C_{11} = 139.5 \text{ Nm}^{-1}\) for the SLMoS\(_2\). Using these two quantities, we get an explicit formula for the critical strain of SLMoS\(_2\),

\[
\epsilon_c = -\frac{4\pi^2 D}{C_{11} L_y^2} \equiv -\frac{43.52}{L_x^2} \equiv -\frac{43.52}{L^2}. \tag{5}
\]

Hereafter, we will use \(L\) to denote the length of the SLMoS\(_2\) instead of \(L_x\).
3. Results and discussions

After the representation of the Euler buckling theory, we are now performing MD simulations to study the buckling of SLMoS\(_2\). All MD simulations in this work are performed using the publicly available simulation code LAMMPS [42, 43], while the OVITO package was used for visualization in this section [44]. The standard Newton equations of motion are integrated in time using the velocity Verlet algorithm with a time step of 1 fs. The interaction within MoS\(_2\) is described by the Stillinger–Weber potential, where the parameters for this potential have been fitted to the phonon dispersion of single-layer and bulk MoS\(_2\) [26]. The phonon dispersion is closely related to some mechanical quantities like Young’s modulus and some thermal properties, so this parameter set can provide a good description for the mechanical and thermal properties of the single-layer MoS\(_2\). Periodic boundary conditions are applied in the two in-plane directions, and the free boundary condition is applied in the out-of-plane direction. Our simulations are performed as follows. First, the Nosé–Hoover [45, 46] thermostat is applied to thermalize the system to a constant pressure of 0, and a constant temperature of 1.0 K within the NPT (i.e. the particles number \(N\), the pressure \(P\) and the temperature \(T\) of the system are constant) ensemble, which is run for 100 ps. The SLMoS\(_2\) is then compressed in the \(x\)-direction within the NPT ensemble, which is also maintained through the Nosé–Hoover thermostat. The SLMoS\(_2\) is compressed uniaxially along the \(x\)-direction by uniformly deforming the simulation box in this direction, while it is allowed to be fully relaxed in lateral directions during the compression.

We shall examine the strain rate effect on the critical strain. Figure 2 shows the stress–strain relation under compression for SLMoS\(_2\) with length 60 Å and width 40 Å at 1.0 K. The curve drops sharply at a critical strain \(\epsilon_c = 0.00939\) when the SLMoS\(_2\) is compressed at a strain rate \(\dot{\epsilon} = 1.0 \mu s^{-1}\).

![Figure 2](image1.png)

Figure 2. Stress–strain relation under compression for SLMoS\(_2\) with length 60 Å and width 40 Å at 1.0 K. The curve drops sharply at a critical strain \(\epsilon_c = 0.00939\) when the SLMoS\(_2\) is compressed at a strain rate \(\dot{\epsilon} = 1.0 \mu s^{-1}\).

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![Figure 3](image2.png)

Figure 3. The structure evolution for SLMoS\(_2\) with length 60 Å and width 40 Å at 1.0 K. The SLMoS\(_2\) is compressed at a strain rate \(\dot{\epsilon} = 1.0 \mu s^{-1}\). The buckling happens at \(\epsilon = 0.00939\). The structure transforms from sinuous into zigzag at \(\epsilon = 0.249\).
The strain rate effect on the critical strain for SLMoS2 with width 40 Å at 1.0 K. The critical strain increases linearly with increasing strain rate for SLMoS2 with length L = 60 Å in (a) and L = 120 Å in (b). Note that the slope (2.7 × 10^{-5} μs^{-1}) of the fitting line in the shorter system in (a) is only a quarter of the slope of 1.0 × 10^{-3} μs in the longer MoS2 in (b), which implies that the strain rate has a stronger effect for longer MoS2.

At 1.0 K. The length of the SLMoS2 is 60 Å in panel (a) and 120 Å in panel (b). In both systems, the critical strain increases linearly with increasing strain rate. The simulation data are fitted to a linear function y = a + bx, where the coefficient a = 9.4 × 10^{-3} and 2.4 × 10^{-3} can be regarded as the exact value (with δ → 0.0) for the critical strain in these two SLMoS2. Using a strain rate of 1.0 μs^{-1}, we get the critical strains 0.00938 and 0.00252 for SLMoS2 with L = 60 Å and 120 Å. As a result, the error due to using a finite strain rate of 1.0 μs^{-1} is 0.2% and 5% for these two SLMoS2. For the coefficient b, this slope of the fitting line in the shorter system in panel (a) is 2.7 × 10^{-5} μs, which is only a quarter of the slope of 1.0 × 10^{-4} μs in the longer MoS2 in panel (b). It indicates that the strain rate has stronger effect for longer SLMoS2, because the frequency of the buckling mode (first lowest-frequency normal mode) is lower in a longer system, leading to longer response time. That is, the buckling mode in a longer SLMoS2 requires longer relaxation time for its occurrence.

Figure 5 shows the length dependence of the critical strain in SLMoS2 with width 40 Å at 1.0 K. The system is compressed at the strain rate of 1.0 μs^{-1} (red squares), 10.0 μs^{-1} (blue triangles), and 100.0 μs^{-1} (black circles). Lines are fit to function y = a + bx, where the coefficient b increases with increasing strain rate. In particular, the coefficient of b = 40.6 Å^2 for δ = 1.0 μs^{-1} is only 6.7% smaller than the prediction from the Euler buckling theory of b = 4π^2D/C_{11} = 43.52 Å^2, where D is the bending modulus and C_{11} is the in-plane stiffness for SLMoS2.
SLMoS2. Furthermore, for the strain rate \( \dot{\varepsilon} = 1.0 \ \mu s^{-1} \), the other coefficient \( a \) is fairly small and there is almost no fluctuation between simulation data, both of which validate the usage of the small strain rate, \( \dot{\varepsilon} = 1.0 \ \mu s^{-1} \). The critical strain for the shortest SLMoS2 (\( L = 60 \) Å) deviates from the fitting curve in all of the three situations. It is due to the linear nature of the Euler buckling theory, while the nonlinear effect becomes important in the short system. The critical strain does not depend on the width of the SLMoS2, because the shape of the buckling mode is uniform in the width direction. Hence, the strain energy is the same in SLMoS2 of different widths. That is why the width parameter does not present in the Euler buckling formula in equation (5).

Figure 6 shows the temperature effect on the critical strain for SLMoS2 with width 40 Å at strain rate 1.0 \( \mu s^{-1} \). Panel (a) is the temperature dependence of the relative critical strain versus temperature for SLMoS2 with \( L = 60 \) and 120 Å. The relative critical strain is scaled by the value at 1.0 K; i.e. 0.00939 and 0.00252 for \( L = 60 \) and 120 Å respectively. Lines are provided as a guide to the eye. The critical strain in both systems remains almost constant at temperatures below 50 K. It increases linearly with increasing temperature for temperatures above 50 K, and the critical strain increases faster in longer SLMoS2. This is due to strong thermal vibration at high temperatures. Panel (b) shows the maximum thermal vibration amplitude versus temperature for SLMoS2 with \( L = 60 \) (black circles) and 120 Å (red squares). According to the equipartition theorem, the maximum thermal vibration amplitude can be fitted to function \( y = \alpha x^{0.5} \). Lines are the fitting results. The maximum vibration amplitude increases with increasing temperature. At higher temperatures (above 50 K), the maximum vibration amplitude is so large that it can disturb the buckling mode; i.e. the strong thermal vibration is able to heal the buckling-induced deformation in the SLMoS2. At the initial buckling stage, atoms are displaced from its original position (following the buckling mode, i.e. the first lowest-frequency normal mode), but atoms are involved in a strong thermal vibration in the meantime. This large thermal vibration amplitude blurs the buckling deformation and the original configuration of the SLMoS2. In other words, the thermal vibration introduces a healing mechanism for the buckling deformation at the initial buckling stage. Similar thermal healing mechanisms have also been observed in the thermal treatment for defective carbon materials [47, 48]. Hence, larger compression strain is needed to incite the buckling phenomenon at higher temperatures.

We end by noting that the present atomistic simulation actually has practical impact, although we emphasized the importance of the strain rate and temperature effects on the buckling of the SLMoS2, which are technique aspects. MoS2 and graphene have complementary physical properties, so it is natural to investigate the possibility of combining graphene and MoS2 in specific ways to create heterostructures that mitigate the negative properties of each individual constituent. For example, graphene/MoS2/graphene heterostructures have better photon absorption and electron-hole creation properties because of enhanced light-matter interactions by the single-layer MoS2 [49]. It has been shown that the buckling critical strain for a graphene of 19.7 Å in length is around 0.0068 [29]. From the Euler buckling theorem, it can be extracted that the buckling critical strain for a graphene of 60.0 Å in length is around 0.00073. Our simulations have shown that the buckling critical strain for SLMoS2 of the same length is 0.0094, which is one order higher than graphene. It indicates that the SLMoS2 can sustain stronger compression than graphene. The higher buckling critical strain for the SLMoS2 is helpful to protect the graphene/MoS2 heterostructure from buckling damage.

4. Conclusion

In conclusion, we have performed MD simulations to investigate the buckling of the SLMoS2 under uniaxial compression. In particular, we examine the importance of the strain rate and temperature effects on the critical buckling strain.
The critical strain increases linearly with increasing strain rate, and it keeps nearly constant at low temperatures. The critical strain increases with increasing temperature at temperatures above 50 K, since the strong thermal vibration is able to repair the buckling-induced deformation. The length dependence for the critical strain is in good agreement with the Euler buckling theory.

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