Elastic bending modulus of single-layer molybdenum disulfide (MoS$_2$): finite thickness effect

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Received 13 August 2013, in final form 6 September 2013
Published 2 October 2013
Online at stacks.iop.org/Nano/24/435705

Abstract

We derive, from an empirical interaction potential, an analytic formula for the elastic bending modulus of single-layer MoS$_2$ (SLMoS$_2$). By using this approach, we do not need to define or estimate a thickness value for SLMoS$_2$, which is important due to the substantial controversy in defining this value for two-dimensional or ultrathin nanostructures such as graphene and nanotubes. The obtained elastic bending modulus of 9.61 eV in SLMoS$_2$ is significantly higher than the bending modulus of 1.4 eV in graphene, and is found to be within the range of values that are obtained using thin shell theory with experimentally obtained values for the elastic constants of SLMoS$_2$. This increase in bending modulus as compared to monolayer graphene is attributed, through our analytic expression, to the finite thickness of SLMoS$_2$. Specifically, while each monolayer of S atoms contributes 1.75 eV to the bending modulus, which is similar to the 1.4 eV bending modulus of monolayer graphene, the additional pairwise and angular interactions between out of plane Mo and S atoms contribute 5.84 eV to the bending modulus of SLMoS$_2$.

(Some figures may appear in colour only in the online journal)

Molybdenum disulfide (MoS$_2$) is a semiconductor with a bulk bandgap above 1.2 eV [1], which can be further manipulated by reducing its thickness to monolayer [2], (or through application of mechanical strain [3, 4]). This finite bandgap is a key reason for the excitement surrounding MoS$_2$ as compared to another two-dimensional material, graphene, as graphene is well-known to be gapless [5]. Because of its direct bandgap and also its well-known properties as a lubricant, MoS$_2$ has attracted considerable attention in recent years [6, 7]. For example, Radisavljevic et al [8] demonstrated the application of single-layered MoS$_2$ (SLMoS$_2$) as a transistor. Several recent works have addressed the thermal transport properties of SLMoS$_2$ in both the ballistic and diffusive transport regimes [9–12], while the mechanical behavior of the SLMoS$_2$ has also recently been investigated experimentally [13–16]. We have also recently performed theoretical investigations considering edge effects on the Young’s modulus of SLMoS$_2$ nanoribbons based on a recently developed Stillinger–Weber (SW) potential [12].

Besides the Young’s modulus, the bending modulus is another fundamental mechanical property. For two-dimensional materials such as graphene or MoS$_2$, the bending modulus is important because it has been shown that the electronic properties of graphene can be strongly impacted by introducing curvature to its topology [17], which points to the important coupling between the mechanical and electrical properties in these two-dimensional materials [18]. The bending modulus also has strong implications for potential future flexible, or stretchable electronics applications involving SLMoS$_2$. 

For graphene, it has been shown that the bending modulus can be analytically calculated directly from an empirical potential. Ou-Yang et al obtained the value for the elastic bending modulus of graphene from a geometric approach [19, 20]. In another analytic work, the exponential Cauchy–Born rule [21] was applied to extract the elastic bending modulus for graphene from the Brenner empirical potential [22, 23]. The bending modulus value from both analytic studies shows good agreement with the experimental data.

Another important benefit of deriving the bending modulus \( D \) directly from the interatomic potential, as done by Arroyo and Belytschko [22] and Lu et al [23] is that in doing so, the need to define an effective thickness \( h \) of SLMoS\(_2\), as is required from shell theory through the well-known relationship \( D = E^{2D} h^2 / (12(1 - \nu^2)) \), where \( E^{2D} = Eh \) is the two-dimensional stiffness and \( \nu \) is Poisson’s ratio, is removed. This is important because the precise definition of the thickness of a monolayer-thick nanostructure, dating back to nanotubes and more recently for two-dimensional graphene, has been an ongoing source of controversy [20, 22, 24–31].

In the present work, by adopting the finite crystal elasticity approach of Arroyo and Belytschko [22], the bending modulus of SLMoS\(_2\) is inherently thickness-independent because it is derived from a surface, and not volume energy density.

Therefore, the objective of this work is to derive an analytic formula for the elastic bending modulus of SLMoS\(_2\) based on our recently developed SW potential [12]. The elastic bending modulus obtained for SLMoS\(_2\) is 9.61 eV, which is larger than the elastic bending modulus of graphene from the Brenner empirical potential [22, 23]. Another important benefit of deriving the bending modulus \( D \) is that it is inherently thickness-independent, which is larger than the elastic bending modulus of graphene [22, 23].

\[ D = \frac{E^{2D} h^2}{12(1 - \nu^2)} \]

where \( E^{2D} = Eh \) is the two-dimensional stiffness and \( \nu \) is Poisson’s ratio [14] and \( \epsilon \) is the strain. Hence, from this estimation, we get an error of 6.5% for our analytic formula in the presence of a mechanical strain of 5%.

From the atomic geometry in figure 1(a), there are the following two constraints on the variables \((b_0, d_0, \phi_0)\):

\[
d_0 = b_0 \sin \phi_0; \quad 2d_0 = \sqrt{3}b_0 \cos \phi_0. \tag{1}\]

As a result, we have \( \phi_0 = \frac{\sqrt{3}}{2} \) and \( d_0 = b_0 \sin \phi_0 = \sqrt{\frac{3}{7}}b_0 \), so we get the bond angle \( 2\phi_0 = 81.787^\circ \) and the Mo–S–Mo interplane spacing \( d_0 = 1.558 \) Å. We denote S atoms sitting in the two planes as S\( ^\pm \).

To investigate the bending properties of SLMoS\(_2\), similar to graphene [22, 23] we homogeneously bend it into a cylindrical surface with radius \( R = 1/\kappa \), where \( \kappa \) is the only nonzero principal curvature. Due to the homogeneous bending, the Mo atomic layer is ideally bent. However, the outer S\(^+\) atomic layer is stretched upon bending, while the inner S\(^-\) atomic layer is compressed. The radii of the cylinder for S\(^\pm\) atoms are \( R = R(1 \pm \kappa d_0) \). As a result, the tensile or compressive strain for these two S atomic layers is \( \epsilon = \pm \kappa d_0 \).

2. Empirical energy density

We have recently parameterized a SW potential for SLMoS\(_2\) [12]. The two-body interaction takes form

\[
V_2 = \epsilon A(\sigma r_{ij}^{-p} - \sigma q r_{ij}^{-q}) e^{(\sigma (r_{ij} - \sigma )^{-1})}, \tag{2}\]
where the exponential function ensures a smooth decay of the potential to zero at the cut-off, which is key to conserving energy in MD simulations.

The three-body interaction is
\[
V_3 = \varepsilon \exp[-\gamma (r_{ij} - a_0) - 1 + \gamma (r_{ik} - a_0) - 1] (\cos \phi_{ijk} - \cos 2\phi_0)^2, \tag{3}
\]
where \(2\phi_0\) is the angle in the undeformed configuration. There are five types of interactions in SLMoS\(_2\) as denoted by red springs (for two-body) and blue springs (for three-body) in figure 1(b). All SW potential parameters can be found in [12].

From the SLMoS\(_2\) configuration, we find the following constraint due to the equilibrium of the Mo and S atoms:
\[
\frac{\partial W}{\partial q_i} \bigg|_{\kappa=0} = 0, \tag{5}
\]
where \(q_i\) is the deformed bond length. Owing to the particular form of the SW three-body potential, we also have:
\[
\frac{\partial W}{\partial \theta} \bigg|_{\kappa=0} = 0; \quad \frac{\partial^2 W}{\partial \theta^2} \bigg|_{\kappa=0} = 0. \tag{6}
\]

Therefore, the SW potential predicts a zero bending modulus for graphene, because as explained in Arroyo and Belytschko [22], the SW potential cannot describe the bending properties of planar, one-atom-thick structures. In particular, the flexural modes, which are related to the bending modulus in graphene, will have zero energy from the SW potential [33]. However, the SW potential is able to describe the bending of SLMoS\(_2\), which has finite thickness and non-planar covalent bonds. This point will be clearly demonstrated in the following analytic derivation of the bending modulus from the energy density \(W\) in equation (4).

3. Analytic derivation of bending modulus

Following Arroyo and Belytschko [22], the bending modulus can be calculated by
\[
D = \frac{\partial^2 W}{\partial \kappa^2}. \tag{7}
\]
Recalling equations (5) and (6), the bending energy can also be written as
\[
D = \sum_q \frac{\partial^2 W}{\partial r_i^2} \left( \frac{\partial \kappa}{\partial \kappa} \right)^2 + \sum_q \left( \frac{\partial^2 W}{\partial \theta^2} \right) \left( \frac{\partial \kappa}{\partial \kappa} \right)^2. \tag{8}
\]
This formula is substantially different from the bending modulus formula in graphene [22]. Specifically, the first derivative here for \(r_i\) and \(\theta_k\) with respect to \(\kappa\) is nonzero owing to the finite thickness of SLMoS\(_2\).

To calculate the bending modulus using equation (8), two quantities \(\frac{\partial^2 W}{\partial r_i^2}\) and \(\frac{\partial^2 W}{\partial \theta^2}\) are required. In the following, we will calculate these two quantities for all six terms in the energy density \(W\) in equation (4). Finally, while SLMoS\(_2\) is a multi-lattice which requires an internal, or shift degree of freedom between the Mo and S planes, we have verified that, similar to monolayer graphene [22, 23], the shift degree of freedom does not contribute to the bending modulus of SLMoS\(_2\).

(1) The first term in the energy density \(W\) in equation (4) is of the form \(V_2(r_{\text{Mo1}})\), which captures the pair FNN interactions between Mo and S atoms. For the first energy term, we have \(\frac{\partial^2 W}{\partial \gamma^2} = 0\). Hence we only need to calculate \(\frac{\partial r_i}{\partial \kappa}\). (To derive this quantity, the two-dimensional SLMoS\(_2\) plane is rolled up onto the cylindrical surface in figure 1(c)), where point A represents atom Mo1 and point B represents the projection of two S atoms (e.g. S\(_5\) and S\(_6\)) onto the Mo atomic layer.
layer. We consider the inner S\(^-\) atom layer. From figure 1(d), one can find the lattice vector to be:

\[
\tilde{r}_q = AS = \begin{pmatrix} (R - d_0) \cos \kappa w_2 \\ (R - d_0) \sin \kappa w_2 \end{pmatrix} = \begin{pmatrix} R \\ 0 \end{pmatrix} - \begin{pmatrix} w_0 Q (\frac{\kappa w_2}{2}) \\ w_2 Q (\frac{\kappa w_2}{2}) \end{pmatrix}.
\]

Using equation (9) the first derivative of the lattice vector is

\[
\frac{\partial \tilde{r}_q}{\partial \kappa} = \begin{pmatrix} -1 \frac{w_0}{2} \\ d_0 w_0 \end{pmatrix}.
\]

The first derivative of the bond length is

\[
\frac{\partial r_q}{\partial \kappa} = \frac{1}{r_q} \frac{\partial \tilde{r}_q}{\partial \kappa} = \frac{-d_0}{2} w_0^2 = -\frac{\sqrt{3}}{7\sqrt{3}} b_0^2 \cos^2 \theta_q.
\]

This is different from the situation in monolayer graphene. We obtain a nonzero value for the first derivative of the bond length because \(\tilde{r}_q \neq 0\). This term is related to the inter-layer spacing \(d_0\), which implies that this nonzero value is the result of the finite thickness of SLMoS\(_2\). For S\(^+\) atoms on the outer cylindrical surface, the only difference is to substitute \(d_0\) by \(-d_0\).

(2) The second term in the energy density \(W\) in equation (4) is of the form \(V_2(R^2)\), which captures the three-body (angular) interactions between Mo atoms in Mo\(_1\)-Mo\(_2\) or Mo\(_1\)-Mo\(_0\). For this derivation, in figure 1(c), point A represents a Mo\(_1\) atom while point B represents one of its SNN atoms (e.g. Mo\(_2\)). All Mo atoms are on the same cylindrical surface, so we get the lattice vector in the cylinder:

\[
\tilde{r}_q = AB = \begin{pmatrix} \frac{-\kappa w_0^2}{2} Q^2 (\frac{\kappa w_2}{2}) \\ w_0^2 Q (\frac{\kappa w_2}{2}) \end{pmatrix},
\]

where the two variables \((w_0, w_1) = b_{Mo}(\cos \theta_q, \sin \theta_q)\), and \(b_{Mo} = \sqrt{3} c_0\) is the distance between two neighboring Mo atoms in SLMoS\(_2\). Using this formula, we find that

\[
\frac{\partial \tilde{r}_q}{\partial \kappa} = \begin{pmatrix} -1 \frac{w_0^2}{2} \\ d_0 w_0 \end{pmatrix}.
\]

As a result, \(\tilde{r}_q \cdot \frac{\partial \tilde{r}_q}{\partial \kappa} = 0\), leading to \(\frac{\partial \tilde{r}_q}{\partial \kappa} = 0\), and thus the SNN Mo atom interactions do not contribute to the bending modulus of SLMoS\(_2\).

(3) The third term in the energy density \(W\) in equation (4) is of the form \(V_3(\theta_{Mo1}^{\sigma}, \theta_{Mo2}^{\sigma})\), which captures the three-body (angular) interactions between Mo and two S atoms in the same plane. For the third energy term, we have \(\frac{\partial^2 W}{\partial \theta_q^2} = 0\). We consider the S\(^-\) atom on the inner cylindrical surface. For S\(^+\) atoms, the derivation is analogous. For this derivation, in figure 1(c), points A and B represent two neighboring S\(^-\) atoms (e.g. S\(_1\) and S\(_2\)) on the inner atomic cylindrical surface. The lattice vector is:

\[
\tilde{r}_q = \frac{-\kappa w_0^2}{2} Q^2 (\frac{\kappa w_2}{2})\frac{\partial r_q}{\partial \kappa} = \begin{pmatrix} -1 \frac{w_0^2}{2} \\ d_0 w_0 \end{pmatrix}.
\]

where due to the compression within the S\(^-\) layer, we have two important relationships:

\[
\tilde{w}_2 = (1 - qd)w_2; \quad \kappa = \frac{1}{R - d} = \kappa (1 + qd).
\]

Here, \((w_2, w_1) = b_S(\cos \theta_q, \sin \theta_q)\), \(b_S = \sqrt{3} c_0\) is the distance between two neighboring S atoms in SLMoS\(_2\).

The first derivative of the lattice vector is:

\[
\frac{\partial \tilde{r}_q}{\partial \kappa} = \begin{pmatrix} -1 \frac{w_0^2}{2} \\ d_0 w_0 \end{pmatrix}.
\]

As a result, we get a nonzero value for the first derivative of the bond length \(\frac{\partial r_q}{\partial \kappa} = -\frac{d_0}{2} w_0^2\). For S\(^+\), an analogous derivation gives \(\frac{\partial \tilde{r}_q}{\partial \kappa} = \frac{d_0}{2} w_0^2\).

(4) The fourth term in the energy density \(W\) in equation (4) is of the form \(V_4(\theta_{Mo1}^{\sigma}, \theta_{Mo2}^{\sigma}), \theta_{Mo3}^{\sigma}\), which captures the three-body (angular) interactions between Mo and two S atoms in the same plane. For the fourth energy term, we have \(\frac{\partial^2 W}{\partial \theta_q^2} = 0\). We consider S\(^-\) atoms. From the definition \(\cos \phi = \frac{\hat{n}_i \cdot \hat{n}_j}{\sqrt{3}}\), where \(\hat{n}_i\) and \(\hat{n}_j\) are two unit vectors for the two bonds forming the angle \(\phi\), we get

\[
\frac{\partial}{\partial \kappa} \cos \phi = \frac{3}{14} \frac{d_0 w_0^2}{b_0^2} (5 - 6 \cos 2\theta_q).
\]

(5) The fifth term in the energy density \(W\) in equation (4) is of the form \(V_5(\theta_{Mo1}^{\sigma}, \theta_{Mo2}^{\sigma}, \theta_{Mo3}^{\sigma})\), which captures the three-body (angular) interactions between Mo and S atoms in different layers. For the fifth energy term, \(\frac{\partial^2 W}{\partial \theta_q^2} = 0\). We also have
\[ \frac{\partial}{\partial x} \cos \phi = 0, \] because homogeneously bending SLMoS\(_2\) results in the distance between two S atomic layers being unchanged, i.e. the bond length S\(_x\)S\(_x\) is unchanged. Thus, the angular three-body interactions between an Mo atom and two S atoms in different planes does not contribute to the bending modulus of SLMoS\(_2\).

(6) The sixth term in the energy density \( W \) in equation (4) is of the form \( V_3(\theta^q) \), which captures the three-body (angular) interactions between S atoms in the same plane. For the sixth energy term, \( \frac{\partial^2 W}{\partial \theta^q} = 0 \). We consider the \( S^\prime \) atom on the inner cylindrical surface. For this derivation, in figure 1(c), point A represents the projection of two S atoms (e.g. S\(_5\) and S\(_6\)), and point B represents the Mo atom (e.g. Mo\(_1\)). The lattice vector and its derivatives are:

\[
\vec{r}_q = S^\prime B = \left( \frac{k w_2^2}{2} Q_2 \left( \frac{k w_2}{2} \right) + d_0 \right)
\]

\[
\frac{\partial \vec{r}_q}{\partial \kappa} = \left( \begin{array}{c} -\frac{1}{2} w_2^2 \\ 0 \\ 0 \end{array} \right) ; \quad \frac{\partial r_q}{\partial \kappa} = -\frac{d_0}{2} b_0 w_2^2,
\]

where \((w_2, w_1) = c_0(\cos \theta_q, \sin \theta_q)\). The derivative of the angle is:

\[
\frac{\partial}{\partial \kappa} \cos \phi = -\frac{3}{7} \times \frac{d_0}{b_0^2 c_0} \left( 1 - \cos 2 \theta_q \right). \tag{19}
\]

We have established above that there are two terms (terms 2 and 5) in the energy density \( W \) in equation (4) that do not contribute to the bending modulus of SLMoS\(_2\). We now evaluate the relative contributions of the other four terms using equation (8) to obtain the bending modulus of SLMoS\(_2\):

\[
D_{\text{term1}} = \frac{27}{49} \times 14 \times b_0^2 V_2'(b_0) = 3.09 \tag{20}
\]

\[
D_{\text{term2}} = \frac{9}{8} \times b_3^2 V_3'(b_3-S) = 3.49
\]

\[
D_{\text{term4}} = \frac{12 \times 27 \times 43}{7 \times 49 \times 49} b_0^3 V_3'(\cos \theta) = 2.75
\]

\[
D_{\text{term6}} = \frac{27 \times 54}{7 \times 49 \times 49} b_0^3 V_3'(\cos \theta) = 0.29
\]

\[
D = D_{\text{term1}} + D_{\text{term3}} + D_{\text{term4}} + D_{\text{term6}} = 9.61 \text{ eV} \tag{21}
\]

where the second derivatives are \( V_2'(\tau_0') = \frac{\partial^2 V_2(q \phi)}{\partial \tau^2} |_{\tau = \tau_0} \) and \( V_3'' = \frac{\partial^2 V_3(\cos \phi)}{\partial (\cos \phi)^2} |_{\phi = 2 \theta_0} \).

For the cycle summation \( \sum_q \), we have used some trigonometric summation identities. If \( \theta_q = \theta_1 + (q - 1) \frac{\pi}{3} \), we have \( \sum_{q=1}^{3} \cos \theta_q = 0, \sum_{q=1}^{3} \cos^2 \theta_q = \frac{3}{2}, \) and \( \sum_{q=1}^{3} \cos^4 \theta_q = \frac{5}{2} \). If \( \theta_q = \theta_1 + (q - 1) \frac{\pi}{3} \), we have following trigonometric identities: \( \sum_{q=1}^{6} \cos \theta_q = 0, \sum_{q=1}^{6} \cos^2 \theta_q = 3, \) and \( \sum_{q=1}^{6} \cos^4 \theta_q = \frac{9}{2} \).

From the final results in equation (21), we find the bending modulus of SLMoS\(_2\) to be 9.61 eV, which is about 7 times larger than the value of 1.4 eV for monolayer graphene [23]. Furthermore, we can clearly demonstrate that this difference arises due to the finite thickness effect, or the fact that SLMoS\(_2\) actually contains three planes of atoms. Specifically, equation (21) shows that nearly 36% of the bending modulus, or 3.49 eV, arises from the contribution of the two-body SNN interactions between S atoms that lie on the same plane. Because there are two planes of S atoms in SLMoS\(_2\), we find that each plane of S atoms contributes about 1.75 eV to the bending modulus. This value is similar to the 1.4 eV value for monolayer graphene [23].

However, due to the three planes of atoms, SLMoS\(_2\) receives additional, out of plane contributions to its bending modulus. Specifically, the FNN Mo–S interactions contribute about 3.09 eV, or 32% of the total bending modulus, while the three-body (angular) Mo–S interactions between Mo and S atoms on the same plane, contributes 2.75 eV, or about 29% of the bending rigidity. Not surprisingly, the three-body interactions between S atoms on different planes contributes only 0.29 eV, or about 3% to the total bending modulus. Overall, the two-body (pair) terms contribute about 6.58, or 68% of the total bending rigidity. This means that the angular (three-body) contribution in SLMoS\(_2\) of about 29% is smaller than the 41% contribution that the dihedral angles were found to make to the bending modulus in monolayer graphene [23].

To validate the analytic results, we compute the bending modulus of SLMoS\(_2\) using the same SW potential using the molecular mechanics method. Figure 2 shows the strain energy density for SLMoS\(_2\) nanotubes. The tubes are obtained by rolling up the SLMoS\(_2\) into a cylindrical structure, with the middle Mo atomic layer purely bent. Both armchair and zigzag tubes are calculated. The energy is calculated for this ideally rolled up tube structure without optimization (energy minimization), because the optimization is not considered in the above analytic derivation. As we have pointed out above, the optimization of the shift degree of freedom between the Mo and S planes of atoms does not contribute to the bending modulus. However, the optimization of the whole unit cell
(with one Mo and two S atoms) can slightly decrease the total energy of the system, and represents a more accurate value. Our analytic value of 9.61 eV is about 16% larger than the value (8.03 eV) obtained from the MM method with optimization and relaxation of all degrees of freedom. The dashed line in figure 2 denotes the analytic result, $W = E^{2D}h^2/(12(1-\nu^2))$. To do so, we note that recently, Bertolazzi et al [13] have found $E^{2D} = 180 \pm 60$ N m$^{-1}$ for SLMoS$_2$, while Copper et al [14] found $E^{2D} = 130$ N m$^{-1}$ for SLMoS$_2$. Given those values, we consider $E^{2D}$ to range from 120 to 240 N m$^{-1}$, while taking the Poisson’s ratio $\nu = 0.29$, (which is obtained from first-principles calculations) [14], and the thickness $h = 2 \times 1.558 = 3.116$ Å, Taking these values gives an experimental range for the bending modulus $D$ from 6.62 to 13.24 eV. Our obtained value of $D = 9.61$ eV clearly fits into this range.

4. Conclusion

In conclusion, we derived an analytic formula for the elastic bending modulus of the SLMoS$_2$, which does not require the definition of a thickness for SLMoS$_2$. The obtained elastic bending modulus is 9.61 eV for SLMoS$_2$, which is significantly larger than the elastic bending modulus of graphene, is found to be within the range of values that are obtained using thin shell theory with experimentally obtained values for the elastic constants of SLMoS$_2$. It is found that the finite thickness of the SLMoS$_2$ plays a key role in determining its bending properties. Specifically, while each monolayer of S atoms has a bending rigidity (1.75 eV) similar to that of monolayer graphene (1.4 eV), the additional pairwise and angular interactions between Mo and S atoms contributes 5.84 eV to the bending modulus of SLMoS$_2$.

Acknowledgments

The work is supported by the German Research Foundation (DFG). HSP and QZ acknowledge the support of NSF-CMMI 1036460. All authors acknowledge helpful discussions with Professor Marino Arroyo.

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