Electronic Supplementary Material (ESI) for Nanoscale Advances.

Supporting Information

Strain Engineering of the Mechanical Properties of Two-Dimensional WS_2

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Buckling modes of a free film–continuum model

As described in the main text (Eq. (8)), the shape of the film under a compressive force satisfies the following equation

$$\frac{E_f I}{1-\nu_f^2}\frac{d^4u}{dx^4}+F\frac{d^2u}{dx^2}=0$$

The non-trivial solution for bending due to buckling satisfies the following solution

$$u(x)=A\sin\left(\frac{2\pi x}{\lambda}\right)+B\cos\left(\frac{2\pi x}{\lambda}\right)+Cx+D$$

where A,B,C and D are constants determined from the boundary conditions and λ is the wavelength of the buckled mode, such that

$$\frac{F(1-\nu^2)}{E_f I}=\left(\frac{2\pi}{\lambda}\right)^2$$

Considering a periodic simulation cell of size L, the buckled shape satisfies the following boundary conditions:

$$\frac{d^nu}{dx^n}(0)=\frac{d^nu}{dx^n}(L)$$

Since we can omit rotation and translation of the whole film in our MD simulation, $C = D = 0$. Thus, it is sufficient to consider the boundary conditions for the deflection and the rotation angle (first derivative). Applying the boundary condition of the solution, we obtain the following equations for the boundary conditions

$$\begin{pmatrix} sin\left(\frac{2\pi L}{\lambda}\right) & cos\left(\frac{2\pi L}{\lambda}\right) - 1 \\ cos\left(\frac{2\pi L}{\lambda}\right) - 1 & - sin\left(\frac{2\pi L}{\lambda}\right) \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

There is a non-unique solution when

$$- \sin^2\left(\frac{2\pi L}{\lambda}\right) - \left(cos\left(\frac{2\pi L}{\lambda}\right) - 1\right)^2 = 0,$$

which leads to a discrete set of solutions for the wave lengths, λ_n, that corresponds to the n-th buckling mode

$$\frac{2\pi L}{\lambda_n} = 2\pi n$$

For a free-standing sheet, the buckling force satisfies

$$\frac{F_n(1 - \nu^2)}{E_f I} = \left(\frac{2\pi}{\lambda_n}\right)^2 = \left(\frac{2\pi n}{L}\right)^2$$

Alternatively, the bucking force in the n-th mode of a periodic sheet of length L is

$$F_n = E_f I\left(\frac{4\pi^2 n^2}{(1 - \nu^2)L^2}\right)$$

Given that $I = \frac{wh^3}{12}$ for a sheet, then

$$F_n = \frac{E_f w h^3}{12}\left(\frac{4\pi^2 n^2}{(1-\nu^2)L^2}\right)$$

and the compressive stress for buckling is

$$\sigma_n = \frac{F_n}{wh} = \frac{E_f h^2}{12}\left(\frac{4\pi^2}{(1-\nu^2)\lambda_n^2}\right) = \frac{E_f h^2}{3}\left(\frac{\pi^2 n^2}{(1-\nu^2)L^2}\right)$$

Alternatively, we can find the compressive buckling strain, such that

$$\varepsilon_n = \frac{\sigma_n}{E_f} = \frac{h^2}{3}\left(\frac{\pi^2 n^2}{(1-\nu^2)L^2}\right)$$

The compressive buckling strain as a function of n/L is shown in Fig. S1.

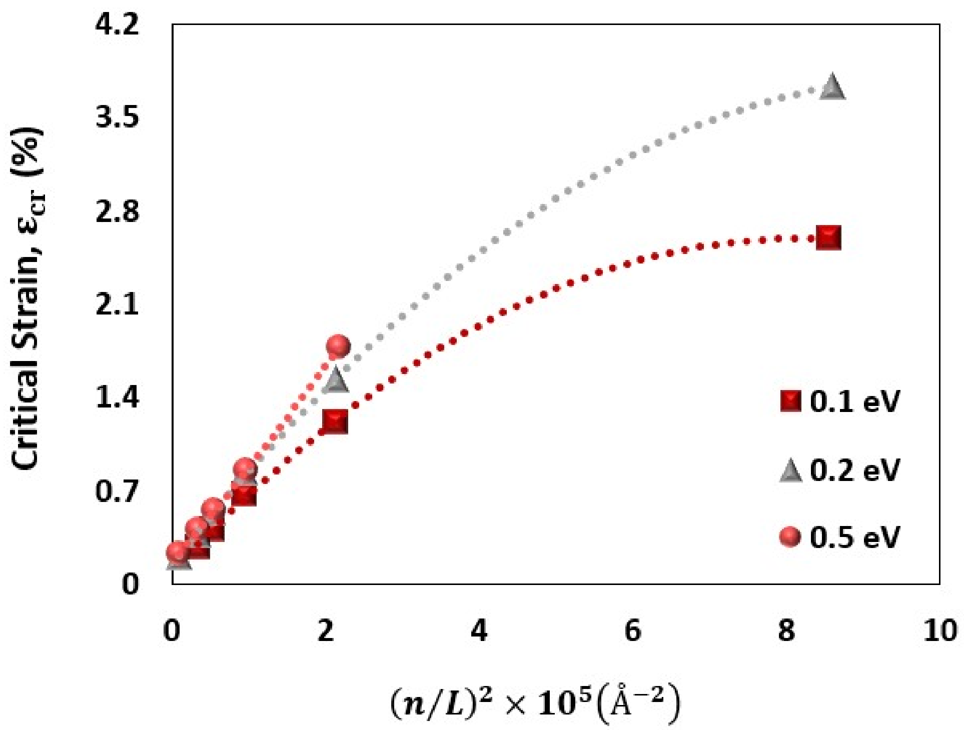

Fig. S1. The buckling strain of a double layer WS_2 film in the MD simulations, for different LJ energies of the intralayer interatomic potential. The lines are a 2nd order polynomial fits, whereas the linear term is used to estimate the slope at large lengths of films (small n/L), from which the effective thickness is estimated.

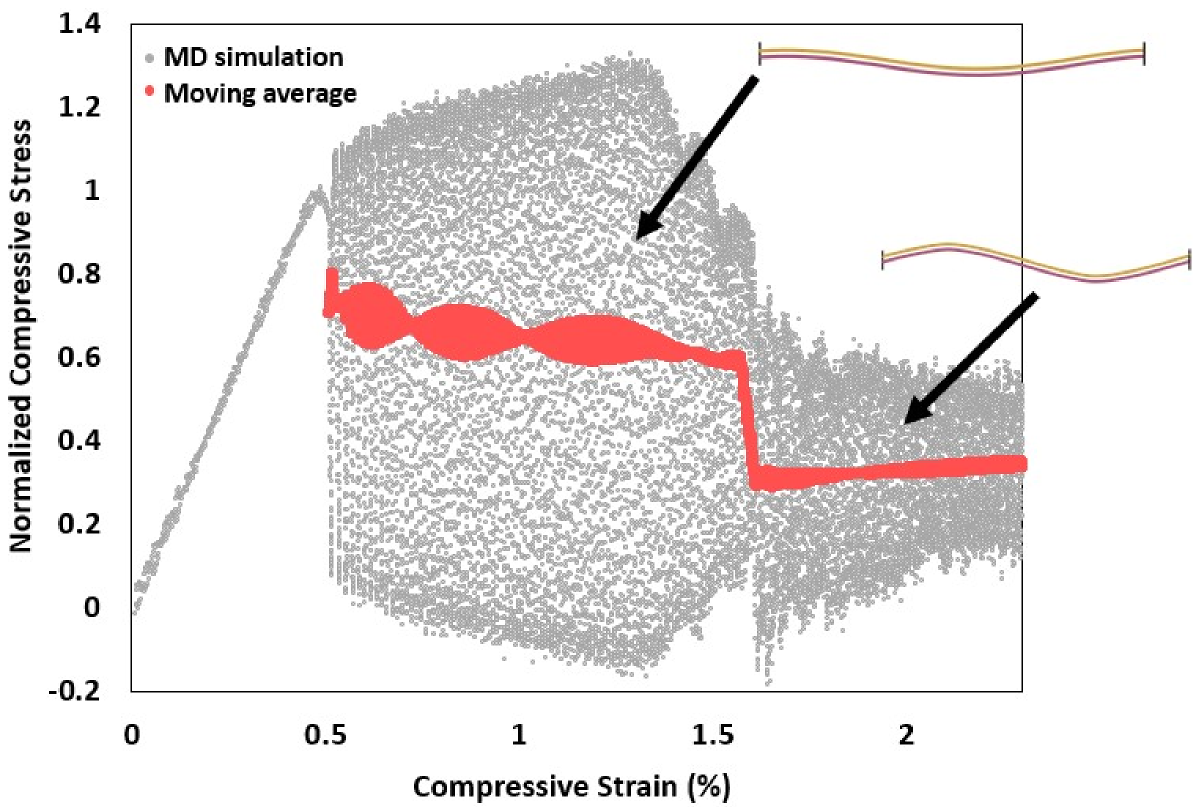

Fig. S2. Stress-strain response of a 540 Ă long double layer WS_2 film (with periodic boundary conditions). To reduce the effect of the fluctuations, moving average is applied to the post-buckling response (red dots). The stress drop as a result of the faceting appears around a strain of 1.5%. The buckled shapes are shown as insets.

Young's modulus of PDMS

We stretched a sample of PDMS, see its stress-strain curve in Fig. S3. The Young's modulus of the PDMS was extracted as $E_s = 845\ kPa$.

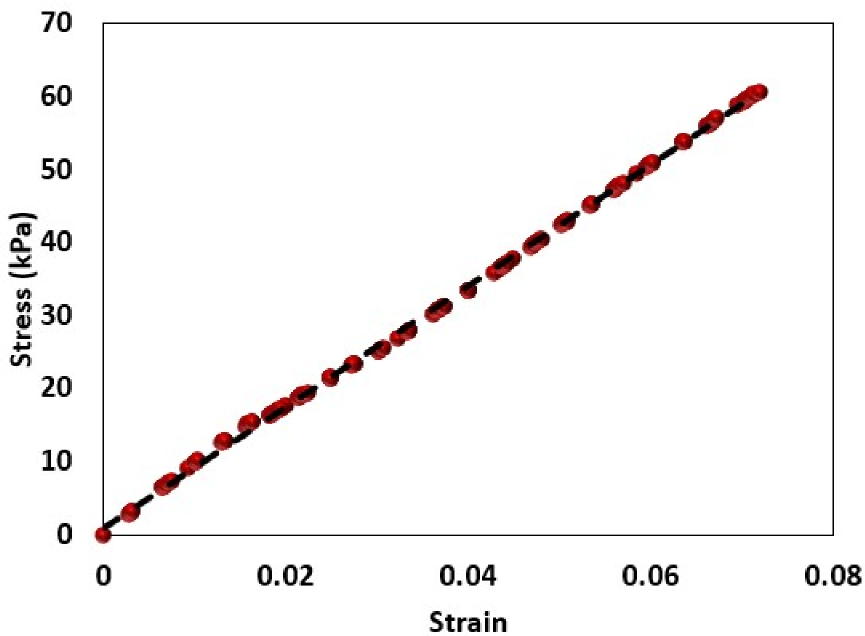

Fig. S3. Measured stress-strain curve of PDMS.

Raman measurement

An example of Raman measurement with no split E_{2g} peak is shown in Fig. S4.

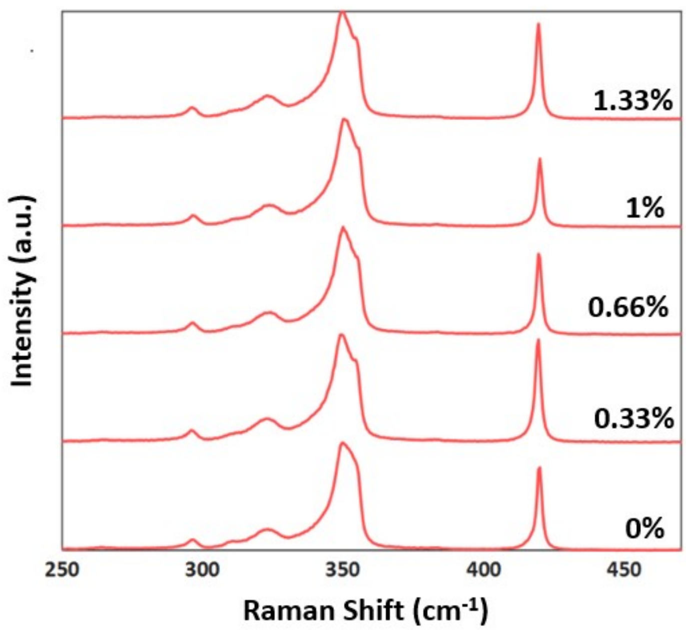

Fig. S4. An example of Raman spectrum with no split E_{2g} peak.