Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


**Supporting Information for:**

# Hysteresis and Its Impact on Characterizing Mechanical Properties of Suspended Monolayer Molybdenum-disulfide Films

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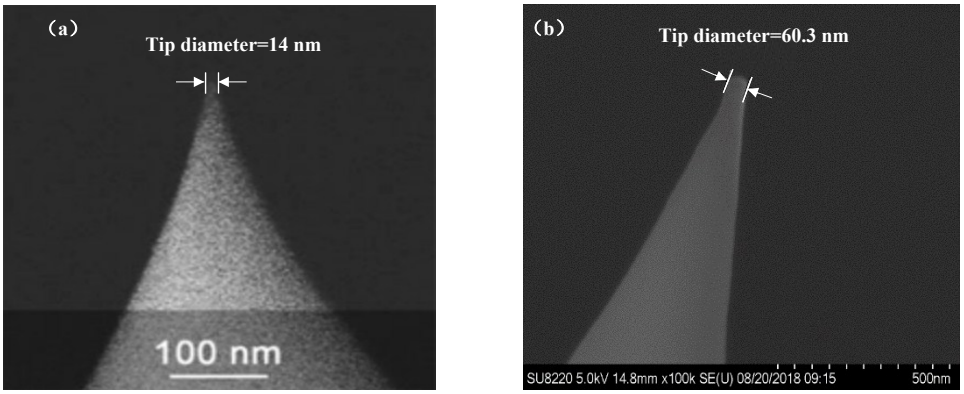


**Figure S1.** Scanning electron micrograph of AFM tip (radius= about 30 nm) (a) before and (b) after use in our experiments. (a) is from the database of manufacturer (Olympus company).

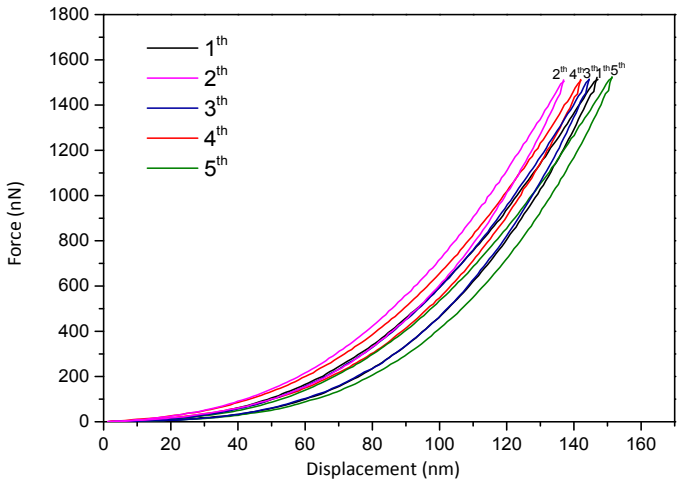


**Figure S2**. The force-displacement curves for a square $MoS_2$ monolayers, with the side length of 1.5 μm and performed at the force of 1500 nN. $1^{th}$, $2^{th}$, $3^{th}$, $4^{th}$, and $5^{th}$ mean the first, the second, the third, the fourth, and the fifth supplemental nanoindentation experiments.

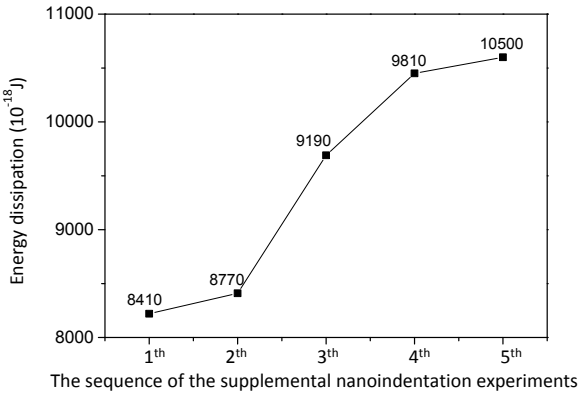


**Figure S3**. Energy dissipations of hysteresis loops in monolayer $MoS_2$ sheets for $1^{th}$ ~$5^{th}$ supplemental nanoindentation experiments.

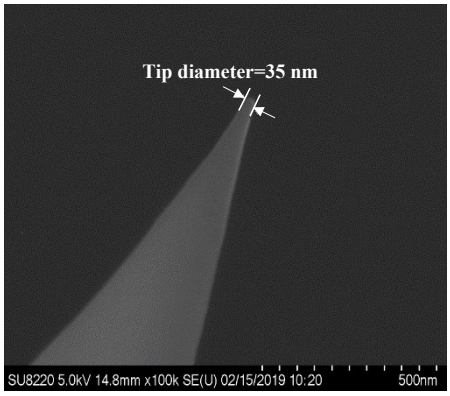


**Figure S4**. Scanning electron micrograph of AFM tip (diameter= about 35 nm) after use in the supplemental nanoindentation experiments. The Scanning electron micrograph of AFM tip before the supplemental experiments is the same as Figure S1 (a).

## MD simultions

In the MD simulations, the monolayer $MoS_2$ film is comprised of a 2D hexagonal honeycomb lattice where a layer of Mo atoms is sandwiched between two layers ( the top and bottom layer) of S atoms, with each Mo atom ionically bonded to six S atoms.[1] In order to efficiently simulate the atomic models, the sizes of tip and the monolayer $MoS_2$ films are scaled down. The rectangular and circular regions with various sizes (80, 100, 120 and 150 Å in diameter or in side length) are defined extending from the center of the films for the nanoindentation simulations, and atoms outside the circular region are fixed as the boundary. A spherical virtual tip with a radius of 3 Å is modeled where there is only repulsive force between tip and monolayer $MoS_2$ sheets. The tip is loaded along the z-axis, and set as a rigid body to avoid the tip wear. The loading rate was set to 0.2 Å/ps, referring to our previous work.[2]

Large-Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) was used to perform the AFM nanoindentation. The atomic interactions in the monolayer $MoS_2$ were determined by the reactive empirical bond-order (REBO) potentials, which has been verified to be more accurate in describing the elastic and mechanical properties of monolayer $MoS_2$.[3-6] The interaction between the monolayer $MoS_2$ and the tip was described by the Lennard–Jones (LJ) potential, which has been demonstrated in our previous works.[2, 4] Before the nanoindentation process, the energy of the system was minimized by the conjugated gradient method, and the isothermal–isobaric (NPT) ensemble controlled by the Nosé-Hoover method was then employed for system relaxation at a temperature of 0.1 K and a pressure of 0.1 bar (the time step is set to 1 fs).

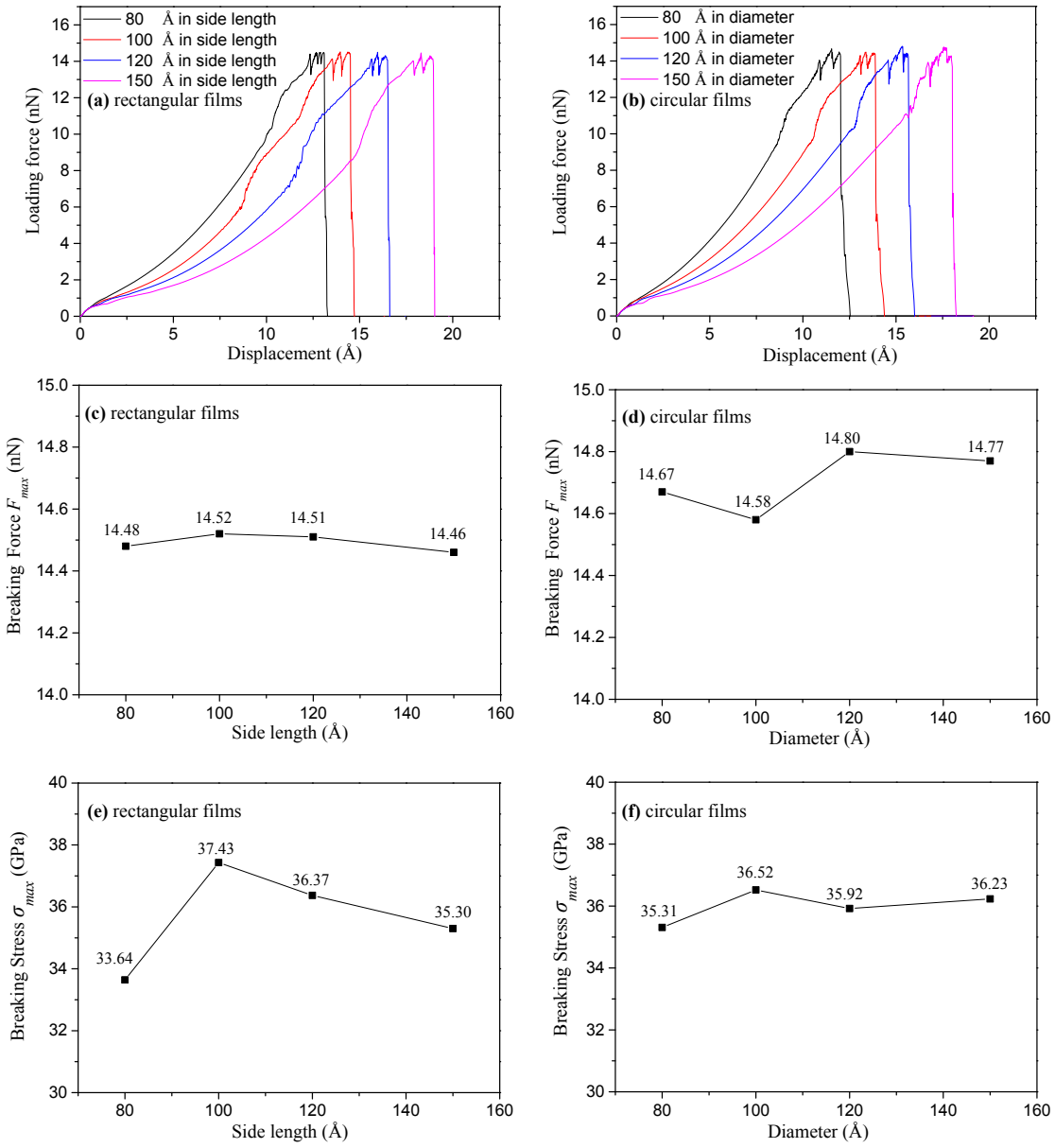


**Figure S5**. The MD simulated loading force-deflection curves, breaking forces $F_{max}$ and breaking stresses $\sigma_{max}$ of the rectangular (a, c and e) and circular (b, d and f) monolayer $MoS_2$ films with various sizes (80, 100, 120 and 150 Å in side length or diameter). The breaking stresses $\sigma_{max}$ are calculated according to the equation 2 in the paper.

## References:


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