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 MoS2 monolayers, with the side length of 1.5 μm and performed at the force of 1500 nN. 1th, 2th, 3th, 4th, and 5th mean the first, the second, the third, the fourth, and the fifth supplemental nanoindentation experiments.

Figure S3. Energy dissipations of hysteresis loops in monolayer MoS2 sheets for 1th~5th supplemental nanoindentation experiments.
MD simulations

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. 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.

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$_2$. 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. 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 $F_{\text{max}}$ and breaking stresses $\sigma_{\text{max}}$ 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 $\sigma_{\text{max}}$ are calculated according to the equation 2 in the paper.
References:
5. S. Xiong and G. Cao, Nanotechnology, 2015, 26, 185705.