

Supplementary

Effect of Compressive Prestrain on the Anti-Pressure and Anti-Wear Performance of Monolayer MoS₂: A Molecular Dynamics Study

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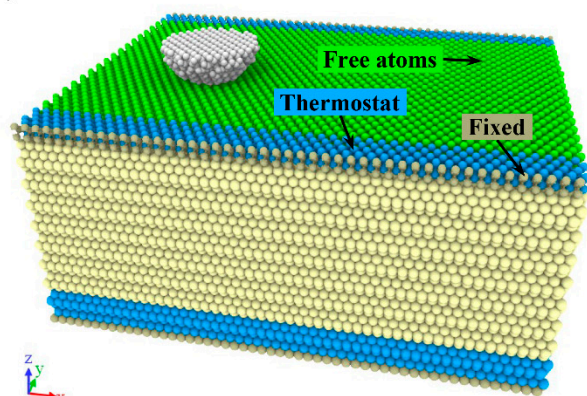
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1. Thermostatting Scheme

(a) Part NVT



(b) All NVT

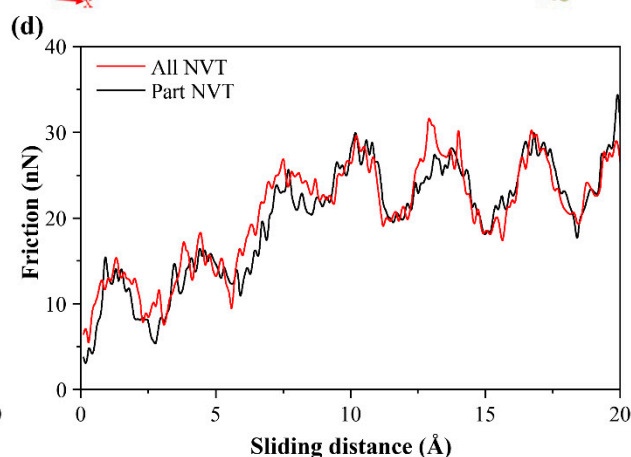
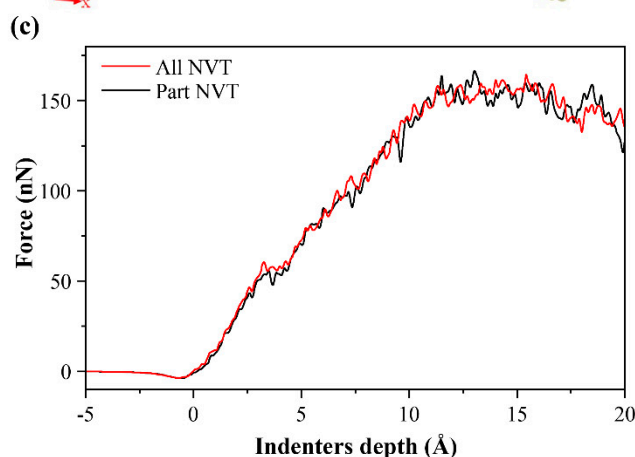
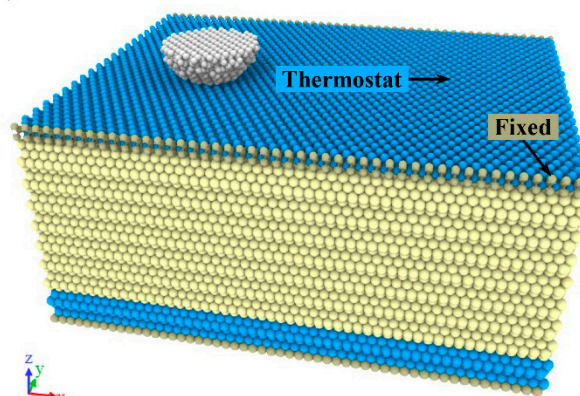


Figure S1. Schematic of two thermostat schemes: (a) Part NVT: the Langevin thermostat is only applied to the MoS₂ atoms close to the fixed region. (b) All NVT: the Langevin thermostat is applied to all free atoms from the MoS₂ layer. Part NVT is adopted in this work. For both schemes, the thermostatting regions in the Pt substrate are the same as that in the main manuscript. (c) The force-depth relations of the MoS₂/Pt substrate during nano-indentation process using Part NVT and All

NVT. (d) The friction-distance curves of the MoS₂/Pt substrate during nano-scratch process using Part NVT and All NVT.

2. Indenting Points and Scanning Lines

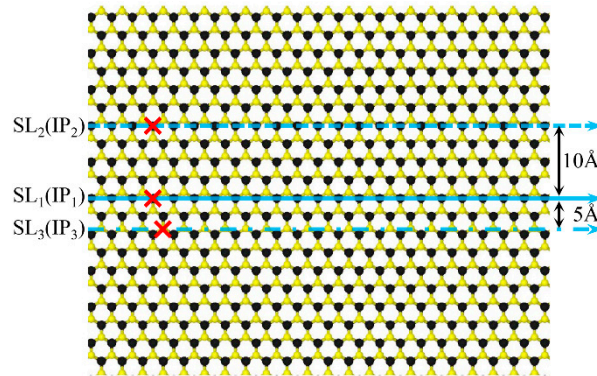


Figure S2. Schematic of indenting points (IP) and scanning lines (SL) on the MoS₂. Each scanning line passes through a corresponding indenting point, which is indicated by red cross.