Fracture Mechanics of Monolayer Molybdenum Disulfide using Molecular Dynamics

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Abstract
Monolayer molybdenum disulfide (MoS2) is a direct bandgap 2D semiconductor that holds great promise for application in nanoelectronic and photonic devices. Due to its bandgap, MoS2 can be used to make transistors and similar electronic gates, making it more versatile than even graphene. We used classical molecular dynamics simulations to study the mechanical properties of monolayer MoS2, focusing specifically on tensile properties and fracture mechanics. A reactive empirical bond-order (REBO) potential was used to model the internal atomic interactions of MoS2. First, we optimized the bond cutoff length parameters of the REBO potential by comparing the calculated tensile strength of monolayer MoS2 with previous computational and experimental studies. The potential was then used to investigate the effects of substrate-material interaction, strain rate, temperature, and defects on the crack propagation of MoS2. We found that while the tensile properties of MoS2 are highly dependent on temperature and stress orientation, substrate interaction has a negligible effect due to weak substrate-potential forces. Furthermore, we showed that crack orientation and strain rates determine the propagation paths of fractures. Finally, we corroborated these results with experimental transmission electron microscopy (TEM) videos of MoS2 fracture mechanics from Warner et al. Our study offers new fundamental insights into the fracture mechanisms of atomically thin materials like MoS2.

Summary
Monolayer molybdenum disulfide (MoS2) is an atomically thin semiconductor that has more favorable electrical, optical, and chemical properties than other 2D semiconductors such as graphene or silicene. It is therefore an excellent candidate for use in a wide range of electronic devices, including computer circuits, cell-phones, and handheld sensors. To prevent the deterioration of such devices, it is critical to understand the mechanical properties of monolayer MoS2. In this work, we studied the properties of monolayer MoS2 using computer simulations based on solving the classical equations of motion for individual atoms. These simulations were used to determine the effects of several critical parameters, including temperature and material defects, on the way monolayer MoS2 responds to strain or undergoes fracturing. Our study provides important insights into the fundamental mechanical properties of monolayer MoS2, contributing to the prediction and prevention of material failure in electronic devices for emerging technologies.