The influences of strain rate on the failure behavior of nanowire by atomistic simulation

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Abstract

Nanowires have received much attention in scientific and engineering fields owing to their outstanding mechanical, electrical and thermal properties. In nanowire researches, the failure modes and the mechanisms of failure have been widely focused on. As the experiments are not easy to carry out at nano-scale, the molecular dynamics simulation plays an important role in investigating the nanowires.

In this presentation, we investigate the dynamical responses, the failure modes and the failure mechanisms of copper nanowires under high strain rates with molecular dynamics simulation. The setup of atomistic models is first thoroughly discussed. Then the cases of loading rates 10^6~10^9 1/s are simulated to investigate the influences. It is found that the yielding stress of nanowires will increase when the strain rate increases, but the magnitudes for different strain rates do not vary significantly. Obvious influences on the failure modes are also observed. The failure is mainly ductile for lower strain rate, and the increase of strain rate will result in embrittlement effect. The mode change can be attributed to inadequate release of dislocations. It is also found that the stress waves generated by the tensile loading are important to the failure mechanism. The combined influential effects by the strain rate and the nanowire size are also investigated.

Keywords: **Nanowire, molecular dynamics, strain rate, failure mechanism**