

# MOLECULAR DYNAMICS SIMULATIONS OF THE TENSILE DEFORMATION OF CU NANOWIRES

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Nanoscale plasticity has drawn significant attention in recent years. Extensive Experimental and numerical studies have been conducted in this field. In previous molecular dynamics (MD) simulations, the Nose-Hoover isothermal procedure was often used to maintain a constant temperature. However, at strain rates on the order of  $10^7\text{s}^{-1}$  or higher, there is not sufficient time for the specimens to exchange heat with the environment. The deformation of nanowires is more close to an adiabatic process rather than an isothermal process. Consequently, more realistic treatments of the issue should entail proper account of temperature increases and should avoid artificial or arbitrary numerical schemes.

The effects of size and strain rate on the tensile deformation of Cu nanowires are analyzed. The analysis uses MD simulations with an embedded atom method (EAM) potential. The cross-sectional dimensions of the nanowires vary from 5 to 20 lattice spacings (or 1.8-7.2 nm). The length of the specimens is 60 lattice spacings (or 21.6 nm). Deformations under spacing strain rates between  $1.67\times 10^7$  and  $1.67\times 10^9\text{ s}^{-1}$  are analyzed. The variation of yield stress with specimen size and deformation rate is studied. It is found that the yield stress (stress at which plastic deformation initiates) decreases with specimen size, while increases with loading rate. On the other hand, ductility (strain at which total separation occurs) increases with specimen size and strain rate. The influences of specimen size are a result of enhanced opportunities for dislocation motion at larger sizes. The influence of rate is due to the dynamic wave effect or phonon drag that impedes the motion of dislocations.

This analysis also focuses on the stress calculation for atomistic systems. Historically, one of the most commonly used methods to calculate stress in an MD system is the virial stress. The virial stress includes a kinetic energy part and an interatomic force part. It has been shown that the kinetic energy term in the virial stress causes it to violate balance of momentum if it is interpreted as a form of mechanical stress. The conclusion is that the interatomic force part of the virial stress alone fully constitutes the Cauchy stress. This new understanding is reflected and used in this paper. In particular, the analysis quantifies the level of errors that may be caused in stress calculation when the kinetic energy term is included. It is found that the relative error varies as the deformation progresses. At the onset of yielding, the level of error is on the order of 5-8%. However, at large plastic strains, the error is typically of the order of 30% and can exceed 100% toward late stages of deformation when fracture initiates.