# TENSILE DEFORMATION BEHAVIOR AND MECHANICAL PROPERTY STUDY OF SIX FCC METALS

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**Abstract**

Nanomaterials have enhanced mechanical properties in comparison to their respective bulk materials. To understand the effect of the size and shape on the mechanical properties of nanomaterials, we used molecular dynamics (MD) methods to simulate the deformation process of copper, gold, nickel, palladium, platinum, and silver nanowires of three cross-sectional shapes (quare, circular, and octagonal) and four diameters (varied from one to eight nanometers).

In this work, the nanowires were subjected to a uniaxial tensile load in the [100] direction at a strain rate of $10^8$ $s^{-1}$ at a simulation temperature of 300 K. The embedded-atom method was employed to describe the many-body atomic interaction energy in metallic systems. The nanowires were stretched to failure and the corresponding stress-strain curves were produced. From these curves, mechanical properties including the elastic modulus, yield stress and strain, and ultimate strain were calculated. In addition to the MD approach, an energy method was applied to calculate the elastic modulus of each nanowire through exponential fitting of an energy function. Both methods used to calculate Young's modulus qualitatively gave similar results indicating that as diameter decreases, Young's modulus decreases.

The atomic structures generated from MD simulations were examined in details to investigate the deformation and yield behavior of each nanowire. It was found that most nanowires yield and fail through partial dislocation nucleation and propagation leading to {111} slip. However, the octagonal platinum nanowire, whose diameter is 5 nm, was found to yield through reconstruction of the {011} surfaces into the more energetically favorable {111} surfaces.