

# TESTING THE ELASTIC PROPERTIES OF SILVER NANOWIRES UNDER BENDING LOADS

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## Introduction

The mechanical properties of nanowires have been extensively examined with experimental and computational techniques in recent years. Mechanical behavior on the nanometer scale differs from that of bulk materials primarily due to the influence of free surfaces. In all materials, surface atoms have a lower coordination and therefore higher energy than bulk atoms. Due to the relatively high ratio of surface atoms to bulk atoms in nanomaterials, surfaces have a greater impact on deformation than in bulk materials.

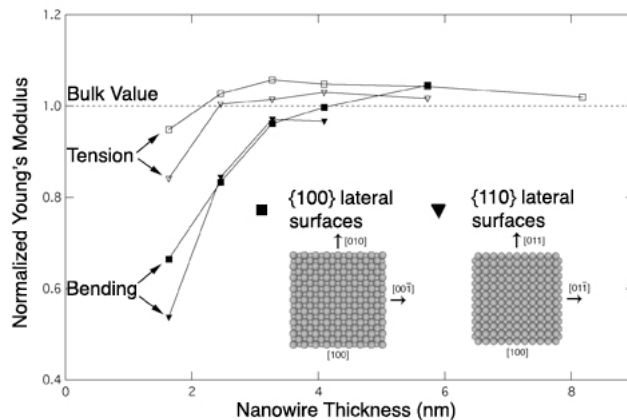
Many experimental studies of the elastic properties of nanowires have been undertaken. Most of these experiments use bending or resonance; tensile tests are difficult to implement on nanometer length scales. On the other hand, computational investigations have primarily utilized tensile tests to study nanowire elastic behavior. This disparity in testing methods raises concerns related to the measurement of elastic properties in nanowires. The objective of the present study is to use computational simulations to investigate the bending and tensile behavior of silver nanowires of varying axial and surface orientation to systematically determine the impact of nanowire structure, geometry, and applied stress state on the resulting elastic response.

## Procedure

All simulations were performed with molecular statics using the embedded atom method (EAM). Four different nanowires with varying axial orientation and geometry were tested (two are shown as insets in Fig. 1). In the bending simulations, three layers of atoms at one end of the nanowire were held fixed while the other end was displaced 0.1 nm vertically downward. The top edge of the displaced end was then held fixed while the nanowire was statically relaxed, and then the bottom edge of the displaced end was held fixed while the nanowire was again relaxed. This incremental process was repeated until a desired maximum deflection had been reached. All static relaxations were performed using a conjugate gradient energy minimization technique. For the tensile simulations, the nanowire was subjected to a ramped displacement profile along the axial direction with 0.2% strain per increment, and then both ends were held fixed while the nanowire was statically relaxed. The Young's modulus was then calculated from both types of simulations using continuum-mechanical methods.

## Results and Discussion

Young's modulus values as a function of nanowire thickness for  $\langle 100 \rangle$  axially oriented square nanowires are shown in Fig. 1.



**Figure 1.** Young's modulus for bending and tensile tests for  $\langle 100 \rangle$  axially oriented square nanowires. All values are normalized by the bulk value (44.3 GPa).

As is evident from Fig. 1, the elastic modulus decreases for both nanowires under both bending and tension as size decreases. For large thicknesses ( $>10$  nm), the elastic modulus approaches the bulk value. At the smaller sizes, modulus values diverge in bending and tension simulations for the same nanowires. This is presumed to be due to the greater influence of surface stress in bending than in tension, because the resulting stress due to a bending load is concentrated at the free surfaces. However, as size increases, the bending and tensile modulus values for the same nanowires approach each other. It should also be noted that at the smallest values, nanowires under the same load with different lateral surfaces exhibit a difference in modulus, which indicates that surface orientation has a magnified effect on modulus at the smallest sizes. In addition to the data in Fig. 1, data for  $\langle 110 \rangle$  axially oriented nanowires was collected; these nanowires show similar trends in modulus values, but they exhibit stiffening instead of softening.

## Conclusions

The elastic modulus was calculated for nanowires with varying geometries and axial orientations under bending and tensile loads. For large sizes, the values approach the bulk; as size decreases, values diverge based on loading method and surface orientation for wires of the same axial orientation. Overall, however, it was demonstrated that bending and tension tests give similar results for wires of appreciable size.