Introduction

Applications
- Moore’s Law: the area covered by a transistor is halved every 18 months
- Molecular electronics: the next technology to succeed silicone

Nanowires
- High surface area to volume ratio
- Atomistically sharp tips
- Higher failure strength than bulk

Figure 1 (left): As early as 1975 limits of Moore’s Law (left) were being recognized, the ultimate limit being quantized matter. Benzene dithiol was the first single molecule to be measured for conductance (right).

Objective

To identify structural motifs in metal nanowires under elongation, and calculate zero-basis conductance of wires as they are elongated to improve the implementation of nanowires in electronic devices.

Methods

Nanowires were elongated at constant tensile strain in vacuum with molecular dynamics simulations
- Elongation rate :: 0.5 m/s
- Temperature :: 10 K & 298 K
- Diameter :: 4 nm
- Length :: 24 nm
- Atom-atom interaction :: TB - SMA

Density Functional Theory was used to calculate the zero-basis conductance of smaller elongated nanowires
- Elongation rate :: 0.5 m/s
- Temperature :: 10 K
- Diameter :: 0.8 nm
- Length :: 2 nm

FCC Metals studied:
- Gold
- Silver
- Copper
- Platinum
- Aluminum

Results

Mechanics
The engineering stress tensor is calculated over the course of elongation in the tensile [100] direction. The yield strength is generally 1 magnitude greater and the Young’s modulus 1 magnitude less than their bulk counterparts.

Figure 2 (above): Image of a copper nanowire undergoing a slip plane dislocation (top) and a gold nanowire undergoing necking (bottom) at 10 K.

Figure 3 (right): Stress-strain curve of gold nanowire at 10 K. Young’s modulus is the slope and yield strength is the maximum of the linear/elastic region.

Figure 4 (above): Average yield strength (left) and Young’s modulus (right) of 15 simulations for each metal at 10 K and 298 K. Both properties are higher at 10 K.

Conductance
There is a clear association with crystal impurities, including slip planes, twin boundaries and necking, and a decrease in conductance.

Figure 5 (left): Zero-bias conductance (top) and minimum diameter (bottom) of metal nanowires made of Au (left), Ag (middle) and Cu (right) under elongation. The jump up in conductance (circled) is a result of the correction of a twin boundary and recovery of the fcc lattice. Other decreases in conductance correspond with a decrease in the minimum diameter, limiting the number of paths for electron transport.

Future Work

- Identify a quantifiable parameter that discriminates modes of deformation to make clear distinctions between the studied metals.
- Test different metals as a function of initial nanowire length.

Acknowledgments

This project was funded by NSF Grant Contract No. DMR-1005023

This research used resources of the NERSC Center, which is supported by the Office of Science of the U.S. DOE under Contract No. DE-AC02-05CH11231.
