Impact of Metal Type on the Deformation and Conductivity of Ultrathin Nanowires

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Introduction

Applications

• Moore's Law: the area covered by a transistor is halved every 18 months

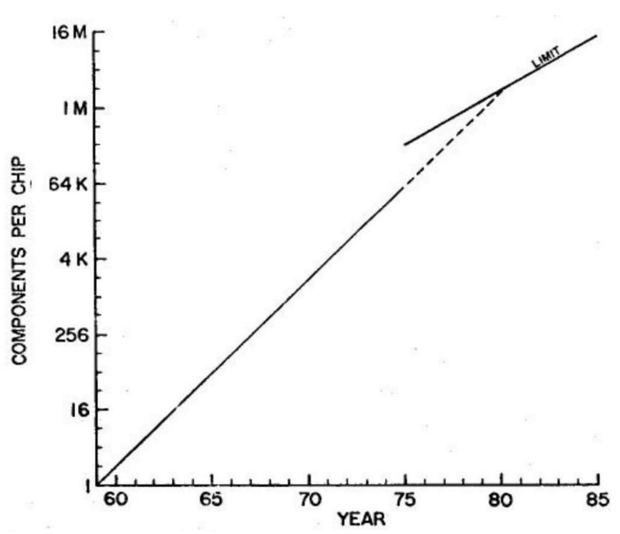
• Molecular electronics: the next technology to succeed silicone

Nanowires

• High surface area to volume ratio

• Atomistically sharp tips

• Higher failure strength than bulk



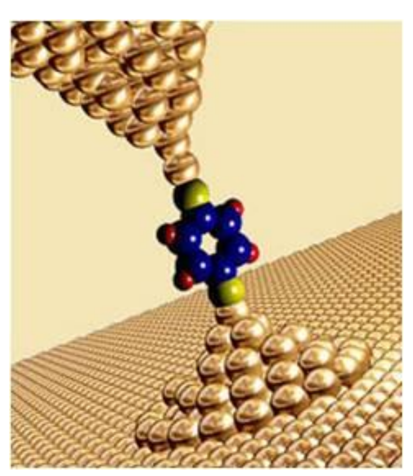


Figure 1 *(left)*: As early as 1975 limits of Moore's Law[1] (left) were being recognized, the ultimate limit being quantized matter. Benzene dithiol was the first single molecule to be measured for conductance (right).

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
- Temperatures :: 10 K & 298 K
- Diameter :: 4 nm
- Length :: 24 nm
- Atom-atom interaction :: TB - SMA

Density Functional Theory was used to calculate the zero-bias 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

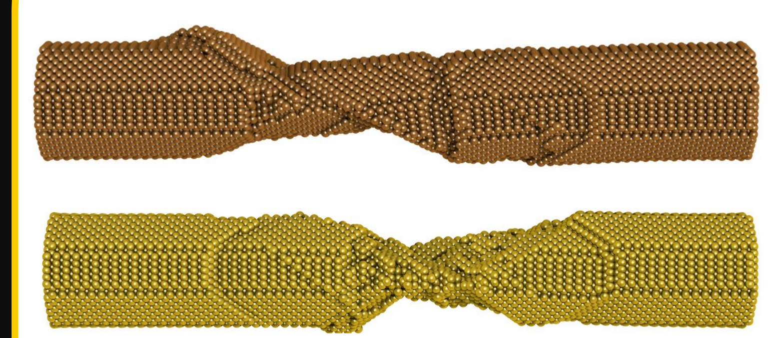
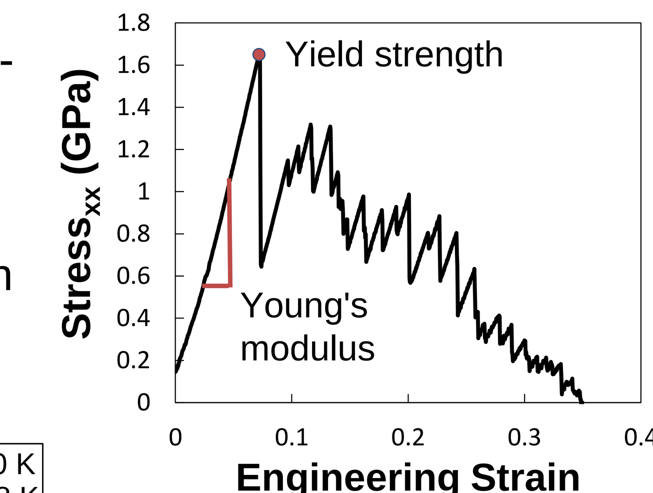


Figure 2 *(above)*: Image of a copper nanowire undergoing a slip plane dislocation (top) and a gold nanowire undergoing necking (bottom) at 10 K.

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 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.



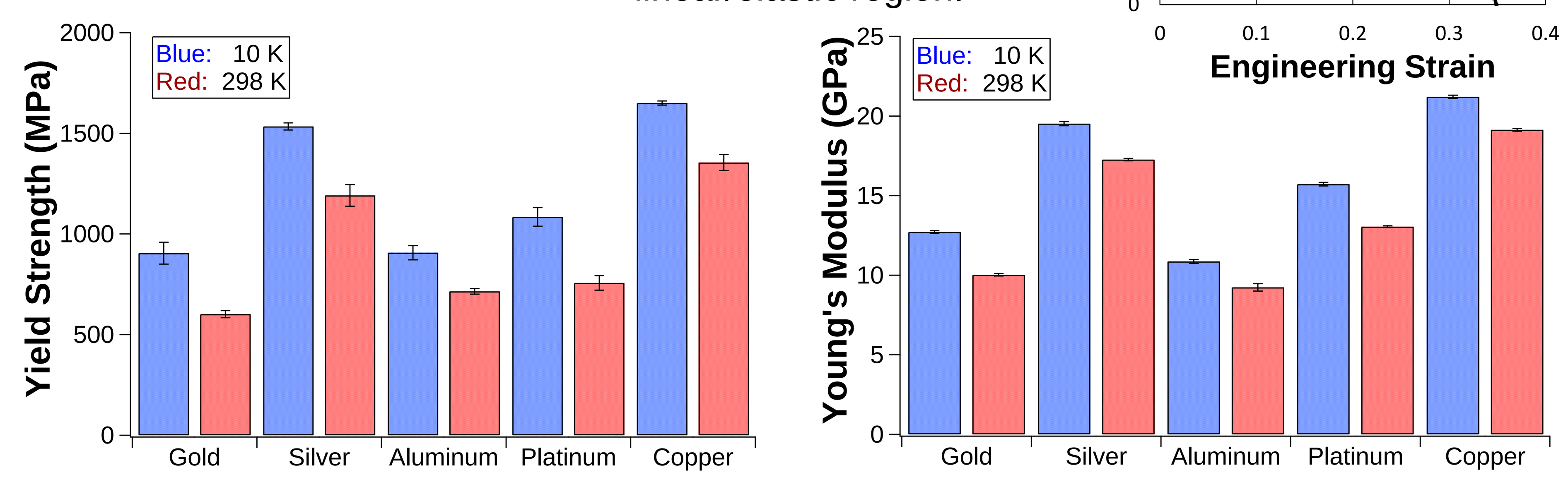


Figure 4 *(above)*: Average yield strength (left) and Young's modulus (right) of 15 simulations for each metal at 10 K and 298 K. Both properties are higher at 10 K.

Conductance

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

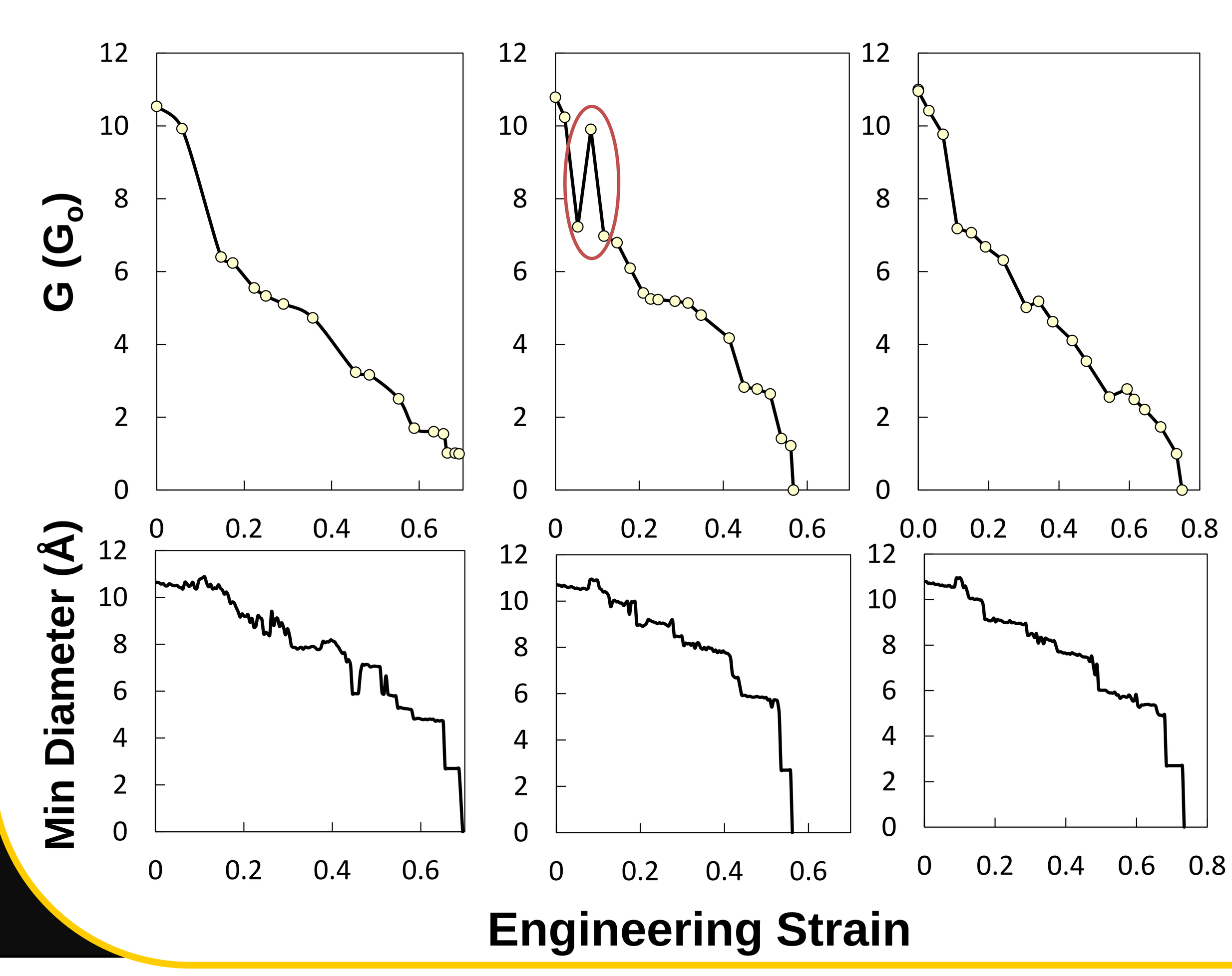


Figure 5 *(left)*: Zero-bias conductance (top) and minimum diameter (bottom) of metal nanowires made of Au (left), Ag (middle) and Cu (right) under elongation. The jump up in conductance (circled) is a result of the correction of a twin boundary and recovery of the fcc lattice. Other decreases in conductance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

Conclusions

• Nanowires exhibit higher yield strength than their bulk counterparts. This is due to the higher surface area and smaller yield strain of the high aspect ratio wires. Wires of this size tend to rely on slip planes and necking to deform under strain.

• As a nanowire elongates, the conductance decreases.

• Drastic changes in the smallest diameter can cause a drop in conductance, due to the fewer paths by which electrons may travel.

• The onset of impurities causes a decrease in conductance.

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

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[1]G. E. Moore, "Progress in Digital Integrated Electronics." © 1975 IEEE. Reprinted, with permission, from Technical Digest 1975. International Electron Devices Meeting, IEEE, 1975, pp. 11-13.

[2]Hadlington, S. (2007, February 21). Organic electricity generator is hot stuff. Retrieved from Royal Society of Chemistry website: http://www.rsc.org/chemistryworld/News/2007/February/21020702.asp