Molecular Dynamics Simulations of Thin Film Conductor Tensile Properties

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Bachelor of Science, School of Engineering

Dylan Culfogienis
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Technical Project Team Members
Dylan Culfogienis

On my honor as a University Student, I have neither given nor received unauthorized aid on this assignment as defined by the Honor Guidelines for Thesis-Related Assignments

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Abstract

This capstone is a series of molecular dynamics tensile tests, simulating homogeneous thin-film materials in submerged aqueous conditions as well as at the interface of aqueous and vacuum conditions. Thin-film gold will be tested in both aqueous and aqueous-vacuum interface conditions. Each material will be tested at different thicknesses. The goal of these experiments is to determine the mechanism of difference in Young's modulus of surface-bound thin films in relation to their thickness. It has been demonstrated by prior research that young's modulus in aqueous-vacuum interface conditions does vary with thickness, however, the mechanism for this variance is unknown. It is hypothesized that the mechanism involves reaction between water and the thin film at the fracture site; we will attempt to confirm this using reactive MD potentials.

This research is relevant to the field of flexible electronics; a common method of creating flexible electronics is thin-film liftoff in aqueous conditions; it can be difficult to predict the behaviour of these thin-film electronics however as their elastic behaviour is different than that of bulk materials. Understanding the mechanism for this difference will allow better prediction of thin film behaviour during liftoff manufacturing.

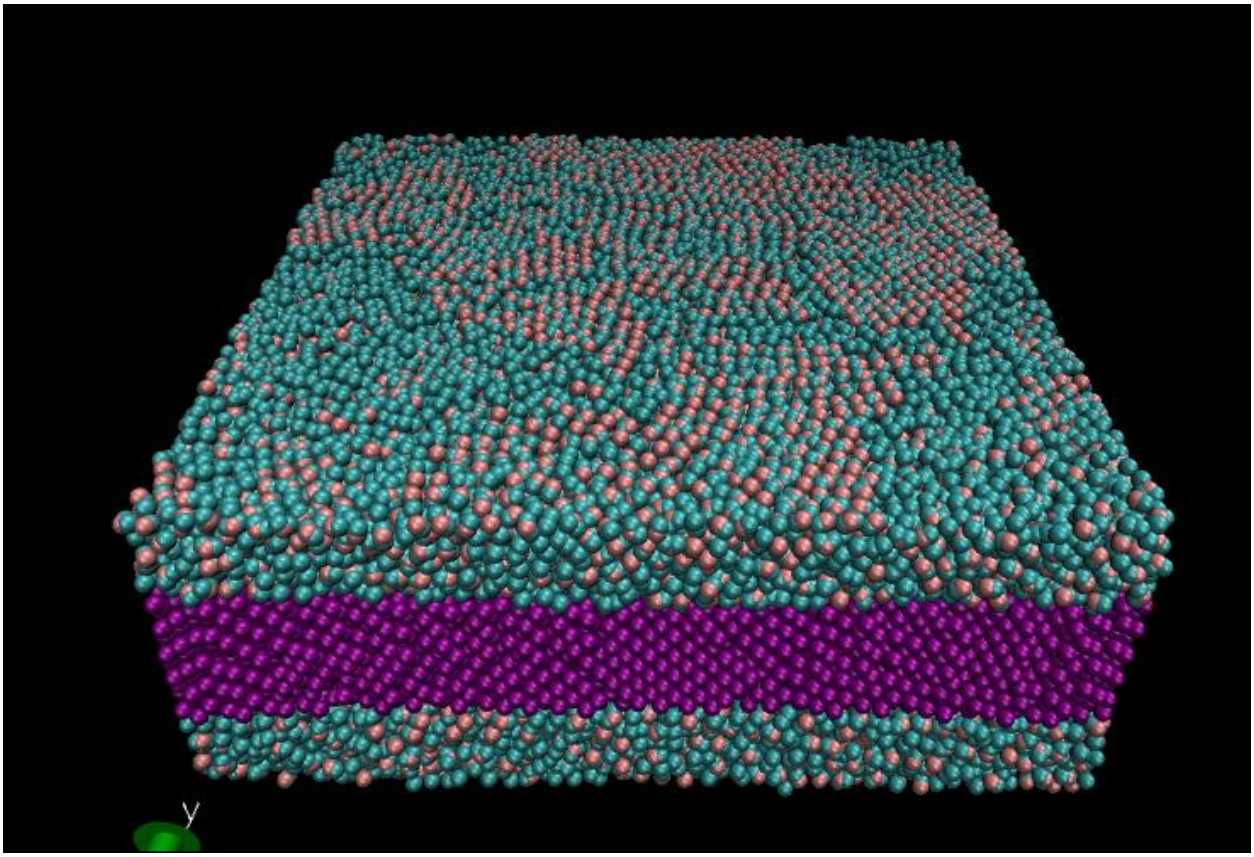
Methods

The LAMMPS classical molecular dynamics simulator is used to model this system. (Plimpton, 1995) LAMMPS has been chosen due to a large abundance of preexisting molecular systems that are similar in nature to the project at hand. It is capable of simulating both water

molecules and FCC metals, as well as the interactions between these two materials, which is sufficient for these experiments.

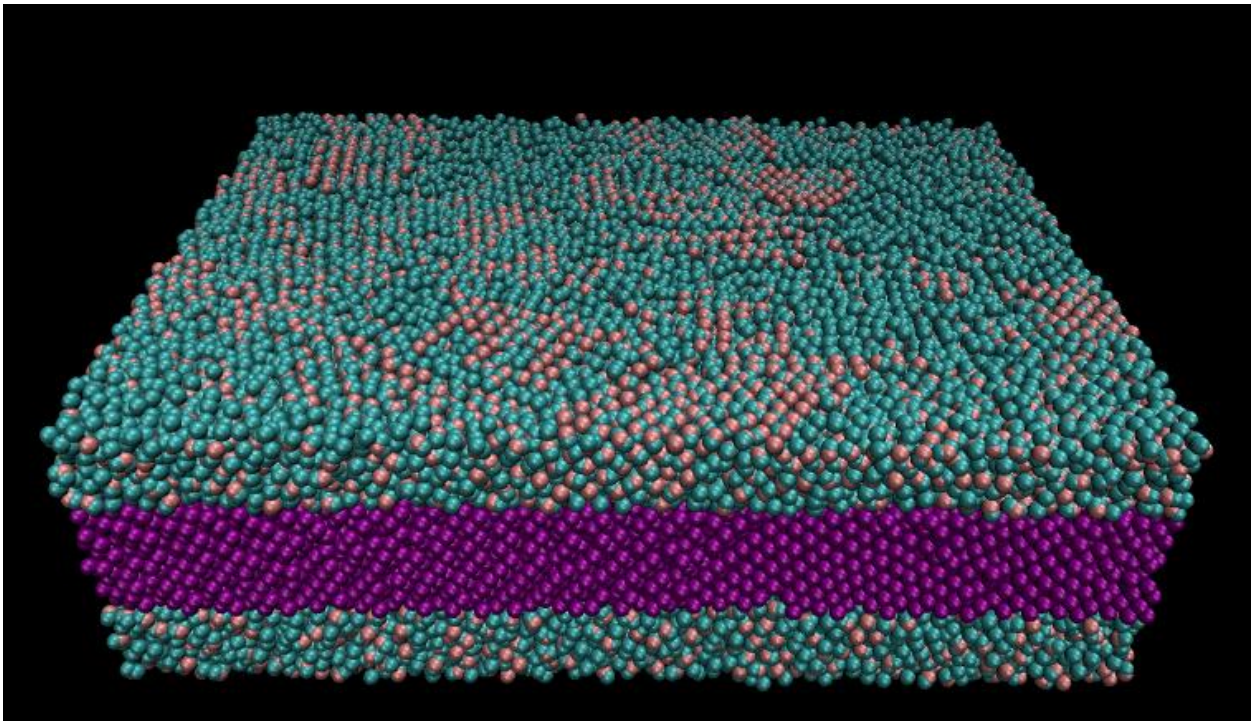
The system is modeled as a small 40x40-unit cell sheet of material of varying thickness, surrounded on both sides by water boxes. Water is modeled using the SPCE water model included with LAMMPS. (Berendsen et al., 1987) FCC metals are modeled using the EAM potential using functions included in LAMMPS (Foiles et al., 1986). The system is periodic on all axes. Such a small system is acceptable as high strains and fracture are not relevant; Young's modulus is the only metric of interest.

The system is assembled using the moltemplate package, and equilibriated via NVE integration (microcanonical ensemble) to 300 Kelvin using a Berendsen thermostat. Equilibriation is done at a timestep of 0.001ps, and runs for 20,000 steps. Equilibriation must be performed in order to ensure that molecules, particularly water molecules, have a reasonable velocity distribution for the temperature the experiment is conducted at.



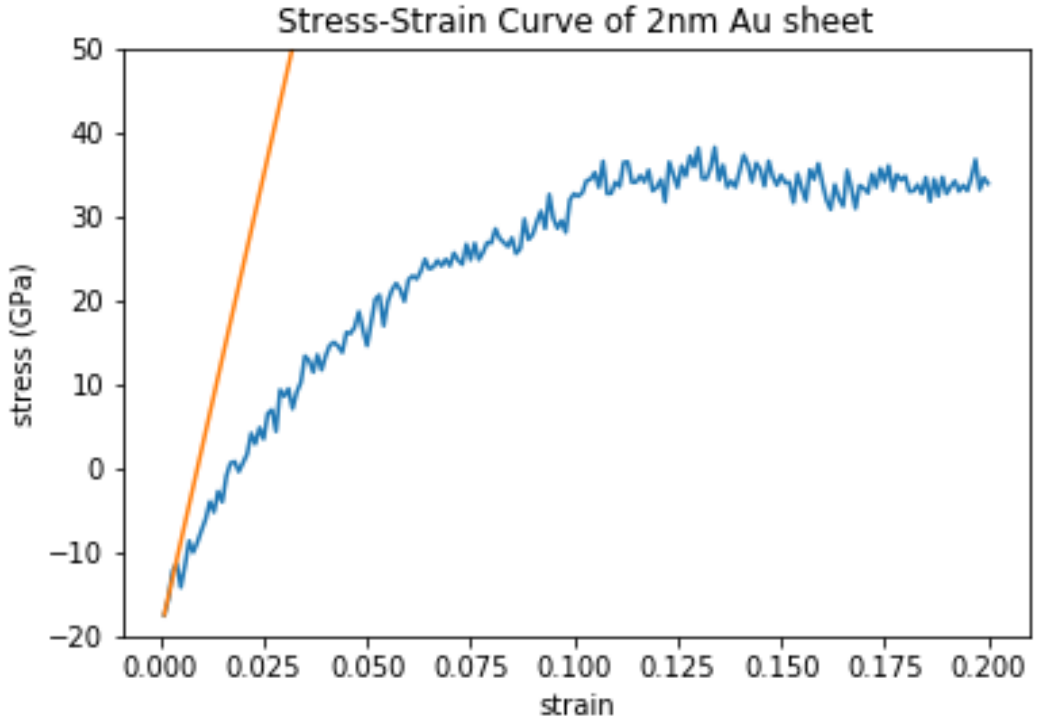
Au system following equilibriation

Once equilibriation is complete, simulations are performed at a timestep of 0.01, using NPT integration, with temperature fixed at 300 Celsius. The tensile test is performed by gradually scaling the system along the X axis, an equivalent effect to a macro-scale tensile test when performed slowly enough that, in an analagous, real tensile test, the system would remain near equilibrium. Both strain and pressure (inverse stress) are recorded. These tensile tests are simulated for 20,000 timesteps, resulting in a final strain value of 0.2.

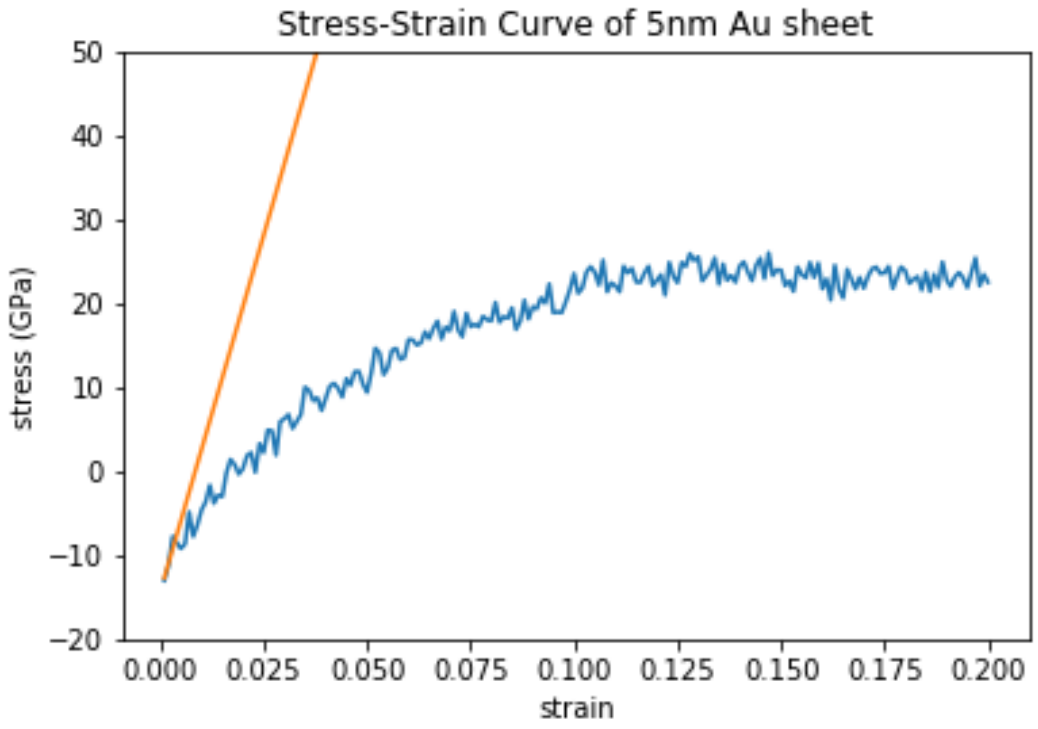


Au system following tensile test

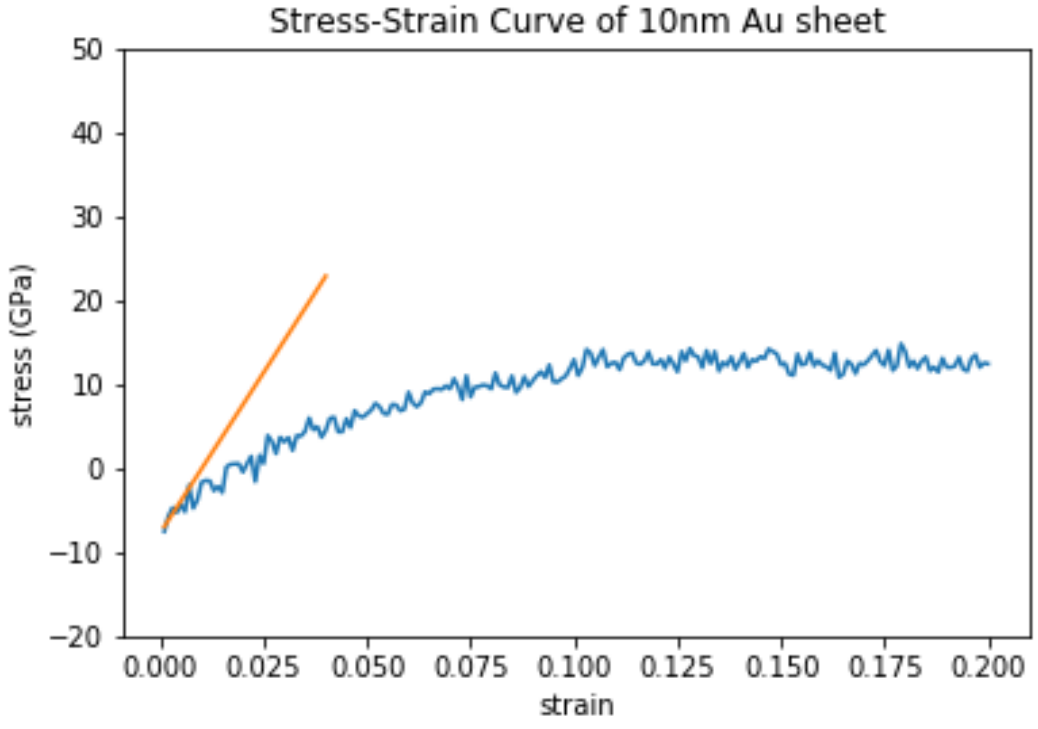
Results and Discussion



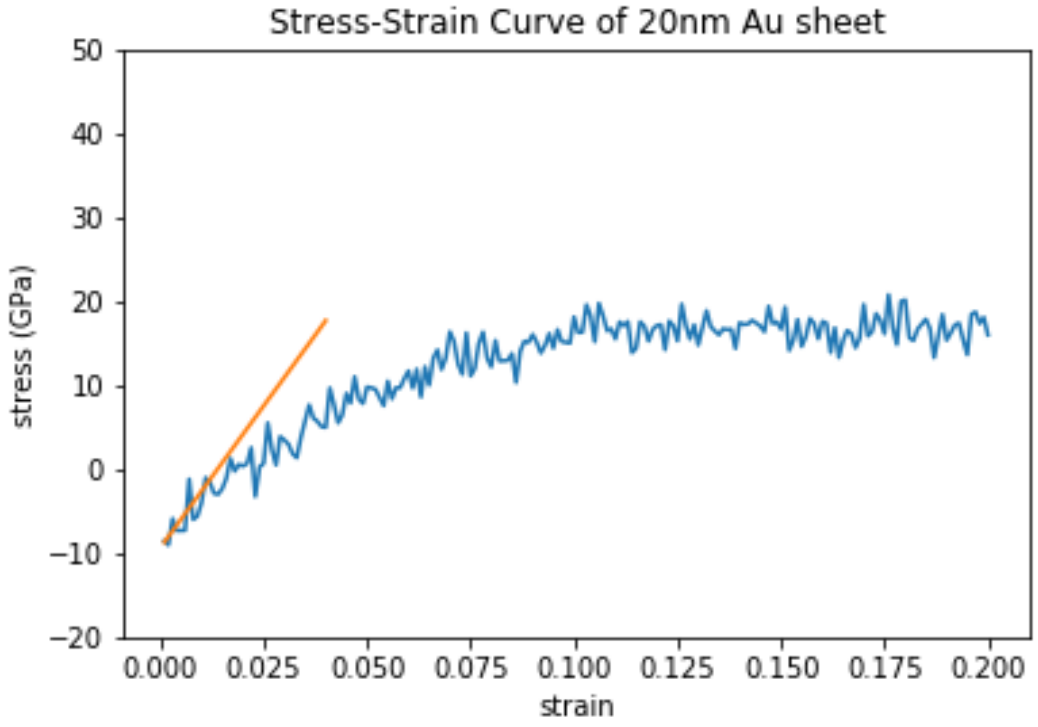
2nm Tensile Test; Y=2174.98



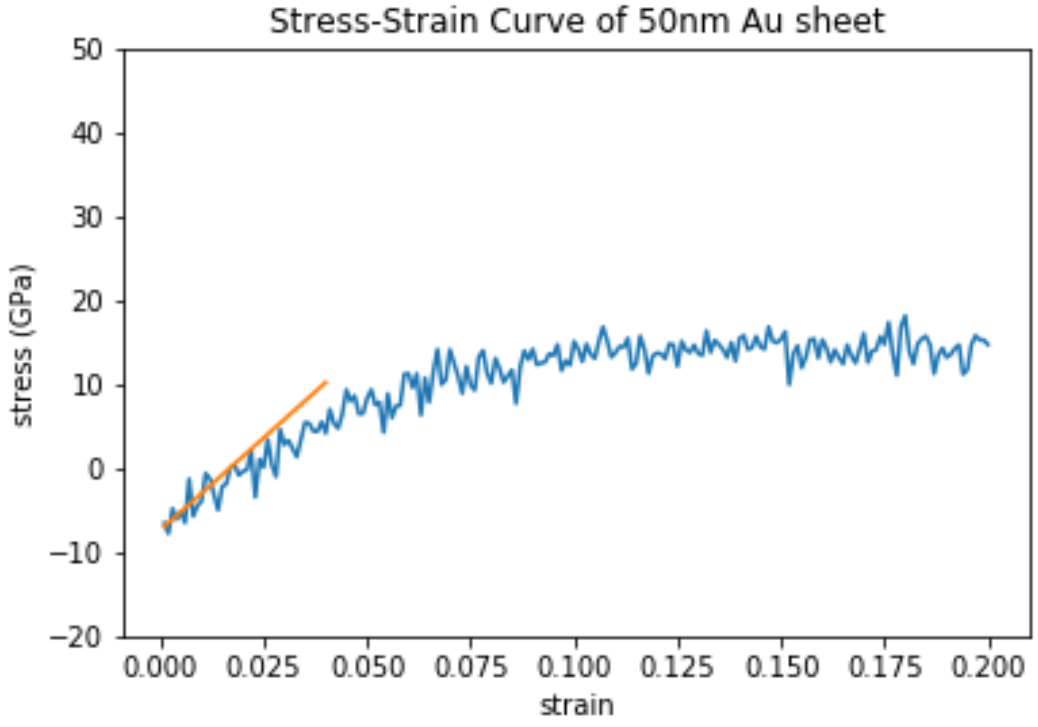
5nm Tensile Test; Y=1696.27



10nm Tensile Test; Y=763.29



20nm Tensile Test; Y=675.48



50nm Tensile Test; Y=439.58

Tensile tests of gold from 2nm to 50nm.

While it appears that there is a trend of decreasing Young's Modulus with increasing film thickness, this is likely not reflective of the actual properties of this system. The bulk Young's Modulus of gold is 79gPa, significantly under any of the recorded Y from this experiment. Furthermore, physical thin films tested by Kim et al., while of a greater thickness than tested films, show a *decreasing* trend in Y with decrease in film thickness, as opposed to an increase.

This lack of physicality is due to an unknown issue with the system setup, which could not be found over the course of the capstone project. Possible candidates include improper setup of pair potential parameters, system bounds that are either too small or too large, and/or improper equilibriation/minimization of system before tensile test. However, multiple significant changes to these parameters showed no improvement in the physical feasibility of results.

Conclusion

The results of the experiment contradict known literature values both for bulk gold and thin-film gold, and target metrics do not reflect any known physical properties of thin films. Thus, the results of this experiment should be disregarded due to technical error.

This topic of study is still one of value, however, due to constraints during the research process, a valid experiment could not be conducted and there are no results of interest to analyze.

Works Cited

Berendsen, H. J. C., Grigera, J. R., & Straatsma, T. P. (1987). The missing term in effective pair potentials. *The Journal of Physical Chemistry*, *91*(24), 6269–6271. https://doi.org/10.1021/j100308a038

Foiles, S. M., Baskes, M. I., & Daw, M. S. (1986). Embedded-atom-method functions for the fcc metals Cu, Ag, Au, Ni, Pd, Pt, and their alloys. *Physical Review B*, *33*(12), 7983–7991. https://doi.org/10.1103/PhysRevB.33.7983

Plimpton, S. (1995). Fast Parallel Algorithms for Short-Range Molecular Dynamics. *Journal of Computational Physics*, *117*(1), 1–19. https://doi.org/10.1006/jcph.1995.1039