MSE SEMINAR

March 16, 2018
113 McBryde Hall
3:30 – 4:30 PM
Refreshments at 3:00 PM

Nathan Beets

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"Deformation mechanisms and scaling relations in the mechanical response of nanoporous gold"

Abstract

Nanoporous gold is a novel catalytic material with promising applications for fuel cell electrodes and actuators. However, the mechanical properties of the material, and how they relate to the morphology, surface tension, and internal stress state is as yet not completely understood. In this study, the authors focused on a predicted asymmetry in the yield stress under tension and compression for nanoporous gold with constant porosity, but with varying surface area to volume ratio using molecular dynamics. The intent was to understand how capillary forces and morphology affect the external vs. internal stress states, and in turn, the ramifications this had on dislocation emission and yielding. The authors conducted a series of mechanical and thermodynamic tests on nanoporous gold samples, nanopillar gold ligaments, and solid gold cubes to ascertain the mathematical formalism to describe said asymmetry how it relates to the surface tension of the samples, and how it aligns with the Gibson-Ashby formalism for scaling diameter-dependent yield stress. An explanation of how internal ligament stress states affect dislocation formation, propagation, and density, and how this fits with the yield stress relation is also put forward, and a theoretical model for yield stress tested, and presented for experimental use and verification.

BioSketch

Nathan Beets is a PhD candidate working under Dr. Diana Farkas. He graduated from Wake Forest University with a B.S. in Physics and a B.S. in Applied Mathematics in 2016, starting at Virginia Tech in August of 2016. In the summer of 2017, he was funded to work at TU Darmstadt to understand the surface effects, thermodynamics and mechanical properties of nonporous gold and silver alloys using Monte Carlo and Molecular Dynamics simulation techniques.

Nathan's research focuses primarily on molecular modeling of bicontinuous and nanoporous alloys, for application in battery and fuel cell electrodes. His work seeks to understand the mathematical relationships of alloy composition, morphology, and interface/surface effects to mechanical stability and thermodynamics herein.