



MECHANICAL ENGINEERING SEMINAR

Monday, 24 February 2025 at 14:30, D. Dan and Betty Kahn Building, Room 217

Also online: [Zoom link](#)

Unraveling Stochastic Mechanical Properties: From Atomistic Modeling to Lightweight Structural Design

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Hosted by: Prof. Alon Wolf

Understanding and predicting mechanical properties from their fundamental building blocks remains a central challenge in the mechanical engineering community. However, this challenge also presents new opportunities for designing materials with tailored mechanical behavior. In this seminar, I will present a series of our recent studies in multiscale materials modeling, focusing on how stochastic mechanical properties emerge across different length scales. Additionally, I will discuss briefly our efforts in modeling the mechanical behavior of metals under high strain rates and the elastic properties of two-dimensional transition metal dichalcogenides.

In the first part of the talk, I will explore how microstructural features drive stochastic mechanical properties at the nanoscale. Specifically, I will introduce a model that describes the statistical distribution of yield strength in nucleation-controlled plasticity, linking it to the activation parameters for dislocation nucleation and its temperature dependence. Using molecular dynamics (MD) simulations, we demonstrate how these stochastic effects manifest in nanoparticle compression and tensile loading of nanowires. Furthermore, I will examine the failure strain distribution in nanowires by presenting simulations of bi-crystalline twinned gold and penta-twinned silver nanowires, illustrating how competition between microstructural mechanisms govern their mechanical reliability.

In the second part of the talk, I will shift focus to lightweight porous structures, where stochastic mechanical properties naturally emerge from their intricate topologies. By generating a large dataset of MD-simulated nanoporous gold structures, we reveal how their mechanical properties correlate with topology and morphology. I will also discuss how incorporating stochasticity into additively manufactured metallic lattice structures enhances their yield strength without increasing weight. Inspired by nature, this approach unlocks new design possibilities for lightweight structures with tunable mechanical properties. I will conclude by demonstrating how MD simulations, in conjunction with finite element modeling (FEM), can inform the development of these next-generation materials.