MECHANICAL ENGINEERING STUDENT SEMINAR

Thursday, November 3 2022 at 13:00, D. Dan and Betty Kahn Building, Auditorium 1.
Online: https://technion.zoom.us/j/94285797004

Mechanical properties of nanoporous gold nanoparticles in molecular dynamics simulations

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Nanoporous structures are used for a variety of applications, and it is desirable to understand their mechanical properties. While most of the studies focus on nanoindentation of bulk nanoporous structures, it was recently proposed to use nanoporous nanoparticles under compression to quantify their mechanical properties. In this work we explore how the different parameters of nanoporous Au nanoparticles are related to their mechanical properties using molecular dynamics simulations. For this endeavor, LAMMPS atomistic simulation was used to simulate compression via indentation of hemispherical nanoporous nanoparticles. Ligament diameter, particle radius, and volume fractions were varied in the simulations, and for each set of parameters, the results of five simulations were ensemble averaged. To analyze the results, the evolution of the true stress was calculated, and correlations were found between the plateau stress and the densification strain and the nanoparticle parameters. We found that out of the three parameters only ligament diameter correlated to plateau stress. Also, an increase in both particle radius and volume fraction, independently, was correlated to an increase in densification rate, which is also correlated to a local increase in the near surface volume fraction. Finally, since obtaining the true stress is difficult experimentally, we discuss how it is related to the engineering stress, showing that it is related to the local densification beneath the indent.

Seminars Coordinator: Assoc. Prof. Matthew Suss.