MECHANICAL ENGINEERING STUDENT SEMINAR

Monday, February 19 2024 at 14:30 (Jerusalem time) and 20:00 (Beijing time)

Online: https://technion.zoom.us/j/94319496398 code: 94319496398

Improving Grain Boundary Mobility in Phase-Field-Crystal Model Using Molecular Dynamics

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Abstract:

The phase-field crystal (PFC) model has emerged as an atomically resolved thermodynamics-based model. It has been shown that both the static materials properties, such as the grain boundary (GB) energy, and kinetic behaviors, such as dislocation motions, are well captured in this method. However, in large scale simulation of grain growth, mobilities for various GBs are not yet included in the PFC model although it is a critical property in microstructure evolutions.

Along with experimental measurements, molecular dynamics (MD) simulations have been widely used in the calculations of GB mobilities in several metal systems. By calculating the GB mobilities from the MD and the PFC separately, and comparing the results for various GB misorientation angles, this work will address the mobility issue in the PFC model by incorporating the mobilities from MD simulations for a few simple GBs for the first time.

Keywords: Grain boundary mobility; PFC; MD; mesoscale simulations.

Note: the seminar will be given in English

Seminars Coordinator: Assoc. Prof. Matthew Suss.