הטכניון מכון טכנולוגי לישראל
TECHNION Israel Institute of Technology

Faculty of Mechanical Engineering
הפקולטה להנדסת מכונות

MECHANICAL ENGINEERING MSc SEMINAR (30 min.)

Monday, September 29 2025 at 14:30-15:00, D. Dan and Betty Kahn Building, Room 217

The effect of grain boundaries in Cu-Zr systems on the energy dissipation during plastic deformation

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Supervisor: Assoc. Prof. Dan Mordehai.

During high-strain-rate plastic deformation, not all plastic work is dissipated as heat; a fraction of the energy is stored in the material. The Taylor–Quinney coefficient (TQC) quantifies the fraction of plastic work converted into heat. To this day, the microstructural origin of the stored energy, namely the energy stored in dislocations and grain boundaries (GBs), remains an open question. In this work, we quantify TQC in Cu–Zr polycrystals using molecular dynamics (MD) simulations. Cu–Zr alloys here are chosen as a model system that permits controlled tuning of GB composition and thickness, which allows isolating the contribution of GBs to the TQC.

We performed MD simulations of simple shear of Cu–Zr polycrystals (0–3 at. % Zr). Zr segregation to grain boundaries (GBs) is induced via hybrid Monte Carlo/Molecular Dynamics (MC/MD); equilibrated cells are then sheared under adiabatic conditions to let dissipation manifest as temperature rise. Composition-dependent heat capacities are calculated and used to compute both integral and differential TQC from the measured temperature and plastic work. We further investigate whether the microstructure of grain boundaries can accommodate a significant portion of the non-thermal energy. The non-thermal remainder is decomposed into energy reservoirs: (i) dislocation energy storage, quantified by dislocation analysis and stacking-fault area, and (ii) grain-boundary energy storage, obtained by identifying GB atoms, reconstructing GB surface/volume, and tracking a characteristic GB thickness versus plastic strain. We found that the energy stored in the dislocation microstructure is insufficient to explain the temperature rise. By tracking the evolution of the GB volume, we find that volumetric changes of the GB network are contributing the energy storage within the GBs. This correlation suggests that early-stage GB thickening accommodates a measurable share of the non-thermal energy. This relationship provides a quantitative handle on where energy goes at high strain rates, enabling better TQC calibration from measurable GB metrics and guiding alloy and process design to balance heating through microstructure tailoring.

Note: the seminar will be given in Hebrew

Seminars Coordinator: Assoc. Prof. Shmuel Gal.