Materials Science and Engineering Department

Spring Seminar Series

Atomistic Insights into Ductile and Brittle Fracture of Metals

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11AM-12PM | Hill Seminar Room (LeBow 240)

Ductile metals typically fail through the nucleation, growth, and coalescence of voids. When metals become embrittled through reductions in temperature or exposure to embrittling agents such as hydrogen, fracture often transitions to an intergranular mode where cracks grow along the grain boundaries. Despite a decades-old qualitative understanding of the mechanisms underlying these processes, physics-based, micromechanistic models for ductile and brittle fracture are lacking. In this talk, recent progress and insights from molecular dynamics (MD) simulations of metal fracture will be discussed. For ductile fracture, the focus is on determination of a criterion and rate law for void nucleation. MD simulations of void nucleation via particle debonding in Al containing a q-particle enable construction of a new nucleation model, suitable for use in continuum porous plasticity models of ductile fracture (e.g., the Gurson-Tvergaard-Needleman model). For brittle fracture, MD simulations reveal a new embrittlement mechanism: embrittlement via a stress-induced grain boundary (GB) complexion transition. The stress state at the crack tip induces a change in GB complexion (i.e., atomic structure) to a low toughness complexion, which then initiates fracture. The thermodynamics and kinetics of this process are quantified, and implications for experimental observations of embrittlement are discussed.

Prof. Ryan Sills received his B.S from Cornell University, his M.S. from the University of Michigan, and his Ph.D. from Stanford University, all in Mechanical Engineering. Prior to joining the faculty in Materials Science and Engineering at Rutgers University in September 2019, he was a Staff Member at Sandia National Laboratories in Livermore, CA for 9 years. At Sandia, he served as a design engineer, researcher, and Principal Investigator for a research program on the mechanics and aging of hydrogen storage materials. He presently leads the microMechanics of Deformation (mMOD) Research Group at Rutgers, which uses multiscale materials modeling to understand how micromechanics influences the mechanical behaviors of materials. Dr. Sills received his Young Investigator Program award from the Army Research Office in 2021 and his NSF CAREER award in 2023. He became Editor-in-Chief of the Journal of Materials Science: Materials Theory in 2024.

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