MM 2: Invited talk Curtin

Time: Monday 9:30–10:00 Location: TC 006

Invited Talk MM 2.1 Mon 9:30 TC 006

Atomistic Mechanisms of Hydrogen Embrittlement — •William Arthur Curtin — EPFL, Lausanne, Switzerland

A number of concepts, such as Hydrogen Enhanced Localized Plasticity and Hydrogen Enhanced Decohesion, have been proposed to explain Hydrogen embrittlement in different metallic systems. Here, we first present atomistic models some of proposed mechanisms and find limited evidence for their operation. We then discuss a new mechanism wherein H accumulates at nanometer scales around any pre-existing crack tip, which shuts off the crack tip dislocation emission and thereby eliminates crack blunting, suppresses ductile failure modes, and fracture occurs by cleavage through the brittle H-rich region. The process is self-sustaining through continual H transport to the crack tip region. We demonstrate operation of this mechanism in Fe-H using direct atomistic simulations. We then connect the nanoscale mechanism to experimental conditions via the kinetics of H diffusion to the crack tip region, and predict embrittlement as a function of loading rate, H chemical potential, temperature, and H diffusion rate. Application of new model leads to predictions of embrittlement across a range of typical Fe-based systems that are in very good agreement with experimental results.