

MM 36: Invited talk Curtin

Time: Wednesday 9:30–10:00

Location: BAR 205

Topical Talk MM 36.1 Wed 9:30 BAR 205
Theory Driven Data Driven Design for Structural Metals —
•WILLIAM A. CURTIN — Laboratory for Multiscale Mechanics Modeling, Institute of Mechanical Engineering, EPFL, Lausanne, Switzerland

A fundamental idea of data-driven design of materials is that the design goal can be adequately represented by some descriptors that, in turn, can be computed by first-principles methods or estimated. For structural metals, the design goals are quantities such as yield strength, work hardening, and toughness or ductility, which are often a function

of temperature and strain rate. The quantities that are most amenable to first-principles computations are zero-temperature elastic and lattice constants, solute misfit volumes, stacking fault energies, solute interactions stacking faults, solute diffusion coefficients, and stable precipitate structures and properties. Few theories quantitatively connect design goals to computable quantities and for structural materials, there is thus an urgent need for theory-driven data-driven design. This talk will present two examples of theory-driven-data-driven design, wherein a fundamental theory is developed, reduced to computable quantities, validated, and then used to guide material selection for enhanced mechanical performance.