MM 27: HV Curtin

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

Invited Talk MM 27.1 Wed 9:30 TC 006

First-principles Predictions of Solute Strengthening in Al and Mg alloys — •William Curtin[1] and Gerard Leyson[2] — [1]Ecole Polytechnique Federale de Lausanne — [2]Brown University

A quantitative, parameter free model to predict the flow stress as a function of temperature and strain rate of such alloys is presented. The model builds on analytic concepts developed by Labusch but introduces key innovations rectifying shortcomings of previous models. To accurately describe the solute/dislocation interaction energies in and around the dislocation core, density functional theory and a flexible-boundary-condition method are used. The model then predicts the zero temperature flow stress, the energy barrier for dislocation motion, and thus the finite temperature flow stress. Predictions of the model are in excellent agreement for a range of Al alloys and basal strengthening in Mg-Al as a function of solute concentration and temperature. This success demonstrates that computational materials science can provide quantitative guidance to materials design for properties controlled by complex interactions of defects, in this case flow stress controlled by dislocation interactions with solutes.