INTERDISCIPLINARY CENTRE FOR ADVANCED MATERIALS SIMULATION

MMM Special Seminar

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Solute Strengthening from First Principles and Application to Al and Mg Alloys

Alloys containing substitutional solutes exhibit strengthening due to favorable solute fluctuations within the alloy that hinder dislocation motion. Here, 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 stresses. The model is used to predict the flow stresses of various Al alloys and Mg-Al alloys undergoing basal slip. Excellent results are obtained for Al-Mg and Al-Mn. Al-Fe with ppm levels of Fe is not predicted well but, using experimental results for Fe, results for the quasi-binary Al-Cr-(Fe) and Al-Cu-(Fe) alloys agree well with experiments. The model is also consistent with the “stress equivalency” postulate of Basinski. Direct application of the model to basal Mg-Al shows excellent results and provides insight on the widely observed “plateau stress'' at high temperatures. This parameter-free model using first-principles input thus provides a basis for achieving the long-sought goal of computational design of alloys, within the context of solute-strengthening mechanisms