DESIGN OF DUCTILITY STARTING FROM FIRST-PRINCIPLES

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Abstract

Low ductility in Al alloys is a major barrier to their replacement of steels in automotive and other applications where failure by localization limits component design. Low ductility in Al-Mg alloys has long been associated with Dynamic Strain Aging – the material is stronger at lower strain rates, which encourages localization and instabilities – but no quantitative or predictive models exist. Here, we present a hierarchical, mechanistic, multiscale model that quantitatively predicts the ductility and enables the design of new higher-ductility alloys. The components of the model, all new to the metallurgy field, are:

(1) first-principles solute/dislocation interaction energies for arbitrary solutes in Al;
(2) predictive theory for solute strengthening in the absence of aging mechanisms;
(3) atomic-scale "cross-core diffusion" mechanism of aging;
(4) effects of cross-core diffusion on two mechanisms of dislocation strengthening;
(5) full thermo-kinetic constitutive model for thermally-activated plastic flow;
(6) implementation with an FEM model to predict coupon-scale response.

The model quantitatively predicts the entire scope of steady-state flow behavior as a function of strain-rate, plastic strain, temperature, and alloy composition in Al-Mg alloys, with all key inputs coming from quantum, atomistic, or dislocation-level computations. In particular, the predicted reduction in ductility of Al-Mg 5182 alloys at room temperature and strain rate of 10^{-3}/s is predicted in good agreement with experiments, tying the ductility loss directly to atomistic-scale phenomena. The model is then used to design new Al alloy compositions that have higher ductility at room temperature while maintaining the same yield and hardening behavior of the commercial alloys.

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