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Simulation of polycrystal deformation with grain and grain boundary effects

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ABSTRACT

Modeling the strengthening effect of grain boundaries (Hall–Petch effect) in metallic polycrystals in a physically consistent way, and without invoking arbitrary length scales, is a long-standing, unsolved problem. A two-scale method to treat predictively the interactions of large numbers of dislocations with grain boundaries has been developed, implemented, and tested. At the first scale, a standard grain-scale simulation (GSS) based on a finite element (FE) formulation makes use of recently proposed dislocation-density-based single-crystal constitutive equations ("SCCE-D") to determine local stresses, strains, and slip magnitudes. At the second scale, a novel meso-scale simulation (MSS) redistributes the mobile part of the dislocation density within grains consistent with the plastic strain, computes the associated inter-dislocation back stress, and enforces local slip transmission criteria at grain boundaries.

Compared with a standard crystal plasticity finite element (FE) model (CP-FEM), the two-scale model required only 5% more CPU time, making it suitable for practical material design. The model confers new capabilities as follows:

(1) The two-scale method reproduced the dislocation densities predicted by analytical solutions of single pile-ups.
(2) Two-scale simulations of 2D and 3D arrays of regular grains predicted Hall–Petch slopes for iron of 1.2 ± 0.3 MN/m$^{3/2}$ and 1.5 ± 0.3 MN/m$^{3/2}$, in agreement with a measured slope of 0.9 ± 0.1 MN/m$^{3/2}$.
(3) The tensile stress–strain response of coarse-grained Fe multi-crystals (9–39 grains) was predicted 2–4 times more accurately by the two-scale model as compared with CP-FEM or Taylor-type texture models.
(4) The lattice curvature of a deformed Fe-3% Si columnar multi-crystal was predicted and measured. The measured maximum lattice curvature near grain boundaries agreed with model predictions within the experimental scatter.

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