

Simulation of subgrain deformation features induced by grain interactions in polycrystals

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We investigate the formation of subgrain deformation structures arising from the constraining effect of grain boundaries on the elastic and plastic deformation fields in polycrystals. We adopt a “full-field” solution approach in which the details of the mechanical fields are accurately resolved by recourse to large-scale simulation. The computational approach is based on a Lagrangian large-deformation finite-element formulation of the continuum three-dimensional problem. The constitutive response of the material inside the grains is described with models of single-crystal plasticity ([3, 2] for FCC and [1] for BCC materials). The only discontinuity taken into account at grain boundaries is the change in the orientation of the crystal. Other important phenomena taking place at grain boundaries such as sliding are left unmodeled. The considerable computing effort is distributed among processors *via* a parallel implementation based on mesh partitioning and message passing. In this approach each mesh partition represents a grain with a different orientation and is assigned to a different processor. Each grain mesh is scalably refined to the required resolution.

We conduct medium to large scale simulations of Taylor-anvil and pressure-shear tests and investigate the computational demands associated with the possibility of capturing subscale deformation features such as localization of slip inside the grains. We show with the aid of specific examples that these demands are greatly in excess of what has been used in previous polycrystalline modeling efforts. In particular, we demonstrate the appearance of localization in the highest-resolution simulation of multicrystals under shear loading and the inability of coarser simulations to capture this microstructural feature. We also investigate the ability of this approach to capture the dependence of the effective plastic response on grain size.

References

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