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Direct Numerical Simulations in Solid Mechanics with Comparisons to Homogenization Theory

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ABSTRACT

Fatigue and fracture processes typically start at stress concentrations, and are highly dependent upon local microstructural details in addition to macroscopic stress levels. Depending upon the relative size of the microstructure (e.g., grain size) and the macroscale structural feature (e.g., fillet radius, hole radius, section thickness), the local stress and strain fields may violate the assumption of scale separation, a key assumption in homogenization theory [1]. As noted by Mindlin [2], ``Higher-order effects can be expected to come into play in linear-elastic solids when the representative length scale of the deformation field becomes comparable to a micro-structural length scale." Homogenization theory, at least for periodic media, predicts the existence of higher-order gradient effects in both the governing field equations and constitutive relations whenever the microstructure is finite [1]. For an infinitesimally small microstructure (first-order homogenization theory), these higher-order effects vanish. Also, homogenization theory predicts the existence of a surface effect, or boundary layer, due to the difference in material confinement at the surface as compared to the interior [3]. Additionally, Beran and McCoy [4] and Drugan and Willis [5] have shown that the governing field equations for the *ensemble-averaged* stress field are nonlocal with the extent of nonlocality governed by the microstructural correlation length. When the correlation length is infinitesimally small, the governing field equations for the ensemble-averaged stress field become local in character, and the ensemble-averaged stress field equals the stress field resulting from the first-order homogenized field equations.

In an era of petascale computing and future exascale computing, it is now possible to perform direct numerical simulations (DNS) in solid mechanics where the microstructure is modeled directly in a macroscale structure. Using this DNS capability, we investigate the macroscale response of polycrystalline microstructures and the accuracy of homogenization theory for upscaling the microscale response. We perform an ensemble of direct numerical simulations in which polycrystalline microstructures are embedded throughout a macroscale structure. A crystal plasticity model is used to represent the grain-scale constitutive response. We idealize the microstructure using a Voronoi tessellation seeded using a maximal Poisson disk sampling process. This seeding process results in an equiaxed grain structure. This microstructure inherently has a correlation length that is less than the mean grain size. For an example, we study at austenitic stainless steel with no texture so that the homogenized response is isotropic. The inherently random DNS results are compared with corresponding simulations based on the deterministic governing equations and material properties obtained from homogenization theory. Evidence is sought for both surface effects and other higher-

order effects as predicted by homogenization theory for macroscale structures containing finite microstructures.

For an example macroscale structure, we chose a tube with a side through-hole, loaded non-proportionally in both tension and torsion. In the linear-elastic regime, we found that the stress results using the homogenized material properties were an excellent approximation, in a weak sense, to both the ensemble-averaged stress field and the spatially filtered stress field of a single realization. Very little evidence was found for either higher-order effects or surface effects. This result is possibly due to the relatively small correlation length inherent in the model polycrystalline microstructure. In the nonlinear regime, a consistent homogenization would require the use of a computational homogenization methodology in which an RVE was embedded within each finite element. Since this capability was not available within our software, we instead fit a standard J2 plasticity model to the plastic response of a single RVE. We then compared the strain fields resulting from the use of this homogenized plasticity model to that from the DNS solutions based on crystal-plasticity. The results differed somewhat. However, for several reasons, we attribute most of this discrepancy to the use of the J2 plasticity model, rather than to higher-order homogenization effects. Future work will entail the use of computational homogenization so that any discrepancy can be properly attributed either to higher-order homogenization effects or to the accuracy of the macroscale constitutive model.

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