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Direct numerical simulations in solid mechanics for understanding the macroscale effects of microscale material variability

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Abstract

A fundamental challenge for the quantification of uncertainty in solid mechanics is understanding how microscale material variability is manifested at the macroscale. 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. Using a massively parallel finite-element code, we perform an ensemble of direct numerical simulations in which polycrystalline microstructures are embedded throughout a macroscale structure. The largest simulations model approximately 420 thousand grains within an I-beam. 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.

Keywords: Polycrystal; Homogenization; Multiscale; Voronoi; Uncertainty quantification; Stainless steel 304L

1. Introduction

Engineered structures composed of metallic materials typically contain complex spatially varying polycrystalline microstructures resulting from the solidification process as well as a series of manufacturing processes such as casting, metal forming (e.g., stamping, forging, rolling), and fabrication (e.g., welding, machining). These manufacturing processes not only alter the initial microstructure but also create complex spatially varying texture (nonuniformly-random

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crystal orientations) [1,2]. A key challenge in quantifying uncertainty in solid mechanics is understanding how the process-dependent microscale material variability is manifested at the macroscale in engineering quantities of interest.

In an era of petascale computing and future exascale computing [3], it is now possible to perform direct numerical simulations (DNS) in solid mechanics, in analogy to DNS turbulence modeling in fluid 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 100 direct numerical simulations in which polycrystalline microstructures are embedded throughout a macroscale structure. The microstructural embedding is accomplished through the use of a voxelation approach and a highly refined finite-element mesh of the macroscale structure with element sizes several times smaller than the grain size. Each finite element is assigned the properties of the grain containing the centroid of the hexahedral element. This approach to microstructural embedding is simple and robust, unlike an explicit microstructural meshing approach in which degenerate elements are invariably created making it difficult to simulate many realizations of the microstructure [4–8]. In this work, we are less interested in detailed stresses near the grain boundaries, but rather with the stress fluctuations above the grain scale.

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 [9]. As noted by Mindlin [10]:

> "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 [9,11–13]. 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 [14–16]. This boundary layer arises due to the break in the periodicity assumption at the surface and due to the satisfaction of displacement or traction boundary conditions using the homogenized material properties. For an infinitesimally small microstructure, the thickness of this boundary layer vanishes. Additionally, Beran and McCoy [17] and Drugan and Willis [18] 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. Using the ensemble of DNS results, we search for evidence of these effects.

The example macroscale structure is an I-beam with holes in the web region and fillets connecting the web and flange. The I-beam is quasi-statically loaded in a torsional mode to create stress gradients throughout the structure along with active stress concentrations in the web region. The example material is stainless steel 304L which possesses an austenitic (FCC) microstructure. For this material, each grain possesses a relatively large elastic anisotropy ratio, making it a seemingly ideal material to display higher-order effects. The microstructure is idealized as a Voronoi tessellation seeded through a maximal Poisson disk sampling process. This seeding process is also referred to as random close-packing [19]. The seeding process and subsequent Voronoi tessellation results in an equiaxed grain structure. The crystal orientation of each grain is assumed to be uniformly random (no texture) and uncorrelated with neighboring grains. This microstructure is in stark contrast to a composite material containing a periodic microstructure with perfect correlation between periodic cells. For the periodic case, higher-order homogenization effects are known to exist [11–13].

In order to explore the effect of a finite grain size and the assumption of scale separation in the homogenized solution, two ratios of web-thickness to grain size are studied: four and eight. For the case of four grains through the web-thickness, each realization of the I-beam contains approximately 60 thousand grains. For the case of eight grains through the web-thickness, each realization of the I-beam contains approximately 420 thousand grains. While only the ratio of grain size to structural size is important for the linear elastic case studied here, we note that for grain sizes on the order of 100 μm, there are approximately 1000 grains per cubic millimeter and 1 million grains per cubic centimeter. Thus, the number of grains considered in this work is still relatively small for structures consisting of many cubic centimeters of material or relatively small grains sizes. Expected future advances in computer resources will