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Delineation of first-order closures for plastic properties requiring explicit consideration of strain hardening and crystallographic texture evolution

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Abstract

Microstructure Sensitive Design (MSD) is a novel mathematical framework that facilitates development of invertible linkages between statistical description of the material's microstructure and its effective properties. Property closures are an important outcome of the MSD methodology, and delineate the complete set of theoretically feasible effective (homogenized) anisotropic property combinations in a given material system for a selected homogenization theory. In recent publications, we have reported first-order closures for the elastic and yield properties of both cubic and hexagonal polycrystalline materials. In this paper, we present major extensions to the previously reported framework to enable rigorous consideration of strain hardening and the concomitant evolution of the crystallographic texture with imposed plastic strain. These new extensions facilitate delineation of first-order closures for properties associated with finite plastic strains (e.g. ultimate tensile strength, uniform ductility). The proposed approach has been successfully applied to an aluminum alloy and a copper alloy, and the results are presented and discussed in this paper.

Keywords: A. Ductility; A. Microstructures; B. Crystal plasticity; C. Numerical algorithms; Property closures

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1. Introduction

Property closures delineate the complete set of theoretically feasible macroscale (homogenized) anisotropic property combinations in a given material system, and are of tremendous interest in optimizing the performance of engineering components. Historically, this problem has been referred to as the G-closure problem by the applied mathematics community (Cherkaev, 2000; Cherkaev and Gibiansky, 1996; Lurie, 2004; Murat and Tartar, 1985). To date, G-closures have been obtained only for a limited set of two-dimensional microstructures comprised of isotropic phases and have been largely focused on properties such as effective conductivity and elastic stiffness. In recent years, a novel spectral framework called Microstructure Sensitive Design (MSD) (Adams et al., 2001; Adams et al., 2004b; Kalidindi et al., 2004; Lyon and Adams, 2004) was proposed and demonstrated to provide *approximations* to the G-closures for a number of combinations of the elastic properties and yield properties of polycrystalline materials (Knezevic and Kalidindi, 2007; Proust and Kalidindi, 2006; Wu et al., 2007) and two-phase composites (Adams et al., 2004a; Kalidindi and Houskamp, in press).

In MSD, we start with a statistical description of the material microstructure using local state distribution functions. The simplest of these, called 1-point distributions, reflect the probability densities associated with realizing specified distinct local states (may be defined as a combination of several microstructural variables that are measurable at the length scale of interest) in the immediate neighborhood of a point thrown randomly into the microstructure. Higher order descriptions, called *n*-point spatial correlation functions, are also possible (Brown, 1955; Torquato, 2002). These distributions are then used to establish quantitative linkages between microstructure and macroscale properties (Adams et al., 2005; Beran, 1968; Kalidindi et al., 2006a; Kroner, 1977; Lyon and Adams, 2004; Proust and Kalidindi, 2006; Torquato, 2002). A salient aspect of MSD is that these linkages are transformed into an efficient Fourier space, resulting in two main constructs: (i) a microstructure hull that includes the complete set of theoretically feasible statistical distributions describing the important details of the microstructure, and (ii) delineation of property closures for a selected homogenization theory. The primary advantages of the MSD approach lie in its (a) consideration of anisotropy of the properties at the local length scales, (b) exploration of the complete set of relevant microstructures leading to global optima, and (c) invertibility of the microstructure–property relationships.

All of the previous reports in the literature on delineation of property closures have focused on a class of properties that treat the microstructure as being static. In consideration of a broader class of plastic properties of metals, we immediately encounter two important features: (i) strain hardening and (ii) concurrent evolution of microstructure due to plastic strain. Prime examples of such properties include the uniform ductility and the ultimate tensile strength. Because of their influence on the toughness exhibited by the material, these properties play an important role in materials selection for critical structural components. Since these properties directly influence the formability (and thereby the success of certain deformation processing operations), they are also of tremendous interest for deformation processing of metals. In order to successfully delineate a broader class of plastic property closures, the framework we presented in previous work (Knezevic and Kalidindi, 2007; Proust and Kalidindi, 2006; Wu et al., 2007) needed to be extended to allow for the evolution of the associated local state variables. In recent work, we demonstrated that the predictive capabilities of the Taylor-type crystal plasticity