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On large-strain finite element solutions of higher-order gradient crystal plasticity

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ABSTRACT

A finite-strain higher-order gradient crystal plasticity model accounting for the backstress effect originating from the existence of geometrically necessary dislocations (GNDs) is applied to plane strain finite element analysis. Different element types are tested to seek out an element formulation that is reliable and useful for solving problems involving severe plastic deformation. In the present finite element formulation, the GND density rates are chosen to be additional nodal degrees of freedom. Different orders of shape functions are employed for the interpolation of displacement rates and GND density rates. Their effects on solutions are examined in detail by considering three boundary value problems: a simple shear of a constrained layer (a film), a compression problem with loading surfaces impenetrable to dislocations, and a tension problem involving shear band formation. In all the cases, the formulation in which eight-node elements with reduced integration and four-node elements with full integration are used respectively for displacement rates and the GND density rates gives reasonable solutions. In addition to the discussion on the choice of finite elements, detailed behavior in gradient-dependent solids, such as the accumulation of GND density and the distribution of backstress on each slip system, is investigated by utilizing the reliable computational results obtained.

1. Introduction

Metals exhibit strongly size-dependent mechanical behavior at the micron or submicron scale. A full understanding of mechanisms of such size effects and their physically-based modeling will contribute to the design of materials with an optimal microstructure providing superior performance for the required purpose and will also contribute to design of micromechanical parts contained in small machines such as micro electro mechanical systems (MEMS). For advanced material modeling toward achieving this goal, crystal plasticity theory (Asaro and Needleman, 1985; Peirce et al., 1983; Taylor, 1938) is promising as a basic framework. Conventional crystal plasticity theory, however, does not account for any size dependence of mechanical properties. Generalizations of models based on crystal plasticity theory to incorporate size effects have been proposed by many researchers. In constitutive models, the size effects have been associated with plastic strain gradients, which correspond to the densities of geometrically necessary dislocations (GNDs) (Ashby, 1970). One method of modeling size effects is to construct a plastic strain-gradient-dependent work-hardening law (Acharya and Bassani, 2000; Ohashi, 2005). Another approach is to extend conventional plasticity models to higher-orders (Arsenlis et al., 2004; Bayley et al., 2006; Borg, 2007; Evers et al., 2004a,b; Gurtin, 2002, 2008; Kuroda and Tvergaard, 2006; Shu and Fleck, 1999; Yefimov et al., 2004a,b). The higher-order-type formulations involve an additional partial differential equation that accounts for strain gradient effects, and therefore require extra boundary conditions.

Higher-order gradient crystal plasticity theories can be subclassified into work-conjugate and non-work-conjugate types (Kuroda and Tvergaard, 2008a). In the work-conjugate type (Borg, 2007; Gurtin, 2002, 2008), higher-order stresses that are work-conjugate to the slip gradients exist in addition to the standard stress, but in the non-work-conjugate types such higher-order quantities do not appear (Arsenlis et al., 2004; Bayley et al., 2006; Evers et al., 2004a,b; Yefimov et al., 2004a,b). It has been shown by Kuroda and Tvergaard (2006, 2008a), in a small strain context, that there is similarity and equivalency between the two types of theories, even though they have different theoretical backgrounds and mathematical representations. The two types of theory are in some cases consistent, depending on the expression for the backstress in terms of the GND densities. These considerations have been extended to a finite deformation context in Kuroda and Tvergaard (2008b).

In the applications of the theories to engineering problems such as advanced material design and microstructure design, a full numerical solution will be necessary in general. The finite element method is still one of the most powerful tools for this purpose. To obtain relevant numerical solutions, a proper choice of finite elements is essential. This is particularly important for finite strain problems involving plastic flow localization, which often appears in the form of shear bands. In addition, solids with crystal plasticity

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