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Gradient crystal plasticity including dislocation-based work-hardening and dislocation transport

Stephan Wulfinghoff*, Thomas Böhlke

Karlsruhe Institute of Technology (KIT), Institute of Engineering Mechanics (Continuum Mechanics), Kaiserstraße 12, 76131 Karlsruhe, Germany

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ABSTRACT

This work aims at the formulation of a gradient crystal plasticity model which incorporates some of the latest developments in continuum dislocation theory and is, at the same time, well-suited for a three-dimensional numerical implementation. Specifically, a classical continuum crystal plasticity framework is extended by taking into account continuous dislocation density and curvature field variables which evolve according to partial differential equations (Hochrainer et al., 2014; Ebrahimi et al., 2014). These account for dislocation transport and curvature-induced line-length production and have been derived from a higher-dimensional continuum dislocation theory. The dislocation density information is used to model work hardening as a consequence of dislocation entanglement. A composite microstructure is simulated consisting of a soft elasto-plastic matrix and hard elastic inclusions. The particles are assumed to act as obstacles to dislocation motion, leading to pile-ups forming at the matrix–inclusion interface. This effect is modeled using gradient plasticity with a simplified equivalent plastic strain gradient approach (Wulfinghoff et al., 2013) which is used here in order to allow for an efficient numerical treatment of the three-dimensional numerical model. A regularized logarithmic energy is applied which is intended to approximate the higher order gradient stress of the statistical theory of Groma et al. (2003).

1. Introduction

On the macroscopic scale, the plastic deformation of single crystal specimens can be characterized by slip along particular crystallographic directions, a critical resolved shear stress being significantly smaller than the theoretical strength (Schmid and Boas, 1935) and by a characteristic work hardening behavior (e.g., Taylor, 1938). These properties can be explained microscopically since the discovery of dislocations (Polanyi, 1934; Taylor, 1934), which shear the crystallographic lattice (Orowan, 1934) and interact through elastic fields (Volterra, 1907).

Besides the discrete picture, dislocations are described in terms of scalar densities on larger scales (Gillis and Gilman, 1965; Essmann and Rapp, 1973), being interpreted as “total line length per unit volume”. In addition, the “effective Burgers vector per unit area” has been formulated in a generalized sense as a dislocation density tensor of second order (Kondo, 1952; Nye, 1953; Bilby et al., 1955; Kröner, 1958).

* Corresponding author.
E-mail address: stephan.wulfinghoff@kit.edu (S. Wulfinghoff).

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A macroscopic continuum crystal plasticity theory, which was formulated by Hill (1966) for the geometrically linear case and further generalized to large deformations, is nowadays widely applied (Teodosiu, 1970; Rice, 1971; Mandel, 1971). In this context, work hardening models often rely on simple dislocation density evolution laws (Franciosi and Zaoui, 1982; Estrin, 1996; Kocks and Mecking, 2003).

Although successful in many macroscopic engineering applications, this type of model is unable to account for size effects typically occuring on the microscale (e.g., Hall, 1951; Petch, 1953). In metals, size effects are often related to plastically inhomogeneous deformations, where the finding that 'smaller is stronger' has been confirmed by numerous experiments (e.g., Fleck et al., 1994; Stölken and Evans, 1998; Dimiduk et al., 2005).

It is possible to obtain a size-dependent model response by introducing an internal length scale into the theory, e.g., by taking into account plastic strain gradients (possibly of higher order) in the constitutive equations (e.g., Aifantis, 1987; Fleck and Hutchinson, 1993). Recent contributions in this field have been proposed, e.g., by Delannay and Barnett (2012), Klusemann et al. (2013), Le and Günther (2014) as well as Mayeur and McDowell (2014), amongst many others.

Physically, the gradient terms are related to geometrically necessary dislocations (Ashby, 1970). This concept has been heavily exploited in numerous gradient plasticity theories (e.g., Fleck et al., 1994; Steinmann, 1996). Gurtin (2000) exploits the principle of virtual power introducing generalized stresses conjugate to plastic strain gradient measures. This implies an extended set of balance equations and allows for thermodynamically consistent models of energetic as well as dissipative generalized stresses (e.g., Cermelli and Gurtin, 2002; Gurtin and Anand, 2005; Gurtin et al., 2007).

Energetic stresses derive from the stored energy function which is often assumed to be decomposed additively, with a defect energy contribution depending on plastic strain gradients. A quadratic defect energy usually leads to size-dependent overall hardening. A size effect on the overall yield strength can be achieved, if the energy is assumed to be non-smooth at the origin (i.e. for a vanishing argument, see Wulfinghoff et al. (2014b)). For example, Ortiz and Repetto (1999) and Ohno and Okumura (2007) assume the defect energy to be a linear function of the Euclidean norm of plastic strain gradient measures. This type of potential has been applied in several finite element simulations and needs a special numerical treatment (Kametani et al., 2012; Hurtado and Ortiz, 2012, 2013; Wulfinghoff et al., 2014b). The logarithmic energy proposed by Berdichevsky (2006) represents another non-smooth example leading to a size-dependent yield strength (e.g., Le and Sembiring, 2008; Kaluza and Le, 2011).

If the dissipative contributions also have a potential structure, global incremental potentials can be formulated (Miehe, 2011, 2014; Hurtado and Ortiz, 2013) representing extensions of local rate variational formulations (e.g., Ortiz and Stainier, 1999; Miehe, 2002). This concept has been applied to geometrically nonlinear gradient crystal plasticity by Miehe et al. (2014). The contribution comprises special finite element formulations being used to simulate three-dimensional systems, partially involving multiple grains.

Svendsen and Bargmann (2010) unified several theories via the application of the rate variational approach including several models which had originally not been formulated in a thermodynamic fashion (e.g., Evers et al., 2004a,b; Bayley et al., 2006), comparing them to the statistical theory of Groma et al. (2003). In some situations, Groma's theory can be approximated based on a logarithmic defect energy as proposed by Forest and Guéninchault (2013) and further developed by Wulfinghoff et al. (2014b).

The micromorphic theory of Forest (2009) reconciles several of the aforementioned gradient-extended theories with so-called 'implicit' models being applied in many contemporary contributions (e.g., Poh et al., 2011; Peerlings et al., 2012). In addition, the micromorphic framework renders the flow rule local.

This property has been exploited numerically, e.g., by Anand et al. (2012), Cordero et al. (2012) and Wulfinghoff and Böhlke (2013) proposing an equivalent plastic strain gradient crystal plasticity theory, which leads to efficient numerics (see also Wulfinghoff and Böhlke, 2012). The model has been further extended to account for grain boundary yielding by Wulfinghoff et al. (2013) closely related to earlier grain boundary models within gradient plasticity (e.g., Aifantis and Willis, 2005; Fredriksson and Gudmundson, 2007).

Kuroda and Tvergaard (2008) define scalar geometrically necessary dislocation densities as nodal degrees of freedom (see also Klusemann et al. (2012) and Kuroda (2013) for a three-dimensional application). In addition, Reddy et al. (2012) investigate a primal-dual formulation (see also Wieners and Wohlmuth, 2011) facilitating a local evaluation of the radial-return algorithm, like the micromorphic approach of Forest (2009). For a discontinuous Galerkin application see Djoko et al. (2007a,b).

In this work, the numerical efficiency of the equivalent plastic strain gradient model is exploited. The model is coupled to 24 additional partial differential equations which govern the evolution of the total dislocation densities in a three-dimensional application to face-centered cubic (FCC) crystals. The peculiarity of the dislocation density evolution equations is given by their ability to account for dislocation transport and curvature-induced dislocation production (Hochrainer et al., 2010, 2014; Hochrainer, 2013; Ebrahimi et al., 2014). The equations originate from a higher-dimensional, kinematical continuum dislocation theory (e.g., Hochrainer, 2006; Hochrainer et al., 2007; Sandfeld et al., 2010) which, under certain assumptions, describes the kinematics of curved dislocations in a highly accurate manner. Besides the dislocation densities, curvature densities are introduced as additional field variables. The theory has been applied in a number of publications (e.g., Sandfeld, 2010; Sandfeld et al., 2011; Schmitt et al., 2013; Schulz et al., 2014). These investigate the potential of the theory to yield a realistic response close to discrete dislocation dynamics simulations (e.g., Weygand et al., 2002; Weygand and Gumbsch, 2005; Aifantis et al., 2009; Senger et al., 2011). However, up to now most applications of the dislocation continuum theory have been restricted to one- or two-dimensional settings with a reduced number of slip systems.

This work aims on a first three-dimensional implementation of the dislocation continuum theory coupled to crystal plasticity involving all 12 slip systems of the FCC-crystal.