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A higher order elasto-viscoplastic model using fast Fourier transforms: Effects of lattice curvatures on mechanical response of nanocrystalline metals

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ABSTRACT

In this work a couple stress continuum based elasto-viscoplastic fast Fourier transform model is developed with the intent to study the role of curvatures – gradient of rotation – on the local meso scale and effective macro scale mechanical response of nanocrystalline materials. Development of this model has led to the formulation of an extended periodic Lippmann Schwinger equation that accounts for couple stress equilibrium. In addition to the standard boundary conditions on strain rate and Cauchy stresses, the model allows imposing non-standard couple stress and curvature rate boundary conditions. Application to representative nanocrystalline microstructures reveals that elastic and plastic curvatures accommodate a part of the local and macroscopic Cauchy stresses. Next, grain boundary interfaces are characterized using curvatures that are representative of their structure and defect content. Depending on the magnitude and distribution of these curvatures, local stresses in the grain boundary neighborhood are generated that activate slip systems besides those fulfilling the Schmid criterion. Generation of both polar dislocations and disclinations as a possible plasticity mechanism in nanocrystalline materials is explored. At the macro scale, this results in a strain rate dependent "softening" or the inverse Hall-Petch effect. The modeling framework naturally captures this grain size effect without any *ad hoc* assumptions.

1. Introduction

Plasticity in nanocrystalline (nc) metals and alloys occurs via an interplay between line crystal defects i.e. dislocations and disclinations, and grain boundary (GB) mechanisms. The dynamics of these interactions is dependent on the local microstructure which for a typical nc material is composed of a large volume fraction of heterogeneously distributed low and high angle GB interfaces (Gleiter, 1989, 2000). Molecular static simulations have indicated that the structure of these GB interfaces

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determines their energy (Hasson et al., 1972; Wolf and Kluge, 1990; Tschopp et al., 2007) which in conjunction with other morphological and textural aspects such as grain size and orientation distribution, plays a major role in defining the energy landscape of nc materials. These provide the driving forces for various non-conventional plasticity mechanisms (Kumar et al., 2003; Dao et al., 2007) resulting in the typical nc macro scale mechanical properties such as improved strength (Hall-Petch effect (Hall, 1951; Petch, 1953)) and increased strain rate sensitivity (Khan et al., 2015; Liu et al., 2015) in comparison with their coarse grained counterparts (Kumar et al., 2003; Dao et al., 2007). Furthermore, below a critical grain size some nc materials exhibit an inverse Hall-Petch or "softening" effect where the material strength decreases (Schiøtz and Jacobsen, 2003; Vliet et al., 2003; Schuh et al., 2002).

Modeling the mechanical response of polycrystalline materials is traditionally pursued using classical continuum based meso-scale crystal plasticity models. Applications to nc materials have generally aimed at demonstrating the grain size effect on the macroscopic response based either on phenomenological assumptions of mechanical behavior of GBs and grain interiors (Carsley et al., 1995; Konstantinidis and Aifantis, 1998; Kim et al., 2000; Fu et al., 2001, 2004; Benson et al., 2001; Kim and Estrin, 2005), GB evolution laws derived from GB mechanisms (Capolungo et al., 2005a, 2005b), or an elasto-viscoplastic response of GBs (Wei and Anand, 2004; Zhu et al., 2005; Wei and Gao, 2008; Jiang and Weng, 2004; Lebensohn et al., 2007). As a consequence of their size independent classical continuum framework, these models are unable to appropriately capture the underlying GB structure. Therefore, these models require introducing an *ad hoc* length scale parameter (typically the grain size) to capture the grain size dependent response.

This problem can be alleviated with the help of distortion gradient plasticity models which intrinsically account for a length scale. These include models that account for the role of strain gradients and rotational gradients i.e. curvatures. While the role of strain gradients on plasticity in nc materials (Aifantis and Willis, 2005; Gurtin, 2008; Aifantis and Konstantinidis, 2009; Aifantis, 2011; Kim and Oh, 2012; Voyiadjis et al., 2014; Aoyagi et al., 2014; van Beers et al., 2015a, 2015b) has received considerable interest over the past decade, the role of rotational gradients i.e. lattice curvatures has received disproportionately less attention. The origin of this imbalance may lie in the fact that only recently experimental characterization techniques have achieved the resolutions to quantify lattice curvatures in nc materials (Rösner et al., 2011; Di Gioacchino and Quinta da Fonseca, 2015; Carter et al., 2015). These studies have revealed that lattice curvatures manifest themselves at locations of GB interfaces, triple junctions, defect cell structures, activation of different slip systems and heterogeneity in slip distribution and intensity on the same slip system. A series of continuum based studies at the nano scale on GBs (Fressengeas et al., 2012) have highlighted that lattice curvatures are necessary to describe GB structure (Upadhyay et al., 2011; Taupin et al., 2013) in order to obtain energy estimates that match those obtained from experiments and molecular statics simulations (Fressengeas et al., 2014) and to model the structure sensitive non-local GB dynamics, for instance shear coupled boundary migration (Taupin et al., 2014).

Deriving motivation from these studies, Taupin et al. (2015) recently proposed a strain and curvature based multi-scale crystal plasticity model to study the role of incompatibilities in lattice curvature and strains on the mechanical response of nc materials. The model, known as phenomenological field dislocation and disclination mechanics (PMFDDM), accounts for the nucleation and dynamics of polar and statistical dislocations and disclinations. It is numerically implemented using a Galerkin-least square finite element approach (Taupin et al., 2015) to study the non-local and size dependent meso scale GB dynamics in bi- and tri-crystalline structures (Taupin et al., 2015).

Modeling representative volume elements (RVEs) of nc materials, however, is difficult to achieve using a finite element based approach; capturing the intricate details associated with GBs that occupy a large volume fraction of nc materials requires employing very fine meshes resulting in a very large stiffness matrix. This, coupled with the numerical complexity associated with solving the finite element problem, motivates the alternative use of fast Fourier transform (FFT) technique. The full field FFT based numerical approach for periodic RVEs was originally developed in a classical continuum framework for composites (Moulinec and Suquet, 1994, 1998) and later extended to viscoplastic (Lebensohn, 2001) and elasto-viscoplastic (Lebensohn et al., 2012) materials. Its advantage is in solving the local problem with a time complexity of $O(NlogN)$.

In light of the above, the main objectives of this work are (a) to develop a numerical implementation of the PMFDDM model using the FFT technique and (b) apply to RVEs of nc materials to understand the role of lattice curvatures on their local and effective mechanical response. In order to facilitate part (b), only the meso scale component of the PMFDDM i.e. evolution of statistical dislocations and elasticity – will be considered. The resulting model is a couple stress continuum based elasto-viscoplastic (CSEVP) model. A couple stress based Green's function is proposed to analytically solve the CSEVP problem. A combined continuum and discrete FFT approach is developed for application to nc RVEs. The CSEVP FFT model allows characterizing initial microstructures using curvatures. This is developed and explored in detail. The role of using a curvature based approach on the local and bulk mechanical response of nc materials is then studied. As will be demonstrated later, characterizing the initial microstructure using curvatures captures the grain size dependent macroscopic strain rate sensitivity and "softening" effect often observed in nc materials.

The paper is divided into sections as follows. Section 2 describes the notations used throughout this work. In Section 3, the governing equations of the CSEVP model are presented along with the technique used to characterize initial microstructures using lattice curvatures. Section 4 develops the FFT implementation of the CSEVP model. The numerical implementation is achieved using a discrete Fourier transform (DFT) technique. Section 5 describes the microstructure, elastic plastic properties and test conditions to study the role of curvatures. In Section 6, the CSEVP DFT model is first benchmarked with respect to the EVP FFT model (Lebensohn et al., 2012) for nc microstructures. Then, the role of initial lattice curvatures on the local and

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