Materials Science and Engineering A 520 (2009) 121–133

Contents lists available at ScienceDirect

Materials Science and Engineering A

journal homepage: www.elsevier.com/locate/msea

# Grain size, grain boundary sliding, and grain boundary interaction effects on nanocrystalline behavior

J. Shi, M.A. Zikry*

*Department of Mechanical and Aerospace Engineering, North Carolina State University, Raleigh, NC 27695-7910, USA*

ARTICLE INFO

*Article history:*
Received 13 March 2009
Received in revised form 6 May 2009
Accepted 7 May 2009

*Keywords:*
Grain boundaries
Dislocation–density grain boundary interactions
Finite elements
Crystal plasticity
Hall–Petch relation
Grain boundary sliding

ABSTRACT

A dislocation–density grain boundary (GB) interaction scheme, a GB misorientation dependent dislocation–density relation, and a grain boundary sliding (GBS) model are presented to account for the behavior of nanocrystalline aggregates with grain sizes ranging from 25 nm to 200 nm. These schemes are coupled to a dislocation–density multiple slip crystalline plasticity formulation and specialized finite element algorithms to predict the response of nanocrystalline aggregates. These schemes are based on slip system compatibility, local resolved shear stresses, and immobile and mobile dislocation–density evolution. A conservation law for dislocation–densities is used to balance dislocation–density absorption, transmission and emission from the GB. The relation between yield stresses and grain sizes is consistent with the Hall–Petch relation. The results also indicate that GB sliding and grain-size effects affect crack behavior by local dislocation–density and slip evolution at critical GBs. Furthermore, the predictions indicate that GBS increases with decreasing grain sizes, and results in lower normal stresses in critical locations. Hence, GBS may offset strength increases associated with decreases in grain size.



## 1. Introduction

It is well known that mechanical properties, such as yield strength, of crystalline materials are closely related to the grain size. Smaller grain sizes can correspond to higher yield and flow stresses in crystalline materials, as indicated by the Hall–Petch relationship [1,2]

$$\sigma_y = \sigma_o + kd^{-1/2}, \tag{1}$$

where $\sigma_o$ is the lattice friction stress to move individual dislocations [3], $k$ is a constant commonly interpreted to represent the stress needed to extend dislocation activity into grains adjacent to regions that have already yielded [4], and $\sigma_y$ is the yield stress of the current material. The Hall–Petch relationship is generally applicable for grain sizes larger than the order of tens of nanometers. There are numerous experimental results that support the Hall–Petch relationship. For face centered crystal (f.c.c.) copper, experimental results by [3–7] have confirmed the Hall–Petch relation when the grain size is larger than 10 nm. When the grain size is less than 10 nm, the Hall–Petch relationship seems to break down, and an inverse Hall–Petch appears to be operative. At this regime, it is suggested that the yield stress of nanocrystals decreases as the grain size decreases, and it attains a lower bound limit corresponding to the yield stress of amorphous materials [8,9].

Grain boundaries (GBs) play a critical role in the yield stress of materials in that normally they can act as barriers or initiators of dislocation activities, and can increase the threshold energy for dislocation movement [10]. The dislocation structures in the GB are very different from those in the grain interior due to various types of partial dislocations [11]. The initial immobile dislocation–density (before deformation) of the GB region is closely related to the misorientation, and for low angle GBs, there is a simple relation that gives the initial GB dislocation–density by accounting for GB misorientation angles [12]. Based on this relation, the initial GB dislocation–densities of polycrystalline materials with various grain sizes can be obtained. Since high strength GBs can repel incoming dislocations and emit dislocations, it is critical to model these GB effects. This is especially significant for aggregates with grain sizes of several nanometers, where GB effects are more significant in comparison with coarse grained aggregates.

There are four major deformation modes that could affect the behavior of crystalline materials: (i) grain boundary sliding (GBS) due to the atomic shuffling of the GB interface, (ii) collective GB migration, (iii) stacking faults, and (iv) dislocation activities in the interface and grain interiors [13]. The first two modes correspond to GB-mediated deformation, and the last two modes correspond to dislocation-mediated deformation. These deformation modes work together in characterizing the overall inelastic behavior of crystalline materials.

* Corresponding author. Tel.: +1 919 515 5237; fax: +1 919 515 7968.
*E-mail address:* zikry@ncsu.edu (M.A. Zikry).

0921-5093/$ – see front matter © 2009 Elsevier B.V. All rights reserved.
doi:10.1016/j.msea.2009.05.012

For coarse grain materials, the plastic deformation is mainly due to the dislocation-mediated deformation such as full and partial dislocation evolutions and annihilations, in which GBs act as barrier of dislocations movement, sink and source of dislocations. This may be understood by considering the sequence of events involved in the initiation of plastic flow from a point source (within one grain) in the polycrystalline aggregates [14]. The strengthening provided by GBs depends on GB structure, misorientations and interactions between dislocations and GBs.

For crystalline materials with grain sizes of several nanometers, the plastic deformation is mainly attributed to the GB-mediated deformation, such as GBS and GB migration. There are generally two different types of GBS. The first is Rachinger sliding [15], which refers to the relative displacement of adjacent grains where the grains retain their original shape but displace with respect to each other. Since polycrystalline aggregates generally have irregular grain shapes, Rachinger sliding has to be accommodated by some intragranular movement of dislocations within the adjacent grains. The other type of sliding is Lifshitz sliding [16], which refers to the boundary offsets that develop as a direct consequence of the stress-directed diffusion of vacancies. The above types of sliding is due to thermal activation process, such as diffusion and atom shuffling, although some MD simulations [13,17] indicate that GB sliding may also happen at 0 K, which indicates that the GBS also contains an athermal component.

One major issue that has been extensively investigated is the understanding on how dislocations interact with GBs. SEM and TEM experimental observations have clearly indicated that dislocations can interact with GBs in different ways through direct transfer, absorption, or transmission across the GB with residual GB dislocations and pile-ups that can result in dislocation emission or the nucleation of intergranular cracks. From these observations, several criteria on dislocation transmission have been proposed for these complex processes [18–22]. For example, Lee et al. have proposed three criteria for dislocation transmission: (i) that the angle between the lines of intersection between the GB and each slip plane must be a minimum, (ii) that the magnitude of the Burgers vectors of the dislocations that remains in the GB must be a minimum; (iii) that the resolved shear stress on the outgoing slip system must be a maximum. These three criteria have been used to understand single dislocation transmissions and to rationalize multiple dislocation activities [23–25]. By understanding these GB effects, there are also experiments directly studying the yield stress of crystalline materials. For example the yield stresses of polycrystalline copper with different grain sizes have been studied, and the Hall–Petch relation has been confirmed [4–6].

Computational simulations have also provided insights of GB activities on different physical scales. Molecular dynamics (MD) simulations have shown that GBs can act as sinks and sources of dislocations [26,27]. Dislocations can be absorbed in the GB causing pile-ups [26,28] and cross-slip [28]. These MD methods provide insights that may not be possible with TEM in-situ observations on the nano-scale. But, severe limitations on time and length scales may render these simulations ineffective on the microstructural physical scale that pertains to the inelastic behavior and yield stress of crystalline aggregates with different grain sizes.

Finite element methods (FEM) and different crystalline plasticity formulations have provided further insights on GB behavior. Ashmawi and Zikry [29] have introduced interfacial GB regions to track slip and dislocation–density transmissions and intersections for a formulation based on dislocation–density based crystalline plasticity. Other investigators [30–32] have coupled FEM with MD formulations for a multi-scale approach. There have been a lot of efforts on modeling the grain size effects using FEM. Fu et al. [33] present a crystal plasticity model, in which plastic flow is a function of grain size incorporating different dislocation accumulation rates in GB regions and grain interiors. The material is modeled as a monocrystalline core surrounded by a mantle (GB region) with a high work hardening rate response defined by Voce equation. Cheong et al. [34] proposed a non-local dislocation-mechanics based crystallographic theory to describe the evolution of dislocation mean spacings within each grain, and grain size effect is studied by FEM incorporated with grain interaction effects. A three-phase micromechanical scheme accounting for stress and strain rate jump at the grain core/grain boundary interface has been developed by Benkassem et al. [35] to describe the size effect in the viscoplastic behavior of pure f.c.c. polycrystalline materials. The above methods consider the dislocation-mediated deformation and use different GB properties in the prediction on yield stress of polycrystals. However, none of the above methods account for important physical mechanism, such as the interactions between dislocations and GB, the initial GB dislocation–densities, and GB-mediated deformation modes, which can render them inaccurate in the modeling of yield stress of nanocrystalline materials.

As a part of this framework, a recently proposed dislocation–density grain boundary interaction (DDGBI) scheme between GBs and adjacent grain interiors has been used. This scheme is based on accounting for three interrelated processes: dislocation–density absorption, emission and transmission. A conservation law for dislocation–density is used to balance dislocation activities within GB regions. A step-by-step illustration of the DDGBI scheme is given by [36,37]. By using this scheme, together with other physical properties of GBs in nanocrystalline materials, the grain size effect of crystalline material can be modeled and predicted. In this investigation, we will use this dislocation–density GB interaction scheme, a GB misorientation dependent dislocation–density relation, and a GBS model to predict and understand the behavior of nanocrystalline aggregates with different grain sizes. We will also investigate how these interrelated GB effects affect aggregates with a preexisting crack. This proposed framework is a bridge to link nanocrystalline phenomena to a microstructural relevant scale that would be associated with nanocrystalline aggregates.

This paper is organized as follows: the crystalline plasticity constitutive formulation is presented in Section 2, which include the computational approach, the proposed dislocation–density grain boundary interaction scheme, the misorientation dependence on initial GB dislocation–density and GBS mechanism; computational results and discussions are presented in Section 3, which include the process to illustrate the DDGBI scheme, the prediction on grain size effects and a discussion on how GBS affect crack behavior in nanocrystalline materials; a summary of the significant results is given in Section 4.

## 2. Constitutive formulation

### 2.1. Multiple-slip dislocation–density based crystalline formulation

In this section, a constitutive formulation for the finite deformation of rate dependent multiple-slip crystal plasticity is outlined. The detailed presentation of this constitutive formulation is given by Zikry and Kao [38].

It is assumed that the deformation gradient can be decomposed into elastic and plastic components, starting from the decomposition of the velocity gradient $V_{i,j}$, into symmetric and anti-symmetric parts as

$$V_{ij} = D_{ij} + W_{ij}, \tag{2}$$

where $W_{ij}$ is the anti-symmetric part, representing the spin tensor, and $D_{ij}$ is symmetric part, representing the deformation rate tensor.