Materials Science & Engineering A 631 (2015) 27–32

Contents lists available at ScienceDirect

Materials Science & Engineering A

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

Examining the evolution of the internal length as a function of plastic strain

X. Zhang [a], K.E. Aifantis [b,*]

[a] Applied Mechanics and Structure Safety Key Laboratory of Sichuan Province, School of Mechanics and Engineering, Southwest Jiaotong University, China
[b] Civil Engineering–Engineering Mechanics, University of Arizona, Tucson, AZ, USA

ARTICLE INFO

Article history:
Received 14 November 2014
Received in revised form
29 December 2014
Accepted 8 January 2015
Available online 14 January 2015

Keywords:
Gradient plasticity
Discrete dislocation dynamics
Internal length scales
Interfaces

ABSTRACT

Recent studies have successfully related gradient plasticity with discrete dislocation dynamics (DDD), providing estimates for the internal length scale parameter and relating it to characteristics of deformation such as the dislocation source length and dislocation source spacing. In those studies the internal length was taken to be a constant throughout plastic deformation, which however may not be physically the case as the dislocation structure evolves with deformation and there have been theoretical models suggesting an internal length that is a function of the plastic strain. In the present study, hence, when fitting the gradient plasticity expressions to the DDD data, the internal length was treated as a 'free' fit parameter for different strain levels, providing different values for the internal length throughout deformation. The results indicate that when deformation occurred in a hardening manner, the internal length decreased with increasing deformation, since the dislocation structure became denser. If however, deformation occurred in a perfectly plastic manner the internal length remained relatively constant throughout the different strain levels.

1. Introduction

Gradient plasticity [1–11] and discrete dislocation dynamics [12–18] have evolved independently over the past thirty years. The underlying physics onto which both formulations are based on are the formation and evolution of dislocations during deformation; gradient plasticity accounts for this in a phenomenological manner through the introduction of the gradient of the plastic strain, while DDD simulations do this explicitly by defining the dislocation structure and monitoring its evolution. Both formulations are in very good agreement with experimental data [19–22], but it was not until recently that a direct comparison between the two took place, indicating that simplified gradient plasticity analytical expressions for the strain profile were in precise agreement with those deduced from the DDD simulations [23,24]. The significance in trying to relate these two approaches is that insight can be obtained regarding the nature of the phenomenological coefficients that come into play in gradient plasticity, particularly the internal length.

The internal length is required for dimensional consistency and it is the characteristic distance over which the gradient effects become more pronounced. It has been proposed that it is related to the dislocation spacing [25], dislocation source distance [24], or grain size [26], while the aforementioned direct comparison between gradient plasticity and DDD simulations has indicated that the internal length cannot be universally related to either the dislocation source length or the dislocation spacing.

In the present study, a new approach is followed in relating gradient plasticity with DDD, by allowing the internal length (l) to vary as a function of the plastic strain. This is achieved by fitting the analytical gradient plasticity strain profile expressions to the DDD data independently with respect to l for different strain levels. Therefore, it is possible to obtain not only how l evolves with plastic strain, but also how it relates to the dislocation parameters.

In addition to l, the interfacial energy parameter γ [6] has been introduced within gradient plasticity to characterize the interface or grain boundary ability to respond plastically to deformation through dislocation transmission or absorption of dislocations. Hence, the evolution of γ as a function of plastic strain will also be examined in the sequel.

2. Summary of discrete dislocation dynamics simulations and gradient plasticity

The DDD data that will be used in the sequel were presented in [23]. A tensile strain was applied on tricrystals with three cubic

* Correspondence to: Department of Civil Engineering and Engineering Mechanics, University of Arizona, Tucson, AZ 85781, USA. Tel.: +1 520 621 2266.
E-mail address: aifantis@email.arizona.edu (K.E. Aifantis).

http://dx.doi.org/10.1016/j.msea.2015.01.011
0921-5093/

grains of size $L=750$ nm; their common axis was the [001] and the misorientation between neighboring grains was 22.5°. The initial dislocation microstructure consisted of randomly distributed Frank-Read sources, which evolved under tension, with a strain rate of 5000 s^{-1}. With the Peach–Koehler stress (f) acting on the dislocations, the movement of the dislocations was controlled through the kinematic equation as

$$m\ddot{x}+\eta\dot{x}=f, \tag{1}$$

where m is the effective mass of dislocations per unit length and it is taken to be $0.51-0.85\times10^{16}$ kg/m, while η is the drag coefficient and it is taken to be 10^{-4} Pa s. In order to investigate the effect of the initial dislocation structure on the internal length scale, three tricrystals which were characterized by different dislocation densities of 3.75×10^{13} m^{-2}, 7.5×10^{13} m^{-2}, and 10.25×10^{13} m^{-2} but had the same dislocation source spacing of 146 nm, were investigated. These dislocation densities correspond to dislocation source lengths of 100 nm, 200 nm, 300 nm and a mean dislocation spacing (inverse square root of dislocation density) of 163, 115, and 99 nm, respectively.

In order to compare gradient plasticity with the DDD data as reported in [23], the analytical expression for the plastic strain profile along the [100] axis of the crystal has to be known. In obtaining the strain profiles two cases were considered: (i) either the grain boundaries were infinitely stiff, inhibiting dislocation transmission or absorption, or (ii) the grain boundaries had a finite strength, which when exceeded allowed for grain boundary-dislocation interactions. Both of these cases have been solved in [23] and it was found that when plastic deformation took place in the grains but the grain boundaries were rigid (infinitely stiff) the plastic strain profile in a crystal comprising of three grains (i.e. tricrystals) was given by

$$\varepsilon_R^P[x]=\frac{\overline{\sigma}-\sigma_0}{\beta_s}\left[1-\cosh\left(\frac{3L/2-x}{l}\right)/\cosh\left(\frac{L}{l}\right)\right]+\frac{\gamma_{sf}}{l\beta_s}\sinh\left(\frac{L/2-x}{l}\right)/\cosh\left(\frac{L}{l}\right)$$
$$\varepsilon_L^P[x]=\frac{\overline{\sigma}-\sigma_0}{\beta_s}\left[1-\cosh\left(\frac{3L/2+x}{l}\right)/\cosh\left(\frac{L}{l}\right)\right]+\frac{\gamma_{sf}}{l\beta_s}\sinh\left(\frac{L/2+x}{l}\right)/\cosh\left(\frac{L}{l}\right)$$
$$\varepsilon_M^P[x]=\frac{\overline{\sigma}-\sigma_0}{\beta_m}\left[1-\cosh\left(\frac{x}{l}\right)/\cosh\left(\frac{L}{l}\right)\right], \tag{2}$$

where σ_0 and $\overline{\sigma}$ are the initial yield stress and applied homogeneous stress, respectively, while γ_{sf} is the parameter to represent yielding of the external surface. The subscripts L, M and R represent the plastic strain and material properties in the left, middle and right grains respectively, while the subscript $i=m$, s distinguishes the difference of the hardening modulus of the middle grain and the surface grains, $\beta_s\neq\beta_m$. The internal length scales of the middle grain and surface grains were chosen to be the same due to the same initial microstructure, $l=l_s=l_m$.

If the grain boundaries were not infinitely stiff, but could deform plastically once a critical stress was applied (grain boundary yield stress σ_{gb}), then the resulting plastic strain expressions before σ_{gb} was reached were given by Eq. (2) but after σ_{gb} was reached they were given by [27]

$$\varepsilon_R^P[x]=\frac{\sigma-\sigma_0}{\beta_s}+A_Re^{x/l}+B_Re^{-x/l}$$
$$\varepsilon_L^P[x]=\frac{\sigma-\sigma_0}{\beta_s}+A_Le^{x/l}+B_Le^{-x/l}$$
$$\varepsilon_M^P[x]=\frac{\sigma-\sigma_0}{\beta_m}+A_Me^{x/l}+B_Me^{-x/l} \tag{3}$$

with A_R, B_R, A_L, B_L, A_M, B_M are constants of integration and can be determined through the boundary condition,

$$A_R=B_L=-\frac{(C_1+C_2)+(C_4+C_5)e^{-2L/l}+(C_4-C_5+C_2-C_1)e^{-L/l}}{4l\beta_sC_6}\mathrm{csch}\left[\frac{L}{2l}\right];$$
$$A_L=B_R=-\frac{(C_1+C_2)+(C_4-C_5)e^{2L/l}+(C_4+C_5+C_2-C_1)e^{L/l}}{4l\beta_sC_6}\mathrm{csch}\left[\frac{L}{2l}\right];$$

$$A_M=B_M=-\frac{(C_1+C_3\cosh\left[\frac{L}{l}\right]+C_5\sinh\left[\frac{L}{l}\right])\mathrm{csch}\left[\frac{L}{2l}\right]}{2l\beta_mC_6}; \tag{4}$$

where

$$C_1=\beta_m\gamma_{sf},\ C_2=\beta_s\gamma_{sf},\ C_3=\beta_m\gamma_{gb}$$
$$C_4=\beta_s\gamma_{gb},\ C_5=(\beta_m-\beta_s)l(\sigma_0-\overline{\sigma}),\ C_6=\beta_s+(\beta_m+\beta_s)\cosh\left[\frac{L}{l}\right], \tag{5}$$

where γ_{gb} is the parameter to represent how difficult it is for dislocation pile-ups to penetrate through the grain boundary, and is used to define the interface energy Φ across the interface Γ.

$$\Phi=\gamma_{gb}\left|\varepsilon_{gb}^p\right|; \tag{6}$$

ε_{gb}^p is the plastic strain at the interface.

3. Relating gradient plasticity and discrete dislocation dynamics

3.1. Rigid grain boundary

The plastic strain profile expression of Eq. (2) was used to describe the plastic strain distribution in the tricrystals with rigid grain boundaries (Figs. 1a, 2a, and 3a). The initial yield stress of the grains can be deduced from the stress–strain plots (Fig. 1 of [23]) as 125 MPa, 62 MPa, and 74 MPa for the samples with a dislocation source length of 100 nm, 200 nm and 300 nm, respectively. The remaining parameters in Eq. (2) β_m, β_s, l, γ_{sf} were obtained by fitting Eq. (2) to the DDD plastic strain profiles of Figs. 1a, 2a, and 3a. The fitted parameters are summarized in Table 1.

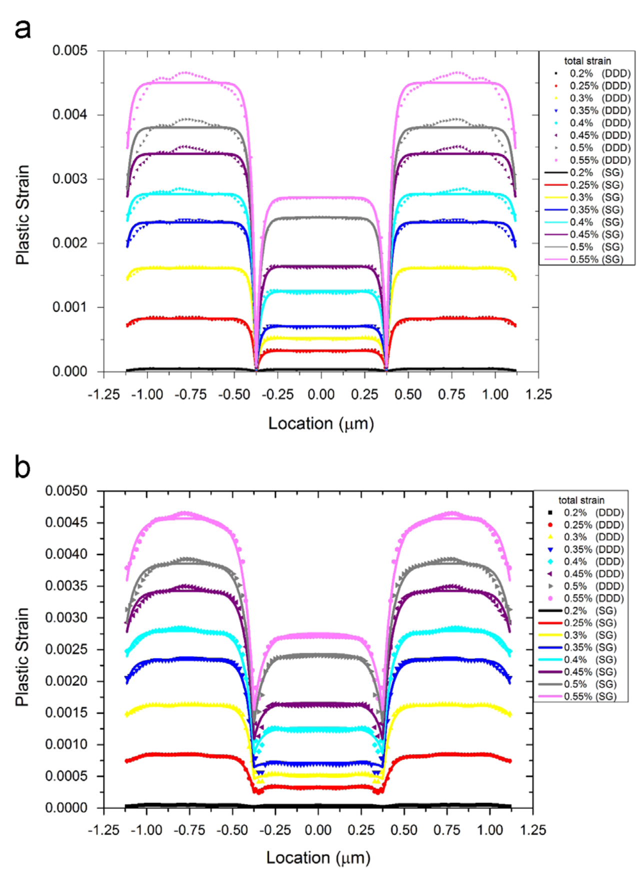

Fig. 1. Gradient plasticity fits for the plastic strain profiles of a tri-crystal with a dislocation source length of 100 nm and (a) rigid grain boundaries which never yield (b) grain boundaries of finite strength.