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Multiscale computational modeling of deformation mechanics and intergranular fracture in nanocrystalline copper

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ABSTRACT

This study presents the development and validation of a two-scale numerical method aimed at predicting the mechanical behavior and the inter-granular fracture of nanocrystalline (NC) metals under deformation. The material description is based on two constitutive elements, the grains (or bulk crystals) and the grain-boundaries (GBs). Their behaviors are determined atomistically using the quasicontinuum (QC) method by simulating the plastic deformation of $[1\,\bar{1}\,0]$ tilt crystalline interfaces undergoing simple shear, tension and nano-indentation. Unlike our previous work (Péron-Lührs et al., 2013) however, the GB thickness is here calibrated in the model, providing more accurate insight into the GB widths according to the interface misorientation angle. In this contribution, the new two-scale model is also validated against fully-atomistic NC simulation tests for two low-angle and high-angle textures and two grain sizes. A simplified strategy aimed at predicting the mechanical behavior of more general textures without the need to run more QC simulations is also proposed, demonstrating significant reductions in the computational cost compared to full atomistic simulations. Finally, by studying the response of dogbone samples made of NC copper, we show in this paper that such a two-scale model is able to quantitatively capture the differences in mechanical behavior of NC metals as a function of the texture and grain size, as well as to accurately predict the processes of inter-granular fracture for different GB character distributions. This two-scale method is found to be an effective alternative to other atomistic methods for the prediction of plasticity and fracture in NC materials with a substantial number of 2-D grains such as columnar-grained thin films for micro-scale electro-mechanical devices.

1. Introduction

Nanocrystalline (NC) materials are known to possess remarkable physical and mechanical properties such as ultrahigh strength compared with their coarse-grained counterparts [1–8]. At this length scale, the plastic deformation is considered to change from intragranular to intergranular by a mechanism in which the grain boundary (GB) character distribution (GBCD) is promoted and controls the NC mechanical behavior [9]. This transition from intragranular to intergranular or GB-mediated plasticity is assumed to control the ductility and fracture behavior of NC materials. However, understanding the evolution of fracture in NC materials is at its infancy experimentally, whereas a failure model at the atomic level is still unavailable. This work aims to develop an atomistically-informed multiscale model for the quantitative prediction of the fracture behavior in NC solids.

Molecular dynamics (MD) simulations have already revealed unusual mechanisms at low temperatures, such as GB sliding and intragranular slip involving dislocation emissions and absorptions at GBs [3,10–14], but suffer from the requirement to consider the dynamics of all atoms, thus imposing drastic limitations on the size of the simulated sample. On the other hand, continuum models, which do not suffer from such limitation, have been mainly limited to the description of grain size dependency [15], strain localization [16,17] and failure processes [15,18]. It appears however that none of these models can predict the plastic deformation of relatively large NC structures while retaining sufficient precision to account for the mechanisms involved at the nanoscale.

In a recent work [19], an original numerical multiscale approach was proposed to gain predictive understanding of the mechanical behavior of NC metals as a function of their GBCD. This model assumes that GBs are embedded in a continuum matrix and

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incorporate full GB elasto-plastic constitutive laws determined by atomistic simulations, thereby paving the way to the simulation and characterization of intergranular fracture in NC materials without the need to fully model all the grains atomistically. In this two-scale framework, the material description was based on the mechanical behavior of two constitutive elements, namely, bulk crystals (or grains) and GBs. The constitutive laws for these two constitutive elements were calibrated atomistically using the quasicontinuum (QC) method [20,21]. An explicit FCC crystal plasticity constitutive model [22] was used for the grains. This formulation improves the original implicit formulation of the forest dislocation hardening model proposed in Ref. [23] and enables large scale computations. The crystal plasticity model was previously characterized using nanoindentation QC simulations [19]. GBs were treated as surfaces of discontinuities with a finite thickness embedded in the continuum. In Ref. [19], parameters of the GBs constitutive model, including plastic and damage responses, were calibrated using the QC method by means of tensile and shear tests, following Refs. [24,25], so as to account for both GB sliding and GB opening modes. However, in that work, the thickness of the GBs was arbitrarily taken as 1 nm [19]. The model is improved here by calibrating the GB thickness parameter, validated against full atomistic results, and tested for intergranular fracture predictions.

Indeed, the objective of the present work is to demonstrate the ability of this two-scale model in predicting the fracture of NC metals for different textures and grain sizes. To this end, we first validate the purely continuum model by comparing it with fully-atomistic QC simulations for two NCs with two different textures, namely high-angle (HA) and low-angle (LA), and two different mean grain sizes. It is found that both models predict the same failure evolution in the GB networks for each texture and grain size. Once the validation step is over, an adequate fitting of the HABs calibration parameters according to their misorientation is proposed. This fitting step allows for the simulation of larger NC with a HA texture consisting of a substantial number of grains without having to run all HABs QC simulations. As an illustration, two NC dogbones, consisting of 103 grains and 251 GBs and presenting the same HA texture with two different mean grain sizes are subjected to tensile loading. These simulations highlight the ability of the two-scale model to predict the intergranular fracture of larger NCs than those conventionally encountered when dealing with pure atomistic simulations, while saving computational time.

The paper is organized as follows. Section 2 presents the details of the two-scale model and the constitutive laws used for grains and GBs. Section 3 is devoted to the QC calibration; GBs QC simulations and nanoindentation tests are presented with a particular focus on the GB width effect. Section 3 also presents the QC results fitting process designed to facilitate HA-type texture simulations. In Section 4, the full calibrated two-scale continuum model is compared to the fully-atomistic QC model for validation. Finally, this methodology is applied in Section 5 to HA-type NC dogbones simulations.

2. The two-scale model

2.1. Constitutive framework

In this section, the continuum framework with embedded GBs is summarized, following the study in Ref. [9]. The main equations for the bulk material are also presented, based on Refs. [22,23,26]. The reader is invited to refer to Ref. [19] for more details.

2.1.1. Grain-boundary constitutive model

The kinematics of the deformation mapping of a GB was developed by considering the GB as a surface discontinuity embedded in the finite element discretization, and is based on the relative motion of the two surfaces $S+$ and $S-$, corresponding to the facets of the tetrahedra on the positive and negative sides, respectively, as shown in Fig. 1a. To this end, the framework presented in Ref. [27] is used. The local stress state is described by the Cauchy stress tensor $\underline{\underline{\boldsymbol{\sigma}}}$ whereas local information about the material deformation is conveyed by the deformation gradient field $\underline{\underline{\epsilon}}$. The material models required to evaluate $\underline{\underline{\boldsymbol{\sigma}}}$ in the bulk as well as the surface traction $\underline{t}$ at the GBs are defined below. The mean deformation mapping is defined as set in Ref. [27]

$$\underline{\tilde{\varphi}} = \frac{1}{2}(\underline{\varphi}^+ + \underline{\varphi}^-) \tag{1}$$

In Eq. (1), $\underline{\tilde{\varphi}}$ is the deformation mapping of the midsurface S, and $\underline{\varphi}^+$ and $\underline{\varphi}^-$ are the deformation mappings of the surfaces $S+$ and $S-$, respectively. By using Eq. (1) we recover the original deformation mapping on both sides of the GB

$$\underline{\varphi}^{\pm} = \underline{\tilde{\varphi}} \pm \frac{1}{2}(\underline{\varphi}^+ - \underline{\varphi}^-) = \underline{\tilde{\varphi}} \pm \frac{1}{2}\underline{\delta} \tag{2}$$

where

$$\underline{\delta} = [\![\underline{\varphi}]\!] = \underline{\varphi}^+ - \underline{\varphi}^- \tag{3}$$

In Eq. (3), $\underline{\delta}$ is the displacement jump at the GB which can be also defined as $[\![\underline{\varphi}]\!]$ the difference between the displacements of the surfaces $S+$ and $S-$, see Fig. 1a. $S \equiv \underline{\tilde{\varphi}}(S_0)$ thus defines the deformed GB and we can obtain directly the initial surface normal $\underline{N}$ from the parametrization $\underline{\tilde{\varphi}} = \underline{\tilde{\varphi}}(s_\alpha)$ of S, where $\alpha = 1$ or 2 and where the coordinates (s_1, s_2) are the natural coordinates of each of the surface elements in a standard configuration, see Fig. 1b and c. Indeed, using the covariant basis vectors ($\underline{a}_\alpha = \underline{\tilde{\varphi}}_{,s_\alpha}$), one has

$$\underline{N} = \frac{\underline{a}_1 \times \underline{a}_2}{\|\underline{a}_1 \times \underline{a}_2\|} \tag{4}$$

The displacement jumps can be decomposed into a GB opening vector and a sliding vector as follows

$$\underline{\delta}_n = (\underline{\delta} \cdot \underline{N})\underline{N} = (\underline{N} \otimes \underline{N}) \cdot \underline{\delta} \tag{5}$$

$$\underline{\delta}_s = \underline{\delta} - \underline{\delta}_n = (\underline{\underline{I}} - \underline{N} \otimes \underline{N}) \cdot \underline{\delta} \tag{6}$$

It is assumed that this kinematics imposes a constant deformation gradient across the thickness h of the GB. This assumption is justified by the low number of atoms within the GB. This gradient of deformation can be expressed in the local orthonormal reference frame

$$(\underline{N}_1, \underline{N}_2, \underline{N}_3) = ((\underline{a}_1/|\underline{a}_1|), (\underline{N} \times \underline{a}_1/|\underline{N} \times \underline{a}_1|), \underline{N}) \tag{7}$$

as

$$\underline{\underline{\epsilon}} = \underbrace{\frac{\underline{\delta}_n \cdot \underline{N}_3}{h}\underline{N}_3 \otimes \underline{N}_3}_{\underline{\underline{\epsilon}}_n} + \underbrace{\frac{\underline{\delta}_s \cdot \underline{N}_1}{h}\frac{1}{2}(\underline{N}_1 \otimes \underline{N}_3 + \underline{N}_3 \otimes \underline{N}_1) + \frac{\underline{\delta}_s \cdot \underline{N}_2}{h}\frac{1}{2}(\underline{N}_2 \otimes \underline{N}_3 + \underline{N}_3 \otimes \underline{N}_2)}_{\underline{\underline{\epsilon}}_s} \tag{8}$$

From Eq. (8), $\underline{\underline{\epsilon}}$ is the sum of two quantities; a normal opening part $\underline{\underline{\epsilon}}_n$ and a sliding part $\underline{\underline{\epsilon}}_s$. In Ref. [19], h, naturally defining a characteristic length scale of GBs in the model, was set to 1 nm following past works [28,29]. However, assigning a fixed value to h does not account for the different thicknesses between each GB type (HAB or LAB) and their impacts on the NC mechanical behavior. Consequently, h is here treated as a parameter obtained from the calibration process. The traction is eventually expressed as