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Strain gradient plasticity analysis of the grain-size-dependent strength and ductility of polycrystals with evolving grain boundary confinement

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Abstract

The loss of uniform elongation with decreasing grain size in polycrystals is analysed using a strain gradient plasticity-based finite-element model involving an enhanced description of the grain boundaries. The grain interiors are modelled by the finite strain version of the isotropic Fleck–Hutchinson theory with one internal length parameter. The grain boundaries are modelled using cohesive zone elements imposing higher-order boundary conditions at the interface between the grain interior and grain boundary layer. The plastic strain rate is initially set to zero at these interfaces to account for their impenetrability to dislocations. With increasing stress levels, the higher-order constraint can be suppressed in order to mimic grain boundary relaxation mechanisms. The model is validated towards experimental data on ferritic steels with grain sizes varying between 100 nm and 10 μm. The model reproduces not only the yield stress evolution, but also the drop of ductility taking place around 1 μm grain size while using a single constant internal length. Relaxation of the grain boundary constraint is needed to correctly predict the response at the smallest grain sizes. The back stress increases with decreasing grain sizes. Additional analysis of bimodal grain size distributions is provided showing a large potential for ductility enhancement.

Keywords: Ferritic steels; Ductility; Hardness; Ultrafine-grained microstructure; Strain gradient plasticity

1. Introduction

A key issue in the development of high-strength single-phase polycrystalline alloys through grain size reduction is the low ductility associated to a poor strain-hardening capacity [1–4]. Ductility is defined here as the resistance to plastic localization. Different solutions exist to restore ductility of sub-microcrystalline metals by processing bimodal grain size microstructures [5–7], through activation of rate-dependent plasticity mechanisms [1,2,7–9], by favouring growth and/or deformation twins [2,8,10–13], through the addition of second-phase particles [14,15], and/or by strain-induced phase transformation [16–18]. Nevertheless, a proper understanding and modelling of the size-dependent loss of strain-hardening in fine and ultra-fine-grained metals leading to very small ductility is still lacking. The dislocation/grain boundary interaction is a very complex problem, due the co-existence of multiple mechanisms such as blocking, annihilation, emission, reflection and transmission, depending on the stress level and character of the grain boundary (GB) [1,19–22]. The convolution of these mechanisms has a direct impact on the rate of recovery near the GB and on setting the magnitude of local strain gradients and of the resulting back stress. One, if not the main, difficulty in the development of continuum models for polycrystals resides in the formulation of coarse-grained representation of the dislocation behaviour near GB.

In the framework of simple one-dimensional models, significant efforts were made to enhance the Kocks–

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Mecking [23] formalism by introducing the effect of GB on the dislocation mean free path [24–26], and by accounting for GB geometrically necessary dislocations (GNDs). The so-called "core & mantle" type models involving a GB layer in which the density of dislocations increases much faster than in the core are able to capture the Hall–Petch effect, see Ref. [1] and references therein. Recent one-dimensional analysis by Sinclair et al. [27] followed by others [15], introduced more realistic representations of the GB and near-GB behaviour. With the introduction of a saturation of the GB dislocation density, involving the relaxation of the impenetrable character of the GB, as well as a back stress evolution law invoking a progressive shielding by the dislocations on the opposite side of the GB, the model quantitatively captures, with a minimum number of adjusting parameters, the loss of ductility associated with a grain size reduction.

Different types of two-dimensional or three-dimensional field models have also been developed in order to simulate the response of polycrystals while explicitly introducing the presence of GBs in order to account for grain size effects. These computational studies are based either on strain gradient plasticity type theories involving [28] or not [29,30] higher-order stresses, on models incorporating explicitly a back stress related to the plastic slip incompatibility [31], or on a discrete description of the dislocation dynamics [32]. All of the aforementioned studies have considered, in a way or another, impenetrable GBs. In the context of strain gradient plasticity theories involving higher-order boundary conditions, impenetrability is enforced through imposing no plastic strain at the GB. The Hall–Petch effect is captured, but not the drop of strain-hardening capacity after small amounts of plastic deformation, except with the model by Beaudouin et al. [33], which correctly predicts an initially low strain-hardening capacity in small grain size silver polycrystal by changing the initial dislocation density. Recently, more advanced continuum descriptions of the interactions between dislocations and GBs have been proposed in the literature, following different directions. Ma et al. [21] developed a polycrystal model involving rules for the transmission of dislocations through GB depending on the crystallographic misorientation, see also Ref. [22]. Gurtin, Gudmunson and their co-workers [28,34,35], followed by several others [36–40], enriched their higher-order theories with a constitutive description of the interface response. These enrichments offer new degrees of freedom to capture the complex and evolving constraints on plastic flow at GBs (and other types of interfaces as well). The present work was conducted in the spirit of these recent developments.

A finite-element model has been set up relying on a finite strain implementation of the strain gradient plasticity theory by Fleck and Hutchinson [41] for the grain interior behaviour. Cohesive zones are used to represent the GB layer, together with evolving higher-order boundary conditions at the frontier with the grain interior, see Fig. 1. The GB layer is extremely thin, on the order of a few atomic spacings, i.e. between 0.2 and 1 nm. This model can thus not be assimilated to a "core & mantle" model, which separates in a somewhat artificial manner the grain interior into two sub-regions. Here the GB layer is considered as made of a truly different structure compared to the grain interior. While applying the load, the grain starts deforming plastically while the GB layer remains elastic. The GBs are considered to be initially impenetrable to dislocations. This is enforced by imposing zero plastic strain at the two interfaces surrounding the GB. The strength of the near GB regions increases rapidly due to the large local plastic strain gradients, generating also a large back stress, with a direct impact on the overall strength of the polycrystal. When the stress on the GB reaches a critical value, the different mechanisms of transmission, nucleation and/or sinking of dislocation at the GB start being activated. This is empirically modelled by relaxing the constraint on both sides of the GB and letting the plastic flow develop at the interface. The back stress then also partially relaxes. From that point on, the confinement of the plastic flow is only controlled by the GB layer behaviour represented by simple linear hardening.

The objective of this paper is twofold. First, a validation of the model is provided by comparing predictions towards experimental data obtained on single-phase ferritic steel. These data, collected recently by Bouaziz [42], cover a wide range of grain sizes from 80 nm up to 80 μm, and involve change of yield stress and ductility both by more than a factor 20. This range of grain size is known to encompass different dislocation-mediated mechanisms [43] from those met: (i) in ultra-fine-grained (UFG) materials with $d < 0.1$–0.2 μm involving limited dislocation storage in the grain interior, no dislocation cell structures, and all the dislocation activity at the GB; (ii) in the transitional behaviour of fine-grained (FG) materials; and (iii) in the traditional regime ($d > 1$–2 μm) involving abundant dislocation storage in the core of the grains. A final validation is provided by running simulations for a bimodal grain size distribution and by comparing the predictions to the results of Wang et al. [5] on Cu, which demonstrate a significant gain in ductility without loss of strength when compared to a monomodal distribution. The second objective is to conduct a parameter study by varying one by one the parameters controlling the GB behaviour in order to unravel their effect on the strength/ductility balance, as well as on the Bauschinger effect.

The paper starts in Section 2 with the presentation of the constitutive model, numerical procedures, and microstructural model. In Section 3, the model is validated, after identification of the material parameters, for single-phase ferritic steel. Then, a parametric study is proposed in order to analyse the effect of the different parameters of the GB model, based on the set of parameters determined for the ferrite. Section 4 addresses the effect of a bimodal grain size distribution in single-phase metals, before concluding.