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Strain gradient plasticity analysis of the influence of grain size and distribution on the yield strength in polycrystals

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ABSTRACT

Plane strain models of polycrystalline microstructures are investigated using strain gradient plasticity (SGP) and a grain boundary (GB) deformation mechanism. The microstructures are constructed using a non-linear constrained Voronoi tessellation so that they conform to a log-normal distribution in grain size. The SGP framework is used to model the grain size dependent strengthening and the GB deformation results in a cut-off of this trend below a certain critical grain size. Plastic strain field localization is discussed in relation to the non-local effects introduced by SGP and a material length scale. A modification of the Hall–Petch relation that accounts for, not only the mean grain size, but also the statistical size variation in a population of grains is proposed.

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1. Introduction

The grain size has a large impact on the yield strength of polycrystalline metals and alloys, as has efficiently been deployed to advance the development of higher strength materials by reducing the grain size. A large amount of experimental evidence exists for this, and to mention a few, the grain size dependent yield stress in Ni for a wide range of experiments are reviewed in Conrad and Narayan (2002) and similarly for Cu in Conrad (2004). In Ohno and Okumura (2007), experiments on Al, Cu, Ni and stainless and IF steels are compiled and also in Bouaziz (2010) data for IF steels and pure iron are reproduced. However, reducing the grain size without control of the grain size variation may not result in the anticipated gain, as an increase in variation seems to counteract a decrease in grain size. Experiments that take into account the importance of the microstructural distribution are not abundant but a few reports related to this is the work of Kurzydłowski and Bucki (1993) on stainless steel, the computational study related to experiments in Zhu et al. (2006) and a study on Ni in Dalla Torre et al. (2002). To what extent the variation in grain sizes affects the overall mechanical properties is not entirely clear as it also depends on the complex features of the grain boundaries. In tests on several sets of Al with similar grain size, but with different characteristics of the grain boundary (GB), Sun et al. (2005) observe that influence of the GB features on the mechanical properties may be significant.

In crystalline metals the microstructure determines many of the mechanical properties. As a corollary the mechanical properties of a material specimen can be controlled if the microstructure can be controlled. The elastic moduli of a polycrystal is determined by the binding energy of the atoms in the crystal lattice, and the microstructure will mainly contribute so that these are averaged out to make the material isotropic on the macroscopic level. For properties pertaining to plastic processes the microstructure has a more profound effect. The difference in yield and post-yield behavior between a single- and polycrystal are far more than a statistical averaging operation. The introduction of grains, and thus also of grain boundaries, enables several microstructural deformation mechanisms that would not be possible in a single crystal. The main deformation features introduced by the presence of GB are the local resistance to plastic flow (i.e. barriers to dislocation motion) and at smaller grain sizes the grain boundaries appear to act as the main channels of inelastic deformation, see for instance the reviews by Kumar et al. (2003) and Meyers et al. (2006).

From a continuum mechanics modeling perspective grain size dependent flow properties can be captured by use of strain gradient plasticity (SGP) theories, see Evans and Hutchinson (2009) for a recent assessment. The use of gradient enhanced theories for modeling is based on current understanding of plastic deformation mechanisms in single- and poly-crystals. It is for instance well established that a geometrically necessary dislocation (GND) density, ρ_{GND}, is proportional to the lattice curvature and therefore to a

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gradient of plastic strain (Nye (1953), Ashby (1970), Arsenlis and Parks (1999) and Kysar et al. (2010)). A dislocation density without a net Burgers vector is characterized as a statistically stored dislocation (SSD) density, ρ_{SSD}, and can be associated with the plastic strain at the material point. In the Taylor hardening model the flow stress on a slip system depends on the dislocation density and since there is no way to distinguish if an individual dislocation is a GND or a SSD both dislocation densities should enter into the hardening relation. Therefore it is reasonable to assume that on length scales where the material experiences large plastic strain gradients, hardening should depend not only upon the accumulated plastic strain, but also on the local plastic strain gradients. Therefore, SGP can be used to capture the increased hardening rate from a large accumulation of GNDs.

Internal barriers to dislocation motion will, during plastic distortion of a structure, introduce local gradients. A common model for this is the so called pile-up model where dislocations of equal sense, i.e. a dislocation distribution with a non-zero Burgers vector, are pinned against a grain boundary. This process of grain boundary strengthening will raise the macroscopic yield point of a material with sufficiently small grains and is usually referred to as the Hall–Petch effect (Hall, 1951; Petch, 1953). This type of initial strengthening due to grain size appears naturally within a SGP framework when explicit grain boundary models are introduced.

In this paper the combined effects of grain size and its variation on the yield strength in polycrystalline metals will be investigated, but we have opted to neglect any contributions due to increased hardening in order to simplify our model. The model explored by the present authors in Dahlberg et al. (2013), based on a strain gradient plasticity framework with internal energetic interfaces allowing for an irreversible sliding/separation deformation mechanism, will be employed. In that study the influence of grain size on plastic flow properties in a *constant sized grain* (CSG) microstructure was investigated by analyzing a columnar grain structure composed of regular hexagons. To generate realistic grain structures with desired size variation, a method based on constrained Voronoi tessellation has been developed. Specifically the isotropic strain gradient plasticity by Gudmundson (2004) will be used for the grain interiors and an interface description for the grain boundaries proposed in Dahlberg and Faleskog (2013) and Dahlberg et al. (2013) which builds on the formulation in Fleck and Willis (2009b). Modeling of grain structures with emphasize on grain size distributions have been performed by Zhu et al. (2006), Berbenni et al. (2007) and Massart and Pardoen (2010). As in this study, grain boundaries are often modeled as thin interfaces. However, very few attempts to combine the two mechanisms of grain boundary sliding and plastic flow resistance. Previous work relevant to this study can be found in Fredriksson and Gudmundson (2007), Pardoen and Massart (2012), Wei and Anand (2004) and Gurtin and Anand (2008).

We start by a short review of experimental observations made to describe grain size distribution and from that a method based on Voronoi tessellation is proposed and employed to construct realistic columnar grain structures. The constitutive framework is described next. Five geometrically different microstructures, in terms of grain size variation, were analyzed and the outcome is presented in the Section on results. Finally some concluding remarks are given.

2. Modeling of polycrystalline grain structures

2.1. Grain size distribution

The population of grains in polycrystalline metals is of stochastic nature, where the grain size, D, can be treated as a random variable. Important statistical parameters characterizing the population of grains are then the mean size, D_0, and the standard deviation, S_{D}, and some notion of the type of distribution. When it comes to the distribution there is now a substantial amount of experimental studies that show that the variation of grain volumes, and also the variation of grain sizes, in metallic materials sufficiently well can be described by a log-normal distribution. This appears to be valid in the whole range from microcrystalline metals (mc: $D_0 > 1$ μm) to nanocrystalline metals (nc; $D_0 < 100$ nm) including ultrafine crystalline metals (ufc) in between. In this context, a useful measure to identify geometrically similar polycrystals is the coefficient of variation, $c_{\mathrm{V}} = S_{\mathrm{D}}/D_0$, as pointed out by Kurzydłowski and Bucki (1992) (they phrase c_{V} in terms of variation of grain volume instead). To mention some experimental observations of interest, reported values of c_{V} in mc metals are: about 0.6 in recrystallized Ti (Okazaki and Conrad, 1972); 0.34–0.88 in recrystallized Al (Rhines and Patterson, 1982); 0.16–0.38 in Zn, Al, and ferritic and austenitic stainless steels (Núñez and Domingo, 1988; Kurzydłowski and Bucki, 1992). Values found in ufc and nc metals are: 0.32–0.46 in Ni-foils (Dalla Torre et al., 2002); 0.34–0.88 Cu, Ni, Fe and Co (Phaniraj et al., 2007 and references therein). In conclusion, the interval $0.2 \leq c_{\mathrm{V}} \leq 0.9$ seems to capture observations made for a vast number of polycrystals with D_0 ranging from mc to nc metals.

A log-normal distribution of grain size, D, is described by the probability density function

$$f_{\mathrm{D}}(D; D_{\mathrm{M}}, S_{\mathrm{N}}) = \frac{1}{S_{\mathrm{N}}\sqrt{2\pi}D}\exp\left[-\frac{1}{2}\left(\frac{\ln(D/D_{\mathrm{M}})}{S_{\mathrm{N}}}\right)^2\right], \tag{1}$$

where D_{M} is the median value (geometric mean) and S_{N} is dimensionless and related to the standard deviation. The distribution (1) is referred to as a number-weighted or true size distribution as opposed to a volume weighted distribution, see discussion in Bucki and Kurzydłowski (1993) and Yu et al. (1998). The expected value (arithmetic mean), here identified as the mean grain size, is defined as

$$D_0 = \int_0^\infty D f_{\mathrm{D}}\,\mathrm{d}D = D_{\mathrm{M}}\exp\left(S_{\mathrm{N}}^2/2\right), \tag{2}$$

and the standard deviation given by

$$S_{\mathrm{D}} = \sqrt{\int_0^\infty (D-D_0)^2 f_{\mathrm{D}}\,\mathrm{d}D} = D_{\mathrm{M}}\exp\left(S_{\mathrm{N}}^2/2\right)\sqrt{\exp\left(S_{\mathrm{N}}^2\right)-1}. \tag{3}$$

Hence, the coefficient of variation can be expressed as

$$c_{\mathrm{V}} = S_{\mathrm{D}}/D_0 = \sqrt{\exp\left(S_{\mathrm{N}}^2\right)-1}. \tag{4}$$

By assuming that the grains are self similar in shape, it follows from the change-of-variable rule that the volume distribution also will be log-normal distributed. Thus, using the transformation $V = k_{\mathrm{V}}D^3$, where k_{V} is defined by the shape of a grain (e.g. $k_{\mathrm{V}} = \pi/6$ for a sphere), the volume distributed coefficient of variation ($c_{\mathrm{V}}^{\mathrm{vol}}$) is related to the size distributed coefficient of variation as $c_{\mathrm{V}} = \sqrt{(1+(c_{\mathrm{V}}^{\mathrm{vol}})^2)^{1/9}-1}$, see derivation in Appendix A. This relation was used to convert reported $c_{\mathrm{V}}^{\mathrm{vol}}$ values in some of the references cited above to the c_{V} values summarized here.

Since the analysis in the current work was limited to planar (2D) columnar grain structures, an area distribution corresponding to

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