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Stress/strain gradient plasticity model for size effects in heterogeneous nano-microstructures

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ABSTRACT

Traditionally, modeling the effect of grain size on the mechanical behavior of crystalline materials is based on assuming an equivalent homogenous microstructure with strength being dependent on the average grain size, for example the well-known Hall-Petch relation. However, assuming an equivalent homogenized microstructure for a highly heterogeneous microstructure can lead to inaccurate prediction of strength and ductility, especially when the gradients in the spatial heterogeneity are severe. In this work, we employ a multiscale dislocation-based model combined with a strain/stress-gradient theory to investigate the effect of spatial heterogeneity of the microstructure on strength and ductility. We concentrate on understanding the effect of various grain size spatial distributions on the mechanical properties of interstitial free (IF)-steel. The results show that by controlling some parameters in the spatial distribution of the microstructure with regions composed of micro-grains and nano-grains one can achieve improved strength and ductility. Based on these results, it is suggested that the mechanical properties of gradient materials can be described by phenomenological relations that include two structural parameters, grain size and grain-size gradient, in contrast to Hall-Petch relation for homogenous materials where only grains size appears in the equation.

1. Introduction

Numerous investigations have shown that the mechanical behavior of metallic materials can be significantly altered by refinement of the microstructure, e.g. (Calcagnotto et al., 2010; Estrin and Vinogradov, 2013). For instance, a polycrystalline material with nano-size grains will have a higher strength than its equivalent micron-size grains. However, the trade-off is that it will also become more brittle (Morris, 2010). For a material with a homogenous microstructure, it is difficult to attain both high strength and ductility. This has been reported by many researchers, e.g. Lu (2014), where it is shown that the strength versus ductility curve, for many classes of polycrystalline materials, follows a so-called ‘banana curve’, shown schematically in Fig. 1. However, recent experimental studies have shown that some heterogeneous microstructures with grain size in the range of a few nanometer up to micrometer can result in both high strength and increased ductility. As an example, a method called surface mechanical attrition treatment (SMAT) has been employed by many researches (e.g (Balusamy et al., 2013; Tao et al., 2003; Yin et al., 2016; Zhu et al., 2004)). To produce materials with heterogeneous

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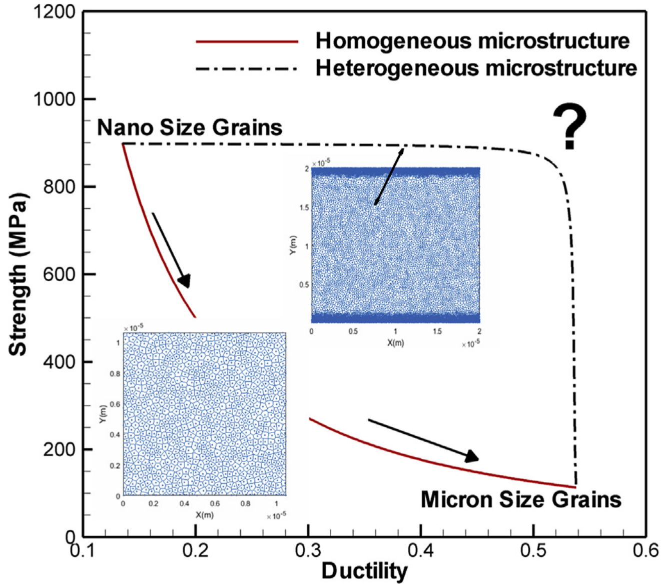

Fig. 1. Strength vs. ductility plot.

microstructures. Other experimental studies showed that this process leads to producing a texture with gradient of grain size ranging from nano grain size close to the surface layer up to coarse grain size about a few micrometers around the middle of the layer. This grain size distribution results in a material having both high strength and high ductility along the tensile direction (Lu and Lu, 2004; Lu et al., 2000; Wu et al., 2002; Yang et al., 2016; Zhao et al., 2006). Furthermore, results obtained from tensile tests showed that when material with a microstructure composed largely of micro-grains is processed so that it also contains nano-regions composed of nano-grains strength and ductility can be improved due to the gradient microstructure (Grange, 1971; Hufnagel et al., 2002). These results suggest that it may be possible to design material with heterogeneous microstructure that may possess both optimum high strength and ductility, as illustrated in the hypothetical curve shown in Fig. 1 (dash line).

Conventional continuum plasticity models cannot capture the effect of the grain size in heterogeneous microstructure. This is because these conventional models do not account for internal length scales and spatial gradient effects. In order to capture size effect, two gradient models, strain-gradient and stress-gradient models, which are based on different dislocation mechanisms and phenomena, have been proposed in the literature. Strain-gradient models account for hardening resulting from the formation of so-called geometrically necessary dislocations (GNDs) to accommodate lattice curvature during non-uniform deformation (Huang et al., 2004; Rhee et al., 1994; Shizawa and Zbib, 1999; Taylor et al., 2002; Wulfinghoff and Böhlke, 2015; Zhu et al., 1997). The effect of the GNDs on flow stress and hardening can be incorporated directly in hardening laws, or in the expression for the dislocation mean-free path, e.g. (Lyu et al., 2015; Ohashi, 2005). The counterpart to the strain-gradient plasticity theory is the stress-gradient plasticity, which is based on the mechanism of dislocation pile-ups against grain boundaries or obstacles under inhomogeneous state of stress (Chakravarthy and Curtin, 2011; Hirth, 2006; Taheri-Nassaj and Zbib, 2015). In a previous study it was shown that these two theories are complementary to each other (Liu et al., 2014) and can be employed in a combined strain/stress gradient model to capture the grain size effect over a wide range of length scale.

Modeling the effect of the grain size in a heterogeneous microstructure requires the introduction of representative volume elements (RVEs) that account for the statistical nature of the microstructure. Currently, there are a few models that account for the statistical nature of the grain size, e.g. (Berbenni et al., 2007; Lehto et al., 2014; Quested and Greer, 2004). Some models discretize the domain into a continuous heterogeneous domain and combine strain-gradient or stress-gradient theory with a finite element method coupled with a Voronoi cell (VCFEM), e.g. (Kabiri and Vernerey, 2013; Vernerey and Kabiri, 2012). However, computational efficiency limits the number of grains that can be considered in the simulations, and this is seen as a problem for modeling heterogeneous microstructure with nano and micron size grain for which a large number of grains needs to be considered. Therefore, in the present work we develop and employ an efficient multi-scale model that combines a visco-plastic self-consistent model (VPSC) with a continuum dislocation dynamic model (CDD) and discrete dislocation dynamic (DDD) model (see flow chart in appendix A). By implementing both strain-gradient and stress-gradient theories in a 2D Voronoi tessellation diagram, with each Voroni cell representing an individual grain, we are able to capture the grain size effect in a heterogeneous microstructure. Although the framework and the theories developed in this work as described in the next section are applicable for any type of polycrystalline material, the focus in this paper is on a typical BCC metal-interstitial free (IF)-steel. There are numerous experimental and numerical studies that have been performed on this material and