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Atomistic and mean-field estimates of effective stiffness tensor of nanocrystalline copper

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ABSTRACT

The full elasticity tensor for nano-crystalline copper is derived in molecular simulations by performing numerical tests for a set of generated samples of the polycrystalline material. The results are analysed with respect to the anisotropy degree of the overall stiffness tensor resulting from the limited number of grain orientations and their spatial distribution. The dependence of the overall bulk and shear moduli of an isotropized polycrystal on the average grain diameter is analysed. It is found that while the shear modulus decreases with grain size, the bulk modulus shows negligible dependence on the grain diameter and is close to the bulk modulus of a single crystal. A closed-form mean-field model of effective elastic properties for a bulk nano-grained polycrystal with cubic grains, i.e. made of a material with cubic symmetry, is formulated. In the model all parameters are based on the data for a single crystal and on the averaged grain size without any need for additional fitting. It is shown that the proposed model provides predictions of satisfactory qualitative and quantitative agreement with atomistic simulations.

1. Introduction

Metal polycrystals are examples of heterogeneous materials in which heterogeneity results mainly from different orientations of local anisotropy axes in each grain. When the size of grains is sufficiently large the continuum mechanics framework is applicable and usually the boundaries between the grains are treated as perfect interfaces that do not require special treatment.

In order to estimate effective properties of a coarse-grained polycrystalline material a micromechanical methodology is used. Besides the classical Voigt and Reuss estimates, the self-consistent model due to Kröner (1958) and Hill (1965) is most often employed. This methodology was successfully extended to the (visco)plastic crystals and large strain regime (Lebensohn & Tomé, 1993; Molinari, Canova, & Ahzi, 1987). Verification of such micromechanical mean-field estimates is usually performed by means of full-field simulations employing either the finite element method (FEM) (Fan, Xie, & Sze, 2010; Kamaya, 2009) or the fast Fourier transform (FFT) technique (Lebensohn, Kanjarla, & Eisenlohr, 2012; Liu, Raabe, Roters, Eisenlohr, & Lebensohn, 2010; Prakash & Lebensohn, 2009).

Nanocrystalline metals are polycrystalline materials with a grain size smaller than 100 nm (Gao, Wang, & Ogata, 2013; Gleiter, 2000). In such materials two phases can be distinguished: grain cores and grain boundaries. The effect of the grain boundaries on the overall properties of a bulk material increases with decreasing grain size

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(Gao et al., 2013; Sanders, Eastman, & Weertman, 1997). At the macroscopic level a nanograined material is still described in the framework of continuum theories. Since there is a need for quick and simple estimates of effective properties, which use only basic knowledge of the material behavior: single grain properties, orientation distribution (texture) within the material volume and the averaged grain size, micromechanical mean-field estimates are also utilized in this case. Most of the mean-field schemes proposed for nanocrystalline materials describe them as composite media made of two or more phases. One phase is the grain core and the other phase (or phases) represents the behavior of the grain boundary. In the early mixture-based model (Carsley, Ning, Milligan, Hackney, & Aifantis, 1995) a nanophase metal was described as a mixture of a bulk intergranular region and a grain boundary built of amorphous metal. The overall strength of the material was obtained as a simple volume average of the strengths of the two phases. In Kim and Bush (1999) a refined mixture model was developed in which the intercrystalline phase was composed of three sub-phases: grain boundary, triple line junctions and quadratic nodes. Additionally pores were considered. All phases were modeled as isotropic and in order to obtain overall elastic moduli the implicit self-consistent relation was used. The concept of grain boundary subdivision into sub-phases was followed by Benson, Fu, and Meyers (2001); Qing and Xingming (2006), although using simple volume averages to obtain the overall Young's modulus and strength, while in the approach presented by Zhou, Li, Zhu, and Zhang (2007) the overall properties were assessed by using subsequently isostrain and isostress assumptions for finding the average response of the grain core and the two grain boundary sub-phases. In Sharma and Ganti (2003) a nano-grained material was described as a crystalline matrix with embedded ellipsoidal flat disks representing the grain boundary. To estimate the overall strength that accounts for grain boundary sliding the disks' stiffness moduli were anisotropic with one modulus vanishing, and the Mori–Tanaka (MT) scale-transition scheme was applied. In Jiang and Weng (2004) the idea of the generalized self-consistent (GSC) model was used to find the strength and stiffness of a nanograined polycrystal: the coating of the spherical grain was assumed to be made of an isotropic material representing the grain boundaries. The grain cores were assumed to be elastically isotropic, while retaining their plastic anisotropy. This idea was followed by Capolungo, Cherkaoui, and Qu (2007) and Ramtani, Bui, and Dirras (2009). In the former model the implicit formulae of the GSC scheme (Christensen & Lo, 1979) were replaced by the explicit relations of the Mori–Tanaka model under the assumption that the grains are embedded in the matrix of the grain boundary phase. Similarly, in Mercier, Molinari, and Estrin (2007) a two-phase elastic-viscoplastic model combined with the Taylor–Lin homogenization theory was used to find the overall yield stress of nanocrystalline copper. The core-shell modeling framework was also used in the case of nanowires (Chen, Shi, Zhang, Zhu, & Yan, 2006). The main difficulty of all these models is related to a valid description of the grain boundary phase(s) and quantification of its volume fraction.

Differently than in the case of coarse-grained materials, in the case of nano-grained polycrystals the use of full-field simulations based on continuum theory for the purpose of verification or calibration of the above-discussed models is questionable. Therefore atomistic simulations based on molecular dynamics are performed to assess the elastic moduli and strength of such materials (Chang, 2003; Choi, Park, & Hyun, 2012; Fang, Huang, & Chiang, 2016; Gao et al., 2013; Mortazavi & Cuniberti, 2014; Schiøtz, Vegge, Di Tolla, & Jacobsen, 1999). An alternative approach is to use refined constitutive models, for example those incorporating scale effects through gradient enhancements, within the framework of FEM calculations (Kim, Dolbow, & Fried, 2012).

In atomistic simulations of elastic properties, usually only the tensile Young's modulus is determined, see e.g. Gao et al. (2013); Schiøtz et al. (1999). It is observed that this modulus decreases with a decreasing grain size. This tendency is qualitatively and quantitatively reproduced by two- or multi-phase micromechanical models after proper adjustment of the grain boundary stiffness and the volume fraction, e.g. (Gao et al., 2013; Jiang & Weng, 2004; Ramtani et al., 2009).

The goal of the present paper is to estimate the effective elastic properties of nanocrystalline copper taking the anisotropy of a single crystallite fully into account. To this end, a series of static molecular simulations are performed to find all 21 components of the stiffness tensor and an anisotropic mean-field core-shell model of a nanograined polycrystal is formulated within the continuum mechanics framework. The results of both approaches are compared.

The paper is constructed as follows. The next section describes the details of the performed atomistic simulations. Section 3 presents the proposed formulation of the two-phase model of a nano-grain polycrystal. Additionally, the isotropisation procedure is outlined for the anisotropic stiffness acquired in the simulations. Section 4 discusses the results of the atomistic simulations and compares their outcomes with the respective mean-field estimates. The paper is closed with conclusions.

2. Computational methods

All molecular simulations were performed using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) (Plimpton, 1995) and a scientific visualization and analysis software for atomistic simulation data OVITO was used to visualize and analyse simulation results (Stukowski, 2010). Due to interest in the static behavior of the material, the molecular statics (MS) approach at the temperature of 0K (Maździarz, Young, Dłuzewski, Wejrzanowski, & Kurzydłowski, 2010; Maździarz, Young, & Jurczak, 2011; Tadmor & Miller, 2011) was used, which is more appropriate in such cases than molecular dynamics (MD). Copper is metal arranged in a face-centered cubic (FCC) structure. The potentials based on the Embedded Atom Model (EAM) have been successful in the description of many metallic systems (Tadmor & Miller, 2011). For analysed FCC copper, the well known EAM potential parametrized by Mishin, Mehl, Papaconstantopoulos, Voter, & Kress, 2001) and taken from NIST Interatomic Potentials Repository (Becker, Tavazza, Trautt, & de Macedo, 2013) was utilized. This potential