EXTENSION OF ANISOTROPIC CORE-SHELL MODEL TO HCP NANOCRYSTALLINE METALS

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Summary Anisotropic core-shell model of a nano-grained polycrystal is extended to estimate the effective elastic stiffness of several metals of hexagonal crystal lattice symmetry. In the approach the bulk nanocrystalline metal is described as a two-phase medium with different properties for a grain boundary zone and a grain core. While the grain core is anisotropic, the boundary zone is isotropic andthe shell has a thickness defined by the *cutoff radius* of a corresponding atomistic potential for the considered metal. The predictions of the proposed mean-field model are verified with respect to simulations performed with the use of the Large-scale Atomic/Molecular Massively Parallel Simulator, the Embedded Atom Model, and the molecular statics method. The effect of the grain size on the overall elastic moduli of nanocrystalline material with random distribution of orientations is analysed.

INTRODUCTION

A class of nanostructured material is considered that is composed of equiaxed nanometre-sized building blocks - crystallites of the same chemical composition and with a characteristic dimension smaller than 100 nm, which differ only by the crystallographic orientation. In such nanostructured material two main phases are distinguished: the grain core and the grain boundaries. The effect of grain boundary zone on the overall properties of a bulk polycrystal is the more significant the smaller is a grain size. Usually at the macroscale level the stress-strain response of nanocrystalline metals is governed by the continuum mechanics theory, and the mean-field estimates are still in use for assessing the bulk properties of nanocrystalline metals. Because of different properties of a grain boundary zone and the grain core, for nano-grained polycrystals two-phase or multi-phase mean-field frameworks are formulated (see [1] for an extensive review).

MODEL FORMULATION

In [1] a two-phase model of elastic nanocrystalline material was formulated in two variants called the Mori-Tanaka(MT) and self-consistent (SC) core-shell model, respectively. As inspired by earlier works [2], an additional phase that forms an *isotropic* coating around the *anisotropic* grain core is introduced. The smaller is the grain this transient zone influences more on the effective properties of polycrystal (Fig. 1). The estimates of overall stiffness by a two-phase model presented in the next section are obtained under the assumption that representative volume element contains infinite set of orientations of random uniform distribution. Under such assumption the overall stiffness tensor $\bar{\mathbf{C}}$ is isotropic and specified by an overall bulk modulus $\bar{K}$ and a shear modulus $\bar{G}$. The effective stiffness $\bar{\mathbf{C}}$ is calculated by embedding the coated grain in the infinite medium of the stiffness $\mathbf{C}_\mathrm{m}$ and next using the procedure of the double-inclusion model, namely

$$\bar{\mathbf{C}} = \left[f_0\mathbf{C}_\mathrm{s}\mathbf{A}_\mathrm{s} + (1-f_0)\left\langle \mathbf{C}(\phi^c)\mathbf{A}(\phi^c)\right\rangle_{\mathcal{O}}\right]\left[f_0\mathbf{A}_\mathrm{s} + (1-f_0)\left\langle \mathbf{A}(\phi^c)\right\rangle_{\mathcal{O}}\right]^{-1} \tag{1}$$

where

$$\mathbf{A}(\phi^c) = (\mathbf{C}(\phi^c) + \mathbf{C}_*(\mathbf{C}_\mathrm{m}))^{-1}(\mathbf{C}_\mathrm{m} + \mathbf{C}_*(\mathbf{C}_\mathrm{m}))\,, \quad \mathbf{A}_\mathrm{s} = (\mathbf{C}_\mathrm{s} + \mathbf{C}_*(\mathbf{C}_\mathrm{m}))^{-1}(\mathbf{C}_\mathrm{m} + \mathbf{C}_*(\mathbf{C}_\mathrm{m}))\,, \tag{2}$$

$\langle\cdot\rangle_{\mathcal{O}}$ denotes averaging over the orientation space and $\mathbf{C}_*(\mathbf{C}_\mathrm{m})$ is the Hill tensor depending on the stiffness $\mathbf{C}_\mathrm{m}$ of infinite matrix and the shape of the coated grain, which is assumed as spherical in the present study. For the MT variant of the core-shell model $\mathbf{C}_\mathrm{m} = \mathbf{C}_\mathrm{s}$ is assumed, while for the SC variant $\mathbf{C}_\mathrm{m} = \bar{\mathbf{C}}$. In formula (1) f_0 is the volume fraction of the transient zone. Assuming the spherical shape of coated grains and denoting by Δ the coating thickness, f_0 is calculated by the formula

$$f_0 = 1 - \left(1 - \frac{2\Delta}{d}\right)^3\,, \tag{3}$$

where d is an averaged grain diameter. The parameter Δ introduces the size effect to the model. In [1] it was demonstrated that Δ can be taken as equal to the *cutoff radius* of the atomistic potential valid for the considered metal. Tensor $\mathbf{C}(\phi^c)$ is the anisotropic local elastic stiffness tensor for the single and depends on the crystal orientation. For cubic crystals studied in [1, 3] it is given by three material parameters For the considered hcp crystals it exhibits transverse isotropy and is specified by 5 independent components, which are the material-specific constants.

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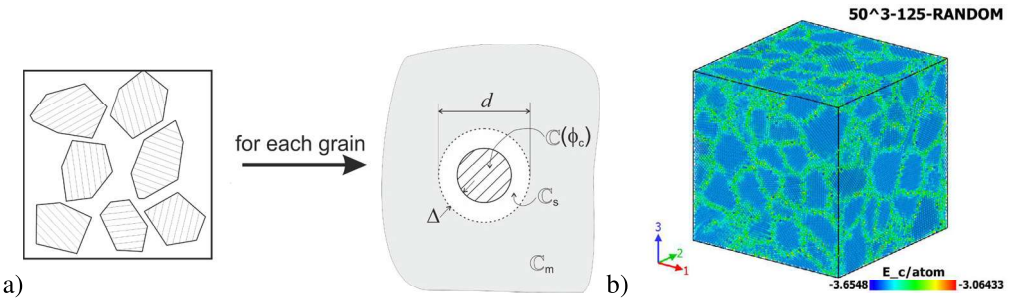

Figure 1: (a) Schematic of a core-shell model, (b) the example of a nanocrystalline sample considered in atomistic simulations.

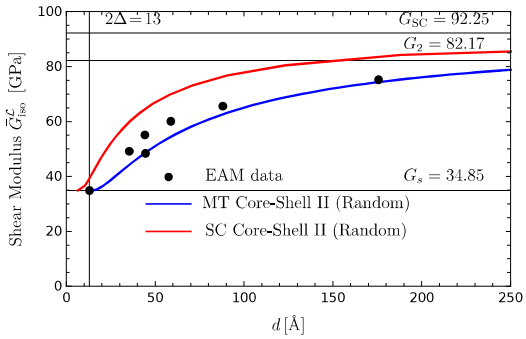

Figure 2: Effective shear modulus - $\bar{G}^{\mathcal{L}}_{\text{iso}}$ as a function of the average grain diameter d obtained by the two variants of the core-shell model - comparison with the results of atomistic simulations for Co.

RESULTS

Predictions of the mean field core-shell model will be compared with the results of atomistic simulations for 6 metals of hexagonal (hcp) lattice symmetry: Co, Zr, Mg, Re, Ti and Ru. The results are obtained by molecular statics using the corresponding EAM potentials taken from the literature [4] and then are analysed and visualized with the Open Visualization Tool OVITO [5]. The methodology for generating polycrystal samples by the Voronoi tessellation method, their pre-relaxation and numerical simulations were described in [1]. In particular, the samples with a different number of atoms per grain are generated, enabling to study the effect of grain size on the elastic stiffness. 21 components of stiffness tensor, of all pre-relaxed structures were computed by the stress-strain method with the maximum strain amplitude set to be 10^{-4}. Using the Log-Euclidean norm the closest isotropic approximation of the obtained tensor is found [1].

There is a known problem at the nano level with how to assume local effective material parameters for the boundary zone between atomistic layers in the local continuum approach (here, K_s and G_s values). Following [3], it is here proposed that elastic properties for the shells themselves are obtained by reducing the size of some generated polycrystal samples, so that the fraction of transient shell atoms is close to unity, $f_0 \to 1$.

Fig. 2 presents the preliminary results obtained for Co nanocrystalline bulk material. Elastic shear moduli obtained by the atomistic simulations and the core-shell model are compared. Good accordance of both predictions, especially fo rthe MT variant, is seen.

CONCLUSIONS

The two-phase core-shell model could provide reliable predictions of elastic properties of nanorystalline metals of hexagonal lattice symmetry. Variation of elastic bulk and shear modulus of polycrystals with random orientation distribution with a grain size is well reproduced as compared to the results of atomistic simulations.

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