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Micromechanical modelling of nanocrystalline and ultrafine grained metals: A short overview

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ABSTRACT

An overview of micromechanical models of strength and deformation behaviour of nanostructured and ultrafine grained metallic materials is presented. Composite models of nanomaterials, polycrystal plasticity based models, grain boundary sliding, the effect of non-equilibrium grain boundaries and nanoscale properties are discussed and compared. The examples of incorporation of peculiar nanocrystalline effects (like large content of amorphous or semi-amorphous grain boundary phase, partial dislocation GB emission/glide/GB absorption based deformation mechanism, diffusion deformation, etc.) into the continuum mechanical approach are given. The possibilities of using micromechanical models to explore the ways of the improving the properties of nanocrystalline materials by modifying their structures (e.g., dispersion strengthening, creating non-equilibrium grain boundaries, varying the grain size distributions and gradients) are discussed.

1. Introduction

During recent decades, growing interest of scientific community has been attracted to the nanostructured materials. The expectations on nanostructuring as a way to enhance material performances and to improve competing materials properties are very high, and some of them have been delivered, indeed.

The extraordinary properties of nanocrystalline and ultrafine grained metallic materials (i.e., materials with the grain sizes of the order of several to several hundred nanometers) include superductility at room temperature, high hardness and high strength to hardness value (which might be 2…7 times higher than in coarse grained materials), lower elastic modulus, negative Hall–Petch slope, enhanced strain rate sensitivity and difference between tensile and compression response [1–5]. The yield strength of nanocrystalline materials can be up to 5…10 times higher than of coarse-grained materials [6]. Other peculiar effect of nanocrystalline materials are the deviation from Hall–Petch relation at ultrafine and nanoscale grain sizes (below 100 nm), which goes into negative Hall Petch slope at about 10 nm, as well as asymmetry of tensile and compressive behaviour and enhanced diffusion properties [7].

In order to predict the service properties of the materials and to explore the potential and reserves of their improvement, computational models linking the macroscale (service) properties and nanoscale structures are necessary. While the atomistics/molecular dynamics seem to be most natural approach to simulate the nanoscale effects and behaviour, they are limited in time and size scales [5], and can be hardly linked to real service conditions (long term loading of large size parts). That is why the continuum mechanical/micromechanics methods attracted the interest of specialists in nanomaterials as a tool for the computational analysis of service properties and usability of the materials.

Still, the continuum mechanical/micromechanical models of materials are based on the inherent assumptions about the large scale difference between the structural elements (atoms, dislocations, polymer chains) and the considered volume, as well as underlying physical mechanisms and homogeneity of deformation (role of dislocations, e.g.). Thus, micromechanical modelling of nanomaterials in fact pushes the borders of traditional continuum mechanics seeking to incorporate non-mechanical, physical effects into the purely mechanical concept.

In some cases, coupling methodologies are employed to combine atomistic and continuum models. Among the different approaches which combined continuum mechanics approach with atomistic modelling, one may mention FEAt by Kohlhoff and collaborators [8], Quasicontinuum (QC) method by Tadmor and colleagues [9–11], coarse-grained molecular dynamics (CGMD) by Rudd and Broughton [12], molecular–atomistic-ab initio dynamics (MAAD) by Broughton et al. [13], and the bridging scale decomposition (BSD) by Wagner and Liu [14]. Among the challenges of

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coupling approaches, one should mention the problem of linking regions and overlap area as well as fictitious boundary effects, due to inconsistencies in the formulation of the potential energy [15]. The coupled methods make it possible to introduce the physically based materials parameters or laws into micromechanical models.

In this paper, we present an overview of micromechanical models of nanocrystalline and ultrafine grained materials, their mechanical behaviour, deformation and strength. Composite models, crystal plasticity based models, grain boundary sliding, the effect of non-equilibrium grain boundaries, etc. are reviewed. The main constraints and challenges in the considered models are discussed.

2. Composite models of nanocrystalline metallic materials

The main structural feature of nanocrystalline and ultrafine grained materials, apart from the small grain sizes, is the high relative volume of grain boundary surface phase. According to Gleiter [1], the differences between the properties of nano – and coarse structured materials are determined by both the low dimensions of grains and the high volume content of the boundary surface phase in nanomaterials. Suryanarayana [16] noted in his review that "nanocrystalline metals can be considered to consist of two structural components – the numerous small crystallites and a network of intercrystalline region" (Fig. 1a shows a real microstructure of ultrafine grained aluminium; Figs. 1bc and 2 show several examples of the unit cell models of nanocrystalline materials).

The relatively thick "grain boundary phase" layers between nanograins led some researchers to the idea to use "composite model" to simulate the deformation behaviour of nanocrystalline material (e.g., two-phase or even three-phase model of a nanocrystalline material, with grains and boundaries, as phases). The easiest approach of micromechanics, based on the rule-of-mixture, has been transferred to the nanocrystalline materials [19,20].

One of the earliest modelling approaches to the analysis of strength of nanomaterials based on the rule-of-mixture was suggested by Carsley et al. [21]. A material is considered as consisting of two phases: squared grains with bulk properties and the boundary phase, which represent a metallic (amorphous) glass material. With this model, Carsley and colleagues studied the grain size softening in nanocrystalline nickel, iron and copper, and observed the change in the Hall–Petch slope at small grain sizes.

Kim, Estrin and colleagues [22–25] applied the rule-of-mixture for two-phase composite (crystalline phase and a grain-boundary phase) to study the plastic deformation and grain size dependence of nanocrystalline metals. Kim developed a micromechanical (cubic unit cell) model of a nanostructured material [22] consisting of a crystallite, boundary phase and triple line junctions (see Fig. 2a). The diffusional (Coble creep and Nabarro-Herring creep) deformation mechanisms were taken into account in the model, as well as the non-crystallographic dislocation glide (only for the grain interior). The grain boundary deformation, controlled by diffusional mechanisms is described as viscous Newtonian behaviour. Viscoplastic constitutive laws, including the dislocation density evolution and diffusion creep (boundary diffusion and lattice diffusion mechanisms) were used for the phases. Inverse Hall–Petch behaviour at low strain rates, when both phases deformation is controlled by diffusion mechanisms, was observed. A composite model with cubic unit cells with four sides and 2 horizontal layers of GB and the cube of grain inside was developed by Zhou et al. [26]. The deformation behaviour of grain interior was described by rate independent plasticity with isotropic hardening law. The deformation of grain boundaries was described by Drucker constitutive equation.

Another version of the composite model is based on the presentation of the "grain boundary phase" as sharp grain boundary surrounded by "grain boundary affected zone" (GBAZ) with varied properties (instead of presenting it as isotropic and homogeneous composite matrix). This concept was proposed by Schwaiger et al. [27], who used a model with two-dimensional grains of hexagonal shape separated by the "grain-boundary affected zone (GBAZ)" (considered as softer "region adjoining the grain boundaries in NC (nanocrystalline) metals where the crystalline lattice is elastically strained despite the ostensible absence of any point defects"). Assuming GBAZ thickness to be 7–10 lattice parameters, and linear hardening constitutive behaviour for the grain interior and the GBAZ, Schwaiger and colleagues simulated the strain-rate sensitivity of nanocrystalline nickel.

On the basis of Schwaiger et al. [27] model, Li and Weng [6] developed a secant-viscosity composite model, where the phases follow unified viscoplastic constitutive law, while the yield stress of grain interior depends on the grain size. The model was applied to predict the strain-rate effect and grain-size dependence of a nanocrystalline nickel.

The main achievement of rule-of-mixture models of nanocrystalline materials consists in the introduction of physical, dislocation density or diffusion based constitutive law of grain boundary phases into the model, and combining it with grain size dependent plasticity for grain interior. This allowed to simulate the inverse Hall–Petch effects and to determine the critical grain sizes even using very simple, cubic micromechanical models.

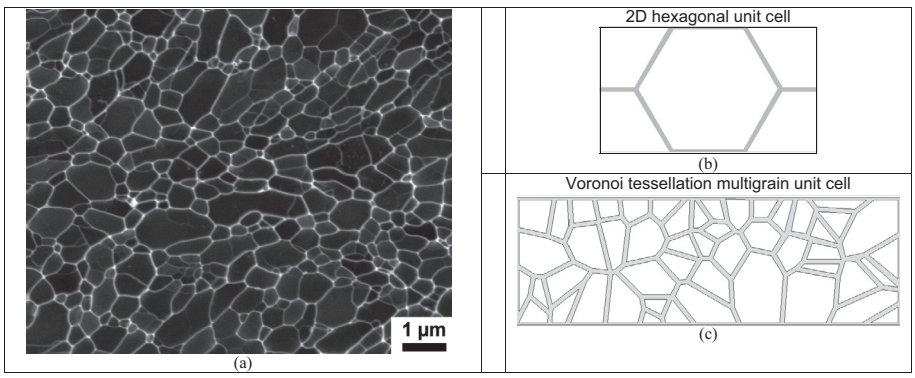

Fig. 1. Real microstructure and unit cell models: (a) Microstructure of heavily deformed commercial purity aluminium [9] revealed using gallium enhanced microscopy [17,18] (courtesy of O.V. Mishin). (b) Hexagonal unit cell idealization, with finite thickness grain boundaries, (c) Voronoi tessellation unit cell, with finite thickness grain boundaries [31].