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# Non-equilibrium grain boundaries in titanium nanostructured by severe plastic deformation: Computational study of sources of material strengthening

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ABSTRACT

A computational model of ultrafine grained (UFG) or nanostructured titanium (Ti), based on a finite element (FE) unit cell model of the material and a dislocation density based model of plastic deformation has been developed. FE simulations of tensile deformation of UFG Ti with different fractions and properties of the grain boundary (GB) phase have been carried out. The effect of different degrees of deviation from the equilibrium state of the grain boundaries (GBs) on the mechanical behaviour of nanostructured Ti have been investigated using the combined composite/dislocation dynamics based model. In particular, the effects of different diffusion coefficients in the GB phase, of a high initial dislocation density in the grain boundaries, as well as of atomic scale precipitates are investigated for affecting the deformation behaviour of UFG or nanostructured Ti.



## 1. Introduction

Nanostructuring of Ti represents a promising method for improving its mechanical properties. Various methods of severe plastic deformation (SPD) have been successfully applied for grain refinement in pure Ti [1–7]. The deformation mechanisms in ultrafine grained and nanostructured metals are different from those of conventional coarse grained metals. From several investigations [1–3], it has been concluded that it is the grain boundary phase (or the regions with changed properties close to the grain boundaries) which determines the unusual properties of nanostructured materials and represents an important resource for the improvement of the mechanical properties of these materials.

In this paper, the effect of the grain boundary phase induced by severe plastic deformation on the mechanical properties of nanostructured Ti is investigated. A series of computational models of materials nanostructured by SPD is developed which take into account plastic deformation by dislocations and allow analysing various non-equilibrium (NE) effects of the grain boundaries. Having established these models, one can explore the possibilities for improving the technologies for nanostructuring.

## 2. State-of-the art: computational modelling of nanostructured and UFG metals

There exist a number of models of mechanical behaviour of nanostructured and ultrafine-grained metals linking their microstructures with their mechanical properties — among them, molecular dynamics simulations [8], studies of dislocation kinetics for the mechanical behaviour of nanostructured metals [9], polycrystal plasticity models [10,11], visco-plastic self-consistent polycrystal plasticity model [12], models coupled with disclination-based grain subdivision criteria [13–16], grain boundary (GB) sliding models [17,18], and so on.

Many of the computational models for nanostructured metals are based on the "composite" model, in which the grain interior (GI) and the GB phase are considered as two different phases [19–24]. Suryanarayana [19] noted that "nanocrystalline metals can be considered to consist of two structural components – the numerous small crystallites … and a network of intercrystalline region". A number of micromechanical (composite) models of nanostructured materials have been developed, among them, the "rule of mixture" model [20], a unit cell model with the phase mixture approach and a three phase model (crystallite, GB phase and quadruple line junctions) [21,22], elasto-plastic self-consistent models based on Christensen and Lo [25] approach [26,27], a 3D Voronoi tessellation based self-similar unit cell with constant GB thickness [28], a hexagonal grain with rate-sensitive GB affected zone (GBAZ) model [29], a number of composite models with GB

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sliding effects [27,30,31] and so on. Generally, the composite models of nanostructured materials provide an efficient approach to the analysis of the mechanical properties of nanometals. Still, the correct description and modelling of the peculiar behaviour of grain boundaries (GBs) represent an open challenge. The interesting point is that the geometrical features (like walls and obstacles) of the nanostructured materials are sometimes included directly at the level of micromechanical models, and sometimes introduced indirectly into the dislocation evolution equations.

In the work presented here, the geometrical features are represented in a micromechanical model and do not enter the dislocation evolution equations of the individual phases. With the developed composite model of UFG Ti the effect of the GB phase, in particular, possible deviation from equilibrium, on the mechanical properties of the materials is analysed.

## 3. Computational model of UFG Ti

### 3.1. FE unit cell model

In this work, UFG Ti, produced by SPD with grain sizes of the order of 50–250 nm is studied. The GB structure evolves during SPD from a deformation structure [32]. Based on the analysis of transmission electron micrographs of UFG Ti, it is suggested to idealise a typical Ti grain as regular hexagon with its main axis aligned with the tensile direction. In this manner the structure appears elongated along the tensile axis despite being composed of equiaxed grains.

In several studies of UFG materials [e.g. 33] it was demonstrated that some regions of the grains adjacent to the GBs demonstrate changed properties. The width of these layers with changed properties around the GB is of the order of 6...8 nm more or less independent of the grain size for grain sizes in the range from 50 to 200 nm [33]. This width includes both the "true" GB and the layer of material with changed mechanical and diffusional properties near the "true" GB layer. In the performed simulations, these layers together with the real GBs will be considered as kind of a representative "GB phase" with a thickness $t$ of 7 nm.

The unit cell model (with periodic boundary conditions) is presented in Fig. 1. The grain size $D$ of the hexagonal grains is taken here as twice the length of a side of a hexagon or equivalently the longest chord length i.e. the distance between the centres of triple junctions as shown in Fig. 1. The area fraction of the GBs is directly calculated from the ratio between the area of the hexagonal grain interior and the total grain area

$$f = 1 - \left(1 - \left(\frac{2t}{\sqrt{3}D}\right)\right)^2 = 2\left(\frac{2t}{\sqrt{3}D}\right) - \left(\frac{2t}{\sqrt{3}D}\right)^2. \quad (1)$$

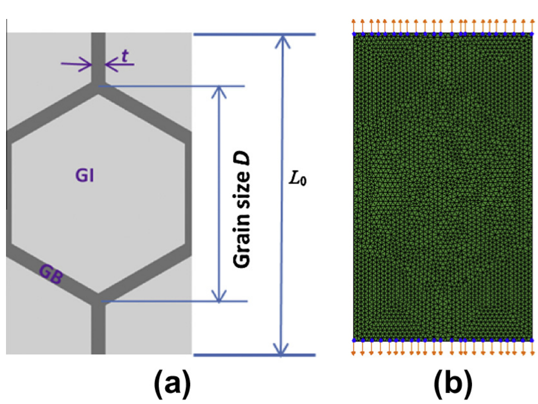


**Fig. 1.** Unit cell model of UFG Ti: (a) GB (dark grey) and GI (light grey) and (b) FE mesh and loading conditions.

6-Node modified quadratic plane strain triangle elements are used to generate the FE mesh of the model. Prescribed displacements (tensile, uniaxial) are applied on both ends of the plate. The nodes on the vertical borders are connected and linked in a set so that the vertical borders move only as a straight line. As a consequence of the boundary condition, the unit cell cannot reflect necking behaviour and the simulations of the work-hardening behaviour can be continued even beyond the potential failure in tensile tests when the Consider criterion is met. The size of the plate is 375 nm × 216 nm, except for the cases for which the dimensions are varied. The simulations are carried out using the commercial FE code ABAQUS Explicit. The subroutine used to calculate the dislocation evolution in grain boundaries and in grain interiors is discussed in the following section.

Uniaxial tensile loading is realised by increasing the prescribed displacements at both ends with constant velocity $v$. In this manner, a nominal strain rate $\dot{\varepsilon} = 2v/L_0$ (where $L_0$ is the length of undeformed plate) is obtained whereas the true strain rate decreases with proceeding deformation. Instead of prescribing the constant velocity instantaneously, the velocity is increased linearly through an initial loading phase in order to avoid undesired oscillations in the numerical results.

### 3.2. Dislocation density based model of UFG Ti deformation

In this section, the evolution equations for the dislocation density in GBs and GIs of UFG Ti are derived. Only quasi-static deformation is considered. It has been experimentally observed [32,33], that at low deformation rates and room temperature the major deformation mode in nanostructured Ti is dislocation slip. TEM examinations in quasi-statically deformed samples revealed twinning only at larger strains. For high strain rates or at lower temperatures however twinning is observed in nanostructured Ti [34]. While twinning is typical for deformation of coarse grained Ti, e.g. [35], it was observed only during the initial stages of severe plastic deformation (as the first or maximal the second pass of ECAP). During later stages only dislocation slip was observed both locally (by TEM) and macroscopically (by texture determination) [36]. Consequently, in the nanostructured state one may neglect twinning in Ti during quasi-static deformation and safely assume that the deformation of UFG Ti is controlled by dislocation glide. Similarly, deformation by partial dislocations as observed in simulations for high strain rates will not be considered.

When combining a micromechanical geometric FE model with dislocation density based evolution equations accounting for the plastic deformation in the material, the evolution equations for the dislocation density must be formulated on a local level. Essentially, the evolution of the dislocation densities in FEs located in the GI do not "know" about the availability and properties of GBs and must not require any information about the deformation behaviour of the GBs other than the caused stress fields (and vice versa); the local evolution equation of the dislocation density is affected only by the local stress fields, the local strain rate, local properties and conditions.

The dislocation density at any point will be changed only by accumulation of additional dislocations or by dislocation annihilation [39,38]. Local storage of dislocations results from the local flux of mobile dislocations carrying the plastic deformation and hence the local plastic strain rate. Dislocation accumulation in GBs and GIs must therefore follow the evolution equations [39]:

$$\frac{d\rho_{GI}}{dt} = k_{GI}\sqrt{\rho_{GI}}\dot{\varepsilon}_{GI} \quad \frac{d\rho_{GB}}{dt} = k_{GB}\sqrt{\rho_{GB}}\dot{\varepsilon}_{GB} \quad (2)$$

$$\frac{d\rho_{GI}}{d\varepsilon_{GI}} = k_{GI}\sqrt{\rho_{GI}} \quad \frac{d\rho_{GB}}{d\varepsilon_{GB}} = k_{GB}\sqrt{\rho_{GB}} \quad (3)$$