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Gradient ultrafine-grained titanium: Computational study of mechanical and damage behavior

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Abstract

A computational model of ultrafine-grained (UFG) titanium with random and gradient distribution based on Voronoi tessellation and the composite model of nanomaterials is developed. The effect of grain size, non-equilibrium state of the grain boundary phase (characterized by the initial dislocation density and diffusion coefficient) and gradient of grain sizes on the mechanical behavior and damage initiation of the UFG titanium are studied in numerical experiments. Using computational experiments, the authors determined the likely damage criterion (dislocation-based model) and found several effects that can positively influence the mechanical response and strength of UFG titanium (homogeneity of grain sizes, dispersoids/precipitates in grain boundaries and initial dislocation density in grain boundaries). It is shown that the homogeneous structures of UFG titanium ensure higher yield stress and lower likelihood of damage than gradient structures. The availability of dispersoids or precipitates in UFG titanium changes its damage mechanisms and delays the evolution of damage.

Keywords: Ultrafine-grained titanium; Non-equilibrium grain boundary; Dislocation density; Finite element simulation

1. Introduction

Titanium is a very promising material for dental and other implants, yet the high requirements of implant properties have led to calls to enhance the properties of titanium, using nanostructuring and, in particular, severe plastic deformation (SPD) technology. Nanostructuring technology allows the fabrication of materials that differ from neat coarse-grained material not only in their grain sizes, but also in a number of other structural features [1–9]. The peculiarity most often mentioned is the high content of grain boundaries (GB) in nano-grained and ultrafine-grained (UFG) material. Another peculiarity of UFG and nano metals (which provokes wide discussion) is the non-equilibrium state of these GB [4,6]. Further, the real nanostructuring technologies cannot always ensure ideally homogeneous structures. Rather, the regions with smaller and larger grains are observed in nanomaterial.

Thus, the question arises: how do the peculiarities of the structures of UFG and nanomaterials influence their mechanical properties and strength, both taken alone and in combination? The goal of this paper is to investigate the effect of the content of GB, non-equilibrium state of GB, inhomogeneous gradient distribution of grains and availability of precipitates in UFG titanium on its mechanical behavior and strength.

To do this, the authors developed a series of computational micromechanical models of UFG Ti, based on Voronoi tessellation and taking into account the dislocation mechanisms of deformation. Varying the grain sizes, grain distributions, diffusion coefficients and dislocation density in GB as well as the degree of structural gradient and precipitate distribution, the authors analyzed the effect of the

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structure of UFG Ti on the mechanical properties and damage initiation.

2. Computational model of deformation and damage of UFG nanotitanium

2.1. Micromechanical modeling of nano- and UFG materials: a short overview

Various approaches are used to simulate the properties of nanostructured and UFG metals, among them molecular dynamics, polycrystal plasticity, dislocation and disclination evolution analyses [10–15]. The advantage of continuum mechanical methods over "physical" methods is that the continuum mechanical models of nanomaterials can easily be linked to the macroscale models of machines and parts, which allow the service properties of products made from nanomaterials to be estimated. In order to model nano- and UFG materials in the framework of continuum mechanics, composite models are often used, where nanomaterials are presented as multiphase composite material, with grain interior (GI), GB phase, triple junctions and pores as different phases.

Table 1 gives an overview of some composite models of nanomaterials. While a composite model of nanostructured materials provides an efficient approach to the analysis of the mechanical properties of nanometals, the correct description and the proper modeling of the peculiar behavior of GB represent an open challenge. The interesting point is that geometrical features (such as boundaries and obstacles) of nanomaterials are sometimes included in composite models at the level of micromechanical models, and sometimes introduced into the dislocation evolution equations.

2.2. Unit cell: Voronoi tessellation with GB of given thickness

In order to represent the nanomaterials' structure, Voronoi tessellation with GB layers was used. As discussed in Refs. [6,7], the thickness of GB for UFG materials (including the "true" GB and the regions of grains adjacent to GB, with changed properties) can be taken as constant, and assumed to be 7 nm (as a first estimation).

The micromechanical finite element (FE) models of UFG materials were generated as follows. First, the MATLAB function voronoi(x,y) was used to generate the Voronoi tessellation of a unit cell. The coordinates of vertices of the Voronoi cells and connectivities were outputted in a text file. With the specially developed FORTRAN program, GB layers of constant thickness were generated along all the borders between cells. The program produced a script file (.scr), which can be read by AutoCAD. The script file includes all the coordinates of the vertices of new Voronoi cells and the connectivity of each new Voronoi cell. In AutoCAD, the script files are run and, as a result, the new Voronoi cells with GB of given thickness are generated. This transformation allows easy and quick modification of the unit cell from ideal Voronoi tessellation to the tessellation with GB. The model is then saved in DXF format and read by ABAQUS. The code developed also allows the calculation of the area fraction of GB, as well as variation in the GB thickness in the model.

2.3. Gradient Voronoi models

In a further series of unit cell models, gradient Voronoi models of nanomaterial with finite thickness GB were generated. In order to generate the gradient Voronoi structures, a FORTRAN program was written. The program first generated the coordinates of the seeds according to the following rule: the horizontal coordinates of each point were uniformly distributed random values (in the range from 0 to the plate width). Vertical coordinates of the points were normally distributed random values, in the range from zero (lower border of the plate) to the upper border. The average of this Gaussian distribution was taken as 0 (i.e. the lower plate border coordinate) and the standard deviation value (called "disperse") was a parameter characterizing the type of gradient. (The algorithm is presented in more detail elsewhere [28].) Small standard deviations (i.e. much smaller than the plate length) mean highly localized distributions of points in the lower region of the plate (i.e. high gradient materials, with very small grains in the lower region and large grains in the upper region). The large standard deviation (i.e. comparable with the plate length) means that the points are distributed over the plate almost uniformly, and, thus, the grain distribution is almost homogeneous. Fig. 1 shows the schema of the seed generation. The seed array was used to generate the coordinates of the vertices of the Voronoi cells and connectivities, and the FE models were generated as described in Section 2.2.

The models were discretized with FE CPE3 (a 3-node linear plane strain triangle). The displacement was applied to the upper and lower horizontal ends of the plates, with a nominal strain rate $0.2\ s^{-1}$. The nodes on the vertical borders were connected and linked in a set so that the vertical borders moved only as a straight line. The simulations were carried out using the commercial FE code ABAQUS Explicit.

2.4. Dislocation density-based modeling of deformation of GB and GI

The deformation of UFG titanium under static loading is controlled by dislocation slip, movement and accumulation. While twinning can play a role for coarse-grained titanium, or at large strains and dynamic loading, it can be neglected in first approximation for the quasi-static loading of UFG titanium [6].

As noted in Ref. [6], the evolution equations for the dislocation density in a composite model of nanomaterials