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A three-dimensional multi-scale polycrystalline plasticity model coupled with damage for pure Ti with harmonic structure design

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ABSTRACT

In this paper, we developed, on the basis of the crystalline plasticity and homogenization method, a three-dimensional multi-scale numerical model to simulate the non-linear and damage behaviors of pure titanium with harmonic structure (HS). The theoretical approach couples a kinematic hardening law for slip systems in the Ti hexagonal crystals; the consideration of the grain size effect modulated by the Hall-Petch law; a special localization-homogenization procedure to allow transforming the microscopic hardening law into the macroscopic constitutive law and avoiding the microstructure meshing of the grains in a bimodal grain distribution; and finally, the Lemaître-Chaboche macroscopic ductile plastic damage model in order to describe the granular damage. This model was implemented into a finite element code by means of the User Defined Material files. The results of the numerical simulation show that the proposed model can predict the crystalline plasticity behavior efficiently for bimodal HS Ti. Moreover, the computing time is optimized and reduced to a very low level.

1. Introduction

A good combination of strength and ductility is a request for many industrial applications. Unfortunately, strength and ductility are antinomies in conventional metallurgy. Thanks to grain refinement processing routes the strength of metallic material can largely be improved (Meyers et al., 2006; Khan et al., 2008; Estrin and Vinogradov, 2013; Okamoto et al., 2014; Ivanisenko et al., 2014 etc.).

However, in most cases, homogeneous ultrafine-grained (UGF) microstructures exhibit improvement in strength but at the expense of ductility (Ma, 2003; Meyers et al., 2006; Dao et al., 2007; Tsuji et al., 2008). As extreme examples nanograined (NG) materials (having grain size lower than 100 nm) are usually reported to exhibit quasi-brittle mechanical properties as they display with very high strength but poor homogeneous deformation. In order to overcome this weakness, research groups (Wang and Ma, 2004; Fujiwara et al., 2008; Dirras et al., 2010 etc.) proposed bimodal grain size distribution strategies for various metallic materials by use of conventional and non-conventional metallurgical routes, such as powder blending and sintering or plastic deformation followed by heat treatments.

Titanium and titanium alloys are excellent candidates for aerospace applications (Boyer, 1996; Leyns and Peters, 2003) or in the biomaterials field (Geetha et al., 2009), owing to their high strength to weight ratio and excellent corrosion resistance. Controlling the amount ω and α phases by thermo-mechanical processes usually strengthens β-titanium alloys. Grain-size refinement process, either by severe plastic deformation alone or combined with cryo-milling, has been used as a means improve the mechanical

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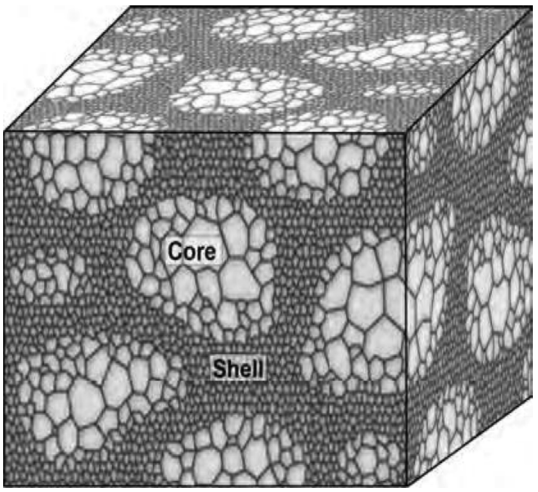

Fig. 1. A schematic illustrating the harmonic structure design (Vajpai et al., 2016).

properties of pure titanium (Ahn et al., 2010; Balasundar et al., 2009; Hong and Hwang, 2012; Kim et al., 2011). Unfortunately, a poor to limited ductility usually mitigate the observed gain in strength (Moskalenko et al., 2017).

As further attempts, several design processes have been proposed to level off mechanical properties of titanium alloys based on twinning-induced plasticity (TWIP) and transformation induced plasticity (TRIP) effects (Ahn et al., 2010; Marteleur et al., 2012) similar to those observed in steels.

Recently the concept of harmonic structure (HS) was proposed by Ameyama and co-workers and successfully applied to titanium and its alloys (Ameyama et al., 2012; Ciuca et al., 2013; Ota et al., 2014). The harmonic structure has a specific topological grain size distribution between the ultrafine and coarse phases, which allows improving the material strength while keeping the material ductility. Schematically, the harmonic structure has a 3D network structure of continuously connected matrix called “shell” with ultrafine grains and dispersive cells formed from a certain number of coarse grains called “core” (Fig. 1). This makes them special and different compared to heterogeneous “nano-micro” bimodal microstructures that are usually produced via various conventional metallurgical processes. High strength without ductility loss has been reported under tensile loading at room temperature of pure Ti (Vajpai et al., 2016).

However, even though the processing and characterization of the titanium alloy with HS design have been well progressed, the effective numerical models have not yet been satisfactorily developed. It is clear that numerical and theoretical studies are needed to assess the mechanisms of the deformation and damage of the materials with HS design. Combined with experimental observations, quantitative information on damage mechanisms at the microscopic level can be obtained. From a theoretical point of view, direct numerical simulation allows detailed description and quantitative prediction on the deformation and damage evolution. In addition, numerical simulations give the necessary feedback that could help to improve and optimize the microstructure design.

The research works on numerical simulations and modeling of the HS materials are still scarce in the available literature. Yu et al. (2015) have conducted multi-scale finite element analysis on deformation behavior of SUS304L with HS design by simulating the core region with truncated octahedrons. In the work of Vajpai et al. (2016), the multi-scale finite element modeling was applied to a bimodal HS Ti with a specific topological distribution of core and shell regions. A representative volume element (RVE) similar to that of Yu et al. (2015) was used. The numerical simulation results of these studies revealed that the initial stages of deformation and strength of the alloys with HS design are governed by the characteristics of the interconnected network of the shell regions whereas the extent of uniform deformation and overall ductility are governed by the ductile core region.

In the present work, we developed, on the basis of the crystalline plasticity and homogenization method, a three-dimensional multi-scale numerical model to simulate the non-linear and damage behaviors of the titanium with harmonic structure (HS). In order to better describe the non-linear behavior of the HS Ti, following ingredients have been included in this work:

1. Crystalline plasticity: From a micromechanical point of view, the slip theory of crystalline plasticity is one of the most faithful descriptions of the constitutive behavior for metals. This theory considers the fact that the plastic deformations are mainly due to crystallographic slips which obey the Schmid resolved shear stress criterion. The flow rule during deformation can be defined by either physically based models (Arsenlis and Parks, 2002; Gao and Huang, 2003; Cheong and Busso, 2004; Ma et al., 2006; Rodríguez-Galan et al., 2015; Chen et al., 2017 etc.) or phenomenological models (Cailletaud, 1987, 1992; Pilvin, 1990; Meric et al., 1991; Han et al., 2015; Hu et al., 2016 among others). In physically based models, dislocation densities are the internal variables that control the critical resolved shear stress evolutions. The physically based models have been widely applied to FCC and BCC materials. However, for HCP materials, such as pure Ti, only a few works exist in the literature mainly due to the difficulty of finding a correct parameterization of the laws for all available slip systems (Alankar et al., 2011).

Barkia (2014) demonstrated that amongst the numerous phenomenological slip models, the kinematic hardening law proposed by Cailletaud (1987) and Pilvin (1990) was appropriate to describe the plasticity behavior of the Ti hexagonal crystals. This microscopic