International Journal of Plasticity 70 (2015) 191–205

Contents lists available at ScienceDirect

International Journal of Plasticity

journal homepage: www.elsevier.com/locate/ijplas

Temperature and stain rate effect on the deformation of nanostructured pure titanium

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A R T I C L E I N F O

Article history:
Received 28 January 2015
Received in revised form 27 March 2015
Available online 14 April 2015

Keywords:
A. Strengthening mechanisms
B. Crystal plasticity
B. Rate-dependent material
C. Finite elements
C. Optimization

A B S T R A C T

The behavior of nanostructured pure Ti has been studied experimentally and theoretically using a crystal plasticity (CP) finite element polycrystalline model. The actual polycrystalline microstructure (grain shape and orientation distributions) was accounted in voxel-based representative volume elements. The crystal behavior was described by a standard CP model with a physically-based description of the plastic slip rate based on the theory of thermally activated dislocation motion. Prismatic, basal and pyramidal <c+a> slip systems were considered. The parameters of the CP model were obtained by combining experimental measurements (i.e. dislocation densities) and an inverse analysis of the macroscopic experimental results. The resulting polycrystalline model was validated by an accurate reproduction of independent experimental tests performed at different temperatures and strain rates. The critical resolved shear stresses (CRSS), predicted by the model for the different slip systems, show the expected increase with respect to those for coarse grained pure Ti. The nanostructured Ti shows lower strain rate sensitivity and activation volumes than coarse grained pure Ti. The ratios between the CRSSs of the different slip systems at room temperature were almost independent of grain size. The model was used to predict the evolution of the CRSSs as a function of temperature and a faster decay of pyramidal CRSS was found compared to prismatic and basal ones.

1. Introduction

Commercially pure Ti (CP-Ti) has been successfully used for fabrication of medical devices due to its high corrosion resistance and biocompatibility (Brunette et al., 2001). Traditionally, the required mechanical properties in materials for implants were reached by alloying. However, the suspicion of long term toxicity problem with elements, such as vanadium, gives rise to new alternative alloys. Nevertheless, there are other strategies under investigation such as the modification of microstructure via grain refinement. It is well known that grain refinement can significantly improve the strength of materials according to the Hall–Petch law (Hall, 1951; Petch, 1953). Various methods of severe plastic deformation (SPD) have been successfully applied for grain refinement in pure Ti, such as equal channel angular pressing (ECAP) (Stolyarov et al., 2001; Ko et al., 2006), high pressure torsion (Sergueeva et al., 2001; Valiev et al., 2003) and hydrostatic extrusion (Pachla et al., 2008). In particular, nanostructured pure Ti (Grade 4) processed via a complex SPD route consisting of ECAP, swaging and drawing showed yield stress of 1240 MPa along the rod axis (Sabirov et al., 2011). However, as drawback of strong crystallographic texture developed during processing a significant anisotropy of the mechanical properties was obtained.

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http://dx.doi.org/10.1016/j.ijplas.2015.04.002
0749-6419/

In order to optimize the beneficial mechanical properties of nanostructured pure Ti, it is necessary to understand the deformation micromechanisms governing the mechanical behavior of SPD processed materials. These mechanisms depend not only on the refined grain size but also on other microstructural features, such as grain boundaries state, defect densities and crystallographic texture (Gunderov et al., 2013). In addition to the microstructure, parameters such as temperature, strain and strain rate critically influence on the mechanical behavior. Although some relevant deformation mechanisms occur at the nanometric scale, the influence of the polycrystalline microstructure on the macroscopic behavior can be accurately captured with a continuum micromechanical description. Particularly, continuum micromechanical homogenization models based on crystal plasticity have been successfully applied to predict the effect of grain orientation distribution and texture evolution in nano Ti (Segurado and LLorca, 2013). This approach can be extended also to include the effect of temperature and strain rate at the crystal level by an appropriate crystal plasticity formulation. In crystal plasticity, each slip system is explicitly considered, and its resistance to the plastic flow (movement of dislocations) is characterized by a critical resolved shear stress (CRSS) evolving with the deformation. The CRSS evolution during deformation can be defined by either phenomenological (Asaro and Needleman, 1985; Bassani and Wu, 1991) or physically-based models (Arsenlis and Parks, 2002; Ma et al., 2006; Cheong and Busso, 2004; among many others). In physically based models, dislocation densities are the internal variables that control the CRSS evolutions, and the flow rule is usually based on the theory of thermally activated dislocation motion. This type of flow rule allows to introduce the effect of temperature and strain rate in the plastic flow under physical considerations and, therefore, to predict naturally the evolution with temperature in CRSSs (Kothari and Anand, 1998). Physically-based models have been widely applied to fcc and bcc materials (Ma and Roters, 2004; Patra and McDowell, 2012). For hcp materials, such as pure Ti, only a few works exist in the literature mainly due to the difficulty of finding a correct parametrization of the laws for all the available slip systems (Ti (Alankar et al., 2011), Mg (Cheng and Ghosh, 2015), Be (Knezevic et al., 2013)).

Ti is an hcp material with an axial ratio of $c/a = 1.587$. The most common deformation modes, in the order of ease of operation, are the prismatic, basal and pyramidal slip systems and the twinning modes (Salem et al., 2005; Gong and Wilkinson, 2009). During the first ECAP pass, deformation twinning is supposed to play a key role in accommodation of a large amount of shear strain, nevertheless, strain is accommodated primarily by dislocation glide processes during the rest of ECAP passes (Shin et al., 2003). In addition, twinning deformation activity in Ti decreases rapidly with the grain size reduction being inactive for grain sizes below 1 μm (Yu et al., 2010). The ratios of the CRSSs in the different slip systems are highly affected by the composition and temperature. The plastic behavior of pure Ti single-crystal as a function of temperature has been widely studied since the 70 s due to high industrial interest (Conrad, 1981). Prismatic glide was studied by direct testing of large Ti single-crystals (Tanaka and Conrad, 1972; Akhtar and Teghtsoonian, 1975; Nemat-Nasser et al., 1999), that reported the CRSS values and available dislocation mechanisms over a large range of temperatures. Basal glide was also studied (Levine, 1966; Akhtar, 1974). All these studies were done on large single-crystal specimens or highly textured polycrystals. In these cases, the behavior can be quite different to the behavior of the grains within the polycrystal due to the differences in the microstructure and the presence of size effects.

Recently, Gong and Wilkinson (2009) measured directly the single crystal properties of CP-Ti (Grade 1) by means of mechanical tests of micron-sized cantilever beams built inside grains with specific orientations. These are the first direct measurements of the CRSSs for each slip system and the ratios between the CRSSs of the different slip systems. This work provides a good benchmark for CP models. However, the absolute values of CRSSs obtained can not be easily extrapolated to other Ti alloys or the nanostructured Ti studied here, due to the differences in the processing route and grain size. Moreover, in the case of nanostructured pure Ti the direct measurement of grain properties is not possible due to the small grain sizes (≤ 0.2 μm). For this reason, an inverse technique to determine single crystal properties from polycrystalline tests can be a good alternative. In this line, an inverse optimization strategy has been recently developed to be used together with crystal plasticity finite element (CPFE) models to obtain the CRSSs of the active slip systems (Herrera-Solaz et al., 2014a). This technique has been successfully applied for hcp metals (Mg alloys) with a strong texture (Herrera-Solaz et al., 2014a,b), and therefore it might be an useful tool in the case of textured nanostructured Ti processed by ECAP-Conform (ECAP-C) and drawing.

Anisotropy in the mechanical behavior and texture of Ti processed by ECAP has recently been studied (Sabirov et al., 2011; Korshunov et al., 2008; Meredith and Khan, 2012). Nevertheless, some deformation kinetics parameters such as strain rate sensitivity and activation volume have not been completely resolved for nanostructured Ti. The strain rate sensitivity of fcc materials (Cu) increases as the grain size decreases, while that of bcc materials (Ta, Fe) shows the opposite trend (Wei et al., 2004; Rodriguez-Baracaldo et al., 2008). Some experimental results suggest that strain rate sensitivity in Ti decrease with the grain size and activation volume does not change drastically with the grain size (Li et al., 2013). However, these results have not been studied for the different slip systems in nanostructured Ti.

Within this framework, the objective of this paper is to determine the behavior of the different slip systems of nanostructured pure Ti processed by ECAP-C and drawing, as well as their evolution with temperature and strain rate. A CPFE polycrystalline model has been used with grain orientations statistically representative of actual texture. The crystal behavior has been modeled using a physically-motivated crystal plasticity model to include the effect of temperature and strain rate. The parameters of the crystal plasticity model were obtained from experiments and using an inverse analysis of macroscopic tests of bars at different temperatures, strain rates and orientations. Finally, independent experimental results were used to validate the single crystal properties and predictive potential of the model (strain rate sensitivity and activation volume).