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Micromechanical modeling of hardening mechanisms in commercially pure α-titanium in tensile condition

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Tensile tests on commercially pure α-titanium show a three-stage behavior giving rise to a well on the strain dependence of the work hardening. An opposite strain rate effect on the well depth is found whether specimens are elongated along the rolling or the transverse direction. Slip lines analysis reveals an initial predominance of prismatic slip, particularly pronounced in specimens strained along the rolling direction. The relative activity of prismatic slip is then observed to decrease with the samples deformation. These results provide grounds for elaboration of an elasto-viscoplastic self-consistent model based on the translated field method and an affine linearization of the viscoplastic flow rule, and capable of explaining such peculiar work hardening behavior. The model considers crystal plasticity and deals separately with mobile dislocation density and dislocation velocity. It assumes lower strain rate sensitivity as well as higher dislocation multiplication rate for prismatic systems. Based on these assumptions, the model reproduces correctly the stress–strain curves and gives sound estimates of Lankford coefficients, prismatic slip activity and textures evolution. Most importantly, the opposite effect of strain rate on the well depth with regard to the orientation of the tensile axis is qualitatively retrieved, which allows putting forward an explanation of the observed phenomena.

1. Introduction

At ambient temperature, Ti has a hexagonal close-packed (hcp) structure which is characterized by a high anisotropy of glide resistance. There is a general agreement that prismatic slip is the easiest deformation mode (Churchman, 1954; Philippe et al., 1995; Zaefferer, 2003; Salem et al., 2005; Wu et al., 2007; Gong and Wilkinson, 2009; Gurao et al., 2011; Li et al., 2013; Warwick et al., 2012; Benmhenni et al., 2013; Gloagen et al., 2013; Barkia et al., 2015). However, less consensus has been found concerning the ranking of other possible slip and twinning systems, especially the corresponding values of the critical resolved shear stress (CRSS) which closely depend on material composition. Their knowledge is however of primary importance for a coherent choice of the parameters used in plasticity models. In particular, glide of <*c*+*a*> dislocations or twinning modes must be involved in the deformation of a Ti crystal so that it could support arbitrary shape changes. Hence, twinning can occur in titanium as observed in many experiments (*e.g.*, Monteiro and Reed-

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Hill (1973); Nemat-Nasser et al. (1999); Salem et al. (2002, 2003, 2006); Nixon et al. (2010); Wang et al. (2010); Ghaderi and Barnett (2011); Gurao et al. (2011); Wang et al. (2012); Li et al. (2013); Becker and Pantleon (2013); Roth et al. (2014); Barkia et al. (2015)). On the other hand, Ti can also deform with a very negligible twin volume fraction (e.g., Nixon et al. (2010); Ghaderi and Barnett (2011); Roth et al. (2014)). The proneness to twinning manifestly depends on material (composition (Monteiro and Reed-Hill, 1973; Li et al., 2014; Barkia et al., 2015), grain size (Ghaderi and Barnett, 2011; Wang et al., 2012), texture (Nixon et al., 2010; Wang et al., 2010; Li et al., 2014)) and loading conditions (temperature (Monteiro and Reed-Hill, 1973; Li et al., 2013, 2014), strain rate (Nemat-Nasser et al., 1999; Gurao et al., 2011), loading mode (Salem et al., 2003; Nixon et al., 2010)).

In particular, twinning is often evoked to explain the strain hardening behavior of Ti (*e.g.*, Salem et al. (2006); Knezevic et al. (2013)). In compression condition, three-stage behavior is notably reported. The initial stage A is characterized by a decreasing strain hardening rate $\Theta = d\Sigma/dE^p$ (where Σ designates the macroscopic stress and E^p the macroscopic plastic strain). It is followed by an increase in Θ during stage B and, finally, a new decrease in stage C. Salem et al. (2002, 2003, 2006) found that the onset of twinning correlates with stage B. Accordingly, they proposed to ascribe the increase in the strain hardening to the effect of twin boundaries on the resistance to dislocation glide, and the decrease in stage C to saturation of the twin volume fraction.

However, recent experiments from Roth et al. (2014) showed that the three-stage character of Ti strain hardening behavior also manifests itself in conditions that induce almost no twinning (twin volume fraction <0.5%), such as tensile loading of commercially pure (CP) α-Ti with 9 μm grain size along the rolling direction. Tests on differently oriented samples showed an ambiguous role of twins in tensile condition. On the one hand, for samples stretched along the transverse direction, these experiments revealed a more significant twin volume fraction (3 to 6%) and a more pronounced tendency to three-stage behavior, which was weaker than in compression tests generally characterized by twin volume fraction an order of magnitude higher (Nemat-Nasser et al., 1999; Salem et al., 2002, 2003, 2006). At the same time, the work hardening rate was considerably stronger all over the deformation curve for samples deformed along the rolling direction, *i.e.*, those with the lowest twin volume fraction. The latter observation is in contradiction with the hardening effect of twins, resulting from the dynamic Hall-Petch effect and/or Basinski effect (Basinski et al., 1997). Such effects could have naturally been conjectured to explain the increase of Θ during stage B of tensile curves, similar to the interpretation applied in the case of compression. Another important observation concerned the effect of the imposed strain rate on the three-stage behavior, which was found to be opposite for the two kinds of elongation directions: the trend to formation of the low hardening stage A was the strongest at the lowest/highest strain rate for samples deformed along the rolling/transverse direction, respectively (Roth et al., 2014). This inversion of the sign of the strain rate effect neither can be explained by the supposed effects of twins. Given the very low twin volume fraction recorded, it was thus conjectured, by Roth et al. (2014), that twins played a secondary role in the tensile deformation of the tested Ti samples. It is noteworthy that such hypothesis is corroborated by some literature results. In the tensile experiments reported by Ghaderi and Barnett (2011), yield point elongation was actually more pronounced for the finest grain size samples, *i.e.*, the ones where twinning was insignificant, and Becker and Pantleon (2013) observed a weaker trend to three stage behavior in tensile condition compared to Roth et al. (2014), in spite of much more intense twinning.

Hence, the data in tensile condition do not support the conjecture of twinning as the mechanism controlling the three-stage strain hardening behavior. Another mechanism could be dynamic strain aging of dislocations caused by their interactions with solute atoms, as suggested by Nemat-Nasser et al. (1999) to explain compression behavior of CP Ti. Nevertheless, this explanation does not apply to ambient temperature because the dynamic strain aging is only essential in Ti in the temperature range of 500–850 K, as shown by Doner and Conrad (1973); Reed-Hill et al. (1995); Lecomte et al. (1997) and discussed by Salem et al. (2002, 2003, 2006). Alternatively, static solute aging of dislocations could account for the initial low work hardening rate during stage A as the occurrence of the Piobert-Lüders phenomenon. However, no propagation of a deformation band was observed by Roth et al. (2014) from high-temporal resolution extensometry performed with the aid of a CCD camera. It was observed instead that the plastic flow started simultaneously in the whole specimen and displayed a high degree of homogeneity, thus invalidating *a priori* this surmise. As a consequence, it is necessary to examine the three-stage hardening character of tensile deformation of CP Ti from the viewpoint of mechanisms based on dislocations glide only. For instance, Conrad (1981) and Naka (1983) both suggested ascribing the yield plateau observed in Ti to fast multiplication of mobile dislocations. In order to explain qualitatively the strain rate effect on the proneness to three-stage behavior, Roth et al. (2014) suggested to take into account that the strain rate sensitivity of stress (SRSS) may be different for different slip families. However, without considering the dislocation multiplication effects, this suggestion led to an unrealistic assumption of a stronger SRSS for prismatic glide, as compared with pyramidal glide.

The objective of the present paper is to propose a model, based on dislocations glide mechanisms, that can account for the work hardening evolution in tensile condition. First, dislocation slip system activity is investigated experimentally, with the objective to provide missing criteria for selection of the relevant mechanisms. Interrupted tensile tests and slip lines characterization in the microscope are used for this task (Sections 2 and 3). Then, an elasto-viscoplastic self-consistent polycrystalline model that integrates mobile dislocation multiplication and different strain rate sensitivities is developed (Section 4). The capacity of the polycrystalline model to reproduce the experimental observations, including stress–strain curves, work hardening behavior, relative slip system activities, Lankford coefficients and textures evolution are analyzed in Section 4. Discussion and conclusions follow.