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Crystal plasticity simulation of strain aging phenomena in α-titanium at room temperature

Arina Marchenko, Matthieu Mazière*, Samuel Forest, Jean-Loup Strudel

Mines ParisTech, Centre des Matériaux, CNRS UMR 7633, BP 87, 91003 Evry Cedex, France

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ABSTRACT

Strain aging phenomena are shown to affect the viscoplastic behavior of commercially pure α-titanium at room temperature. A yield stress anomaly corresponding to static strain aging was experimentally observed when the material was loaded in the transverse direction. At low strain rates small serrations on the stress-strain curves, typical for the Portevin-Le Chatelier effect are observed for the material loaded in the transverse and rolling directions at room temperature. The presence of a stress peak is attributed to the interaction between activated <*c*+*a*> slip systems with the atoms of interstitial oxygen. The Portevin-Le Chatelier effect is presumably due to the non-planar core of screw-type dislocations. A phenomenological strain aging model is combined with a comprehensive description of slip systems active in HCP crystals in order to take into account the role of crystal plasticity in static as well as dynamic strain aging. Finite element simulations are performed on polycrystalline aggregates with various numbers of grains accounting for the elastic and plastic anisotropy of α-titanium. The simulations of static strain aging do not show formation and propagation of macroscopic shear bands. Instead, a complex strain localization phenomenon is taking place within some grains and specific associations of grains, which leads to the formation of meso-Lüders bands. The results of dynamic strain aging simulations predict the initiation and propagation of macroscopic Portevin-Le Chatelier bands even in the presence of positive apparent strain rate sensitivity.

1. Introduction

High strength in combination with low density and good corrosion resistance make titanium (Ti) and its alloys widely used metals in aerospace, chemical and petrochemical industries. Among them, commercially pure (CP) α-Ti is of a great interest due to its high environmental resistance and good workability. Pure α-Ti has a hexagonal close-packed crystal structure with a c/a ratio of 1.586 at ambient temperature. Strong plastic anisotropy due to crystallographic texture and the possibility of twinning is responsible for the complexity of the deformation behavior of α-Ti. Three slip system families with Burgers vector of <*a*>-type $<\bar{2}110>$ gliding in basal (0001), prismatic $\{10\bar{1}0\}$ or first-order pyramidal $\{10\bar{1}1\}$ planes constitute a set of 12 slip systems including only 4 kinematically independent ones (see Fig. 1). Some additional *non* <*a*>-type deformation mechanisms such as pyramidal <*c*+*a*> dislocation slip and four twinning systems accommodate the plastic deformation along the *c*-axis (Lütjering and Williams, 2007). Prismatic <*a*> slip was found to be the easiest in CP-Ti, thus governing the

* Corresponding author. Tel.: +33 1 60 76 30 78; fax: +33 1 60 76 31 50.
E-mail address: matthieu.maziere@ensmp.fr (M. Mazière).

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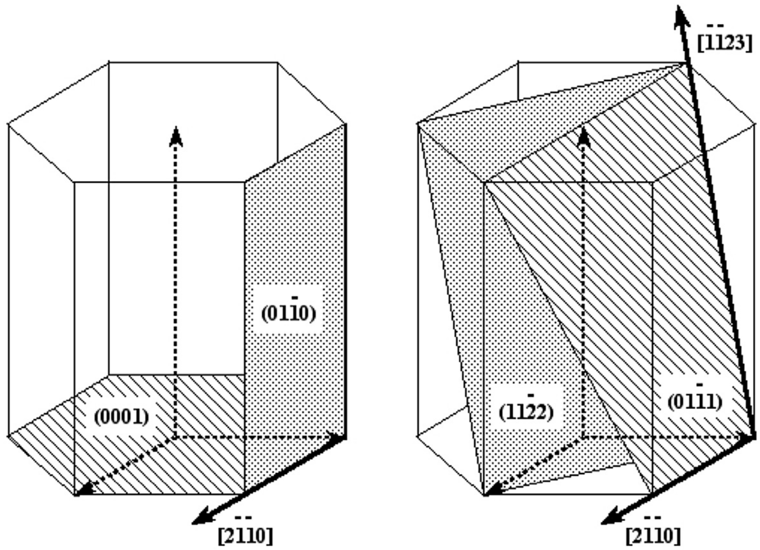

Fig. 1. Slip systems in α-titanium, after Guillot et al. (2001).

room-temperature plastic deformation. The relative ease of prismatic slip was explained by the lowest stacking fault energy for the <*a*>-dislocations associated with a non-planar dislocation core structure (Legrand, 1984).

A large number of studies devoted to the mechanical behavior of Ti has been conducted over the past few decades. In particular, the phenomena of dynamic and static strain aging and the underlying physical mechanisms have been the subjects of numerous investigations and of some long-standing debates.

Strain aging is usually associated with interactions between dislocations and point defects, i.e. vacancies, self-interstitials, substitutional and interstitial impurities. Solute atoms can migrate to dislocations and then segregate in or near their core, thus inhibiting the dislocation motion. In order to move the dislocation away from the solute rich regions, an extra stress is required to overcome attractive dislocation-defect interactions. At sufficiently high temperatures and/or low strain rates, the point defects can migrate back to dislocations, thus causing repeated locking−unlocking processes called dynamic strain aging (DSA). These intermittent and unstable localized strain bursts lead to the discontinuous yielding phenomenon known as Portevin-Le Chatelier (PLC) effect, characterized by serrations on the tensile stress-strain curve. At a given temperature and impurity concentration, the average flow stress needed to unpin dislocations, increases with decreasing strain rate or increasing waiting time of dislocations. As a result, the flow stress of the material vs. strain rate is decreasing and may even become negative, leading to the so-called negative strain rate sensitivity (NSRS), according to Kubin and Estrin (1991). When the imposed strain rate falls into the range of NSRS, the initiation and propagation of plastic strain rate localization bands in multiple sites of a specimen can be observed during the straining process (Hull and Bacon, 1984).

Static strain aging (SSA) is usually manifested by a marked yield point or a stress peak on the stress-strain curve when a prestrained specimen is unloaded and aged for a preset time and then reloaded. When dislocations cooperatively break away from their obstacles, strain localization bands called Lüders bands are formed at one site of the specimen and spread through the sample (Kubin et al., 1992).

Titanium and its alloys always contain some residual impurities such as nitrogen, oxygen, carbon, hydrogen. Rosi and Perkins (1953) were the first to report strain aging phenomena in CP Ti at elevated temperatures and they attributed it to the segregation of nitrogen atoms. According to Doner and Conrad (1973), pinning being controlled by diffusion, the activation energy of the process at the atomic scale is that for the diffusion of the solutes responsible for the pinning. The investigation of SSA in CP Ti at elevated temperatures by Donoso and Reed-Hill (1977) indicates that the activation energy of the process is in good agreement with that for the diffusion of oxygen in Ti. At intermediate and low temperatures, Conrad (1981) ascribed the yield peak in CP Ti to dislocation multiplication mechanisms. An alternative explanation of the yield peak in CP Ti observed at room temperature was recently proposed by Roth et al. (2014) who suggested that distinct slip systems have different strain-rate sensitivities. The tendency for the yield peak formation was explained by the initially dominant activity of pyramidal slip with a critical resolved shear stress (CRSS), resulting in a higher yield stress.

The significance of DSA in CP Ti at elevated temperatures was studied by Doner and Conrad (1973), Garde et al. (1972). They suggested that interstitial oxygen interacting with mobile dislocations through bulk diffusion can be responsible for DSA above 600 K, while DSA around 350 K might be due to hydrogen that has a higher diffusivity. According to Senkov and Jonas (1996), solute hydrogen reduces the extent of DSA in titanium at high temperatures by weakening the interaction between dislocations and impurity atoms thus causing material softening. Nemat-Nasser et al. (1999) argued that the activation