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Twinning in pure Ti subjected to monotonic simple shear deformation

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ABSTRACT

The aim of this paper is to provide a thorough study on the occurrence and importance of deformation twinning in simple shear deformed pure α-Ti. A statistically relevant inspection of the morphology of the deformation twins in relation to the applied strain/deformation is performed. The investigated microstructural aspects are the twin volume fraction, the twin thickness distribution and the resolved shear stress distribution on the twin plane. All these aspects are examined as a function of the twin types and two initial textures.

Monotonic simple shear experiments are carried out for three different loading directions with respect to a direction linked to the initial crystallographic texture. EBSD and TEM observations reveal the presence of $\{10\bar{1}2\}$ and $\{11\bar{2}2\}$ twins. The statistical analysis reveals that $\{10\bar{1}2\}$ and $\{11\bar{2}2\}$ twins have a similar average thickness around 1.9 nm, but the $\{10\bar{1}2\}$ twins show a far larger spread on their thickness and can grow to almost the size of the original parent grain. Correlation of the twin fractions with the RSS analysis shows that RSS is an acceptable method explaining the difference in twin fractions for different textures and orientations. A detailed analysis shows that $\{11\bar{2}2\}$ twins occur in average with a smaller volume fraction but with a higher RSS, indicating they are more difficult to nucleate or grow compared to $\{10\bar{1}2\}$ twinning. In general a higher RSS value on the twin plane is not connected to a higher twin thickness; only in the case of $\{10\bar{1}2\}$ twins the highest RSS values show clearly thicker twins.

1. Introduction

Pure titanium which has a hexagonal close packed (hcp) structure at room temperature, exhibits twinning as a prevalent deformation mechanism to accommodate imposed strains [1–8]. These twins are necessary to accommodate a strain component in the direction of the c-axis of the unit cell by twinning on a pyramidal plane and hereby introducing a shear with a c-component [9,10]. Different types of twinning are possible, the most observed ones in Ti being the $\{10\bar{1}2\}$

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$\langle 10\bar{1}\bar{1}\rangle$ tensile twin and the $\{11\bar{2}2\}\langle\bar{1}\bar{1}23\rangle$ compression twin [9–15]. Tensile twinning relates to the aspect of introducing a positive shear strain along the c-axis of the parent grain and compression refers to a negative component along this c-axis. Other types of twinning *e.g.* $\{10\bar{1}1\}\langle\bar{1}012\rangle$ and $\{11\bar{2}1\}\langle 11\bar{2}\bar{6}\rangle$ can occur depending on the temperature and type of deformation [16,17]. The actual mechanisms and energies needed to nucleate and grow these twins are still under discussion and might differ from the considered type. Theoretical models for the mechanisms involved [8,15,18–22] substantiated with experimental evidence [4,11,13,23,24] are available and this especially for the $\{10\bar{1}2\}$ and $\{11\bar{2}2\}$ types of twins which are observed most frequently. Nevertheless, there are still many aspects that need a dedicated study in order to obtain a better and more complete understanding of the nucleation and growth mechanisms involved. Recent work on this topic is proposed by [25] where the authors studied the atomic structure of the nucleus of a $[10\bar{1}1]\ \langle\bar{1}012\rangle$ twin in Mg by atomistic simulations using density function theory (DFT) and an empirical potential. At mesoscale, twin activation and their competition with other slip systems are important factors when incorporating twinning mechanisms in models simulating the mechanical behavior and texture change during deformation. An example of such a simulation is the viscoplastic self consistent (VPSC) approach [26] which allows the incorporation of twin systems in the case of hcp materials [27,28].

Calculation of the resolved shear stress (RSS) or resulting Schmid factor for a certain slip system in combination with a critical resolved shear stress to activate this system is commonly used to predict which system is active or to justify why one system is preferred above another one. This approach is often transposed to twin systems [2,4,6,29–31] which are then considered as a conventional slip system with a plane (twin plane) and slip direction (twin shear direction) being unidirectional in contrast to regular slip systems. In the case of twinning the existence of a critical resolved shear stress for nucleating or propagating a twin is still under discussion and might strongly depend on the type of twin. In order to apply an RSS based technique to predict or simulate the occurrence of twinning, its validity should be justified. One way to obtain information is to study the deformed microstructure in a direct way using for example transmission electron microscopy (TEM) [11,22–24,31,32]. Another approach is to look on a larger scale and to obtain more relevant statistical data of the twin morphology by using for example electron backscatter diffraction (EBSD) analysis [2–5,10,29,31]. Both approaches lead to complementary data. Up to now most statistical studies on the occurrence of twinning in Ti and other hcp materials are performed on simple compression or tension samples. Other macroscopic stress states involving, more than one principal stress component like simple shear are less common. To the authors' knowledge, only two studies are available analysing the presence of twinning in simple shear deformed titanium [10,33]. However, the morphology of the twins is not studied in depth in this work. The goal of the current paper is to provide an in-depth statistically relevant study which could be useful for optimizing or confirming micromechanical models. In this work, the influence of the initial texture on the type of twins and their fraction will be studied using EBSD and some additional TEM analysis. An RSS calculation will be applied to predict the occurrence of twins and these results will be correlated with the observed twin types and fractions. In addition, special attention is paid to the thickness distribution of twins and its correlation with the RSS value. This approach is similar to the one used in order work studying twin growth and nucleation in Zr [4] and Mg [34].

2. Experimental

Monotonic simple shear tests are performed using the setup described in [35]. For EBSD observations, the samples are prepared using mechanical grinding followed by electrochemical polishing with a mixture of 59% methanol, 35% butoxyethanol and 6% perchloric acid at a potential of 35 V. The method is tested on undeformed recrystallized material to make sure no twins are introduced by mechanical polishing. To study the presence of twins, EBSD measurements are performed at 20 kV with a stepsize of 0.6 μm (or 0.3 μm or 0.5 μm for some cases) and scanned areas with an approximate size of 40▯10^3 μm^2. For determining the texture, larger scan areas up to 1 mm^2, with a stepsize of 2 μm are used.

TEM observations are performed on a CM20 microscope operated at 200 kV and 3 mm samples are prepared by mechanical grinding and a final electropolishing step with the twin-jet technique using the same electrolyte as in the case of the EBSD preparation but with a potential of 18 V and at a temperature below −20 °C.

For conducting the monotonic simple shear experiments [36], samples cut following different orientations with respect to the rolling direction from two pure titanium rolled plates having a different initial texture are prepared. The two plates are, from now on, being referred to as P1 (plate 1) and P2 (plate 2) respectively. On each plate three reference axes are conventionally fixed as RD, TD and ND. Plate P1 is characterized by a typical split-basal texture as indicated in Fig. 1a by the (0001) pole figure obtained by EBSD (see also [33]). This pole figure is in good agreement with the pole figure obtained by XRD measurements obtained from larger areas (Fig. 1b) justifying the use of EBSD measurements to estimate the texture. In the case of plate P2, the RD and TD directions are taken as indicated in Fig. 1c. The initial texture of P2 is more isotropic and a (0001) pole figure is given in Fig. 1c. For both textures, only the (0001) pole figures or distribution of the c-axis are given because their initial orientation and final reorientation are of particular important in the case of twinning. The assumed isotropic plate P2 still shows a not fully symmetric distribution of the c-axis *versus* the ND direction; however the (0001) pole distribution asymmetry in the RD-TD plane is small. Nevertheless, this asymmetry will be used further on to explain differences in twin fraction.

3. Results

3.1. *Mechanical Behavior*

Simple shear tests are performed in three different directions with respect to the RD direction of each plate; those three shear directions form respective angles with RD equal