



# Initiation and accommodation of primary twins in high-purity titanium

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## Abstract

Uniaxial compression tests were carried out at room temperature and at strain rates of 0.001, 0.01, 0.1 and  $1 \text{ s}^{-1}$  on samples of high-purity titanium. The initial texture was favorably oriented for contraction twinning. The double-differentiation method was employed to detect the initiation of twinning as well as of dynamic recrystallization. Critical strains of about  $-0.24$  and  $-0.65$  were determined, respectively, for these two mechanisms. The relevant mechanisms were identified by means of electron backscatter diffraction (EBSD) techniques. At a true strain of  $\epsilon = -0.3$ , two main kinds of primary twins,  $\{11\bar{2}2\}$  contraction and  $\{10\bar{1}2\}$  extension, were observed and second-generation twins were also identified by means of the EBSD analysis. The presence of low Schmid factor (SF) ( $<0.2$ ) twins was established as well as the absence of potential high SF ( $>0.4$ ) twins. The appearance of the low SF twins is explained in terms of the low accommodation work required in the neighboring grains; this involves prismatic glide in the present case. The absence of the potential high SF twins, on the other hand, is justified as requiring the operation of a combination of several difficult deformation modes: basal glide, pyramidal glide, and twinning.

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## 1. Introduction

The deformation of titanium is more complicated than that of cubic metals because of the hexagonal close-packed (hcp) structure of Ti. Pure  $\alpha$ -Ti has a  $c/a$  ratio of 1.587, which is less than the ideal ratio of 1.633 [1]. As a result, prismatic glide is favored over basal glide [2,3]. Deformation twinning is also an important deformation mode, together with two types of pyramidal glide ( $\langle a \rangle$  and  $\langle c + a \rangle$ ) [4–11]. There are two competing effects of deformation twinning on the stress–strain response: (i) hardening and

(ii) softening [12]. Whether the occurrence of twinning leads to increases or decreases in the work-hardening rate depends on the initial texture and strain path [13–16]. Both softening [17–20] and hardening [12,21,22] effects have been observed. Here, double differentiation of the flow curve was employed to detect the initiation of twinning [23] and dynamic recrystallization (DRX) [24], as both of these mechanisms led to softening in the present case. This interpretation was confirmed by means of scanning electron microscopy and electron backscatter diffraction (EBSD) techniques.

In Ti, the most common twinning systems are the  $\{11\bar{2}2\}\langle 11\bar{2}\bar{3} \rangle$  contraction twins (CTs) and the  $\{10\bar{1}2\}\langle 10\bar{1}\bar{1} \rangle$  extension twins (ETs) [13,21,25,26]. Six geometrically equivalent second-generation variants can form within each primary twin. Consequently, there are

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36 possible second-generation CTs within primary ETs and 36 possible secondary ETs within primary CTs. The most commonly employed criterion for twin variant selection in hexagonal materials is the Schmid rule. Its applicability has been investigated recently in both Ti [27–29] and Mg [30–34] alloys. Generally, it has been reported that the twin variants with the highest resolved shear stresses on their habit planes and along their shear directions are selected because they have the highest Schmid factor (SF) values [15]. However, some non-Schmid behaviors have also been reported in commercial-purity Ti [29,35] and high-purity Ti [25], where twins with the highest SFs are absent while variants with lower SFs appear instead. Similar results have been reported regarding the formation of primary contraction  $\{10\bar{1}1\}$  and double  $\{10\bar{1}1\} - \{10\bar{1}2\}$  twins in Mg [30,31,34]. These non-Schmid behaviors have been explained in terms of the development of the high internal back-stresses induced by the accommodation strains required to permit twin formation. These prevent growth of the potential twins associated with the high SFs. Conversely, if the back-stresses are low, then the work of accommodation is small, permitting the twins associated with the low SFs to form [30,31,36].

The accommodation strains associated with twin formation were first described by Mahajan and Chin in 1973 [37]. The accommodations that potential twins are trying to impose on their neighbors are calculated by rotating the twinning shear displacement gradient tensor into the crystallographic reference frames of the neighboring grains [30,31]. This variant selection criterion has been shown to account quite successfully for the appearance of twins in deformed Mg alloys. However, in Ti, the mechanism of twin variant selection is still poorly understood. Although Schuman et al. [28] and Wang et al. [29] proposed a twin variant selection rule for commercially pure titanium T40, their approach was limited to the energy expended within the matrix grain and did not consider the possible interactions between potential twins and the neighboring grains. Generally, dislocation glide or twinning is required in the grain neighbors to relax the accommodation strains that the twin tries to impose on its neighbors.

In the present work, variant selection was investigated in cylindrical samples that were deformed in uniaxial compression. The primary twins were mainly CTs, although some ETs were also observed. The second-generation twins were mainly ETs and formed within CTs; nevertheless, a few contraction twins generated in ETs were also detected. In this paper, the accommodation strain principle is employed to account for the selection of primary twins in high-purity Ti and its alloys. The factors governing variant selection during the formation of secondary and tertiary twins are discussed in a separate publication [38].

## 2. Experimental method

The material used in this investigation was high-purity  $\alpha$ -Ti (99.99%). The as-received material was a rolled plate

10 mm thick. This material was annealed at 530 °C for 1 h to produce an equiaxed grain structure with an average grain size of 16  $\mu\text{m}$  (see Fig. 1a).

Uniaxial compression tests were performed on a servo-controlled MTS machine at McGill University. Cylindrical specimens 8 mm in diameter and 9 mm long were machined from the as-received plate; their orientations with respect to the latter are shown in Fig. 1b. The compressive load was applied along the normal direction (ND) of the plate. The rolling direction was marked on each specimen to distinguish it from the transverse direction (TD) during machining.

The initial texture is presented in Fig. 1c in terms of (0001), (10–10) and (11–20) pole figures. These indicate that most of the c-axes lie within  $\sim 30^\circ$  of ND, with a spread towards TD. During deformation, these grains were subjected to c-axis contraction, which promoted formation of the  $\{11\bar{2}2\}\langle 11\bar{2}3\rangle$  CTs. The experiments were conducted at room temperature at strain rates of 0.001, 0.01, 0.1 and  $1\text{ s}^{-1}$ , and true strains ranging from  $-0.3$  to  $-0.9$  were applied.

The deformed samples were prepared for orientation imaging microscopy (OIM) by sectioning each sample perpendicular to the rolling direction using a diamond saw. The samples were ground with 320, 600, 1200 and 4000 silicon carbide papers and then electropolished in a solution of 10 ml perchloric acid and 90 ml methanol at  $-30^\circ\text{C}$  using a 17 V DC power supply. EBSD analysis was performed on a Hitachi SU-8000 scanning electron microscope equipped with a field emission gun to determine the natures of the twin boundaries and to detect the formation of new equiaxed DRX grains. For this purpose an acceleration voltage of 20 kV, a working distance of 15 mm and a  $70^\circ$  sample tilt angle were employed, and the data were processed using the HKL Channel 5 software.

### 2.1. Determination of the initiation of twinning and DRX

For analysis of the flow curves, the flow stress at 2% strain was identified as the “yield stress” and the curves beyond this point were fitted with ninth-order polynomials using MATLAB software. The double-differentiation method was then employed to detect the critical stresses associated with initiation of the operative softening mechanisms (in addition to dynamic recovery). This was done by determining the points of inflection in plots of the strain-hardening rate as a function of the stress. In order to identify the mechanism associated with each minimum, samples deformed to strains just beyond the respective critical strain were prepared. Cross-sections perpendicular to the rolling direction were cut from the deformed specimens and polished as described above to determine the mechanism associated with each critical strain.

### 2.2. Calculation of the accommodation strains

The critical resolved shear stresses (CRSSs) of the various deformation modes in high-purity Ti, i.e. prismatic

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