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Growth of $\{11\bar{2}2\}$ twins in titanium: A combined experimental and modelling investigation of the local state of deformation

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ABSTRACT

In this work we combine experiments and simulations to study the residual deformation state near twins in titanium at different stages of the complete twin growth process, including the twin tip: (i) far from a grain boundary, (ii) approaching a grain boundary, and (iii) intersecting with a grain boundary. High resolution electron backscatter diffraction (HR-EBSD) was used to characterise the local residual stress state and dislocation density distributions. Schmid factors were calculated from both the global deformation state (i.e. remote loading) and local deformation state (i.e. from high angular resolution EBSD). Crystal plasticity finite element modelling was used to simulate the stress field close to twins during loading and unloading. These simulations indicate that while the magnitudes of the localized stress fields close to twin boundaries are reduced upon removing the far field load, the major features of the stress fields in these regions are dominated by accommodation of the twin and thus persist from the peak load state to the unloaded state. We find a good correlation between the active twin variant and the maximum local Schmid factor, while the external loading (i.e. global Schmid factor) plays a less important role. These findings are useful in determining which twins will grow when a sample is deformed, and this has important implications for in service performance as well as texture evolution during mechanical processing.

1. Introduction

Deformation twinning is a very important and frequently occurring deformation mechanism in hexagonal close packed (HCP) metals [1]. Twin formation produces large shear within the crystal lattice [2] and the interaction of deformation twinning with grain boundaries can lead to damage nucleation [3]. For the HCP metals there are at least 7 types of twins [4], including 4 $\{\bar{1}01K\}$ types and 3 $\{\bar{2}11K\}$ types where K = 1, 2, 3, 4 for the former and 1, 2, 3, for the latter, and for each type there are 6 variants. These twin types can be initiated to accommodate contraction or extension strain along the <c> axis of the crystal, and whether a particular twin type is due to contraction or extension correlates with the c/a ratio of the material [5]. For titanium, with c/a ratio of ~1.588 [6], 4 types of twins are commonly observed [3,7] among which the $\{10\bar{1}2\}\langle\bar{1}011\rangle$ and $\{11\bar{2}1\}\langle\bar{1}\bar{1}26\rangle$ are extension twins and the $\{11\bar{2}2\}\langle11\bar{2}\bar{3}\rangle$ and $\{10\bar{1}1\}\langle10\bar{1}\bar{2}\rangle$ are contraction twins. The crystallographic relationships between these twins and their parents can be found in Ref. [7].

Nucleation of a twin could be associated with formation of zonal dislocations [8,9] by dissociation of lattice dislocations under suitable stress states [10]. Large bodies of research have treated twin nucleation as a critical resolved shear stress (CRSS) governed process [11–14] akin to the activation of dislocation sources. However, the viability of treating twin nucleation with Schmid factor criteria needs to be re-evaluated, as some investigations have discovered non-Schmid behaviour of twin nucleation [10,15–17]. The 'Schmid factor' referenced above is defined based on the external macroscopic loading, which we will refer to as 'Global Schmid factor (GSF)' in this work. This highlights that when a polycrystal is deformed, the local, i.e. microstructurally resolved,

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stress state can differ significantly from the external loading [18]. It is therefore necessary to probe the local stress state and relate the 'Local Schmid factor (LSF)' to the observed twin variant selection. Local stress measurement techniques that enable experimental evaluations of the LSF currently include: 3D-XRD [19], Differential Aperture X-ray Laue Micro-diffraction (DAXM) [20], High energy Transmission Laue Micro-diffraction (HETL) [21], and High (angular) Resolution EBSD (HR-EBSD) [22,23].

Wang et al. [24] and Abdolvand et al. [25–27] have statistically investigated the effect of stress heterogeneity on twin variant selection and stress partitioning between parent and twin crystals. Based on *in-situ* X-ray measurement of local stresses averaged over the parent grain they have suggested that LSF is the predominant factor influencing twin variant selection rather than GSF, and therefore CRSS criteria might still hold for the twinning process if it is to be assessed on a length scale local to the microstructural feature. However Wang et al. [24] point out that '*Stress close to the twin interface may be different from the grain-averaged stress*'. Apart from the local stress state at the twin-parent interface, the deformation compatibility across a grain boundary, i.e. the effects of neighbouring grains, have also been found to affect twin variant selection [16,28,29].

The process of twin growth has been classified as two steps by Yoo and Lee [5]: the lengthwise propagation along a twin shear direction, and the thickening process perpendicular to a twin invariant plane. The former is controlled by mobility of twinning dislocations [5] while the latter is dependent upon a continuous supply of zonal dislocation at the twin-parent interface [30]. The twin growth process is very fast and often has been treated as an instantaneous process [31]. Therefore, experimental characterisation of this process has rarely been reported. In this research we use HR-EBSD to capture the residual stress and GND density distribution (after removal of external loading) local to twin tips in different scenarios: (i) twins fully imbedded in the interior of a grain far away from any grain boundary, (ii) twins that have propagated across the grain interior and have tips near grain boundaries, and (iii) twins intersecting with grain boundaries. CPFE simulations are also performed to assess whether or not the residual stress field near the twin-parent interface in an unloaded specimen gives a reasonably interpretable indication of the nature of that stress field at peak loading.

2. Methodology

2.1. Experimental procedures

The material used in this research is Grade I commercial purity titanium (kindly supplied by Timet UK), the chemical composition of which is shown in Table 1.

Tensile test samples were cut from the as-received material using electron discharged machining followed by heat treatment at 830 °C for 24 h with furnace cooling to establish a grain size of ~300 μm with a low residual stress state (the geometry of these tensile samples has been reported elsewhere [6]).

The samples were then mechanically ground to 4000 grit followed by chemical mechanical polishing using colloidal silica (60 nm particle size) with intermittent etching using a solution consisting of 1% HF and 10% HNO_3 in water until a crisp grain shape was visible in optical microscopy under polarized illumination. The polished sample was deformed in tension to 1% plastic strain (~235 MPa), monitored using *in-situ* digital image correlation. The DIC was performed by marking both ends of the gauge section with high contrast markers whose displacements were tracked by a high speed camera mounted to the tensile testing rig (Shimadzu AGX-10 tensile testing machine). The sample was loaded at a cross-head displacement rate of 1 μm/s (7×10^{-5}/s strain rate) and then unloaded for HR-EBSD measurements. Various regions of interest featuring a twin tip in the interior of a grain, a twin tip near a grain boundary, and a twin tip intersecting with a grain boundary were scanned using a Zeiss Merlin FEG-SEM system and Bruker e-flash high resolution (1600 × 1200 pixels) EBSD detector. The working distance was 18 mm and scanning was performed using 14 nA beam current under 20 kV excitation voltage. At each beam position, a 1600 × 1200 pixel image of the diffraction pattern was captured with 1 s exposure time and stored as 12 bit images for offline analysis.

2.2. Elastic strain and GND density calculation from HR-EBSD

The strain and geometrically necessary dislocation (GND) density analysis are based on cross-correlating the diffraction patterns. In this process, a reference point was picked far away from the twin lath and toward the interior of the grain, where it was assumed that the stress was relatively low and uniform. For each diffraction pattern, 50 regions of interest (ROI) with 256 × 256 pixel size were selected with one at the middle of the pattern, 19 others surrounding it in a ring and the remaining 30 randomly distributed. These regions of interest on each of the test patterns were compared with the corresponding parts on the reference pattern [32] and their shifts were measured with a sensitivity of ~0.02 pixels [22]. These pattern shifts were used to fully determine the displacement gradient tensor (DGT) with the assumption that the normal stress perpendicular to the sample surface is zero [33]. Very often, lattice rotation local to some microstructure features, such as mechanical indents and deformation twins, can be very high (>10°), under such situations the elastic strain can no longer be accurately recovered due to large diffraction pattern shifts [23] and rotations. Therefore, it is necessary in the first step to estimate a finite rotation matrix from an initial diffraction pattern correlation and rotate the test pattern closer to the reference pattern. A second cross correlation analysis is then applied to the remapped pattern to determine the lattice strain [23]. The deformation gradient tensors from the first and second passes of cross correlation were combined to give a total deformation gradient $\boldsymbol{F}$ from which the Green strain tensor ($\boldsymbol{E}$) was obtained: $\boldsymbol{E} = 1/2(\boldsymbol{F}^{\boldsymbol{T}}\boldsymbol{F} - \boldsymbol{I})$. These elastic strain fields were then used to calculate stress fields using elastic constants (in GPa) for titanium: $C_{11} = 162.4$ $C_{33} = 180.7$ $C_{44} = 117$ $C_{66} = 35.2$ $C_{13} = 69.0$ [34]. Polar decomposition of $\boldsymbol{F}$ into the product of rotation and stretch tensors using singular value decomposition method enables the (finite) lattice rotation to be determined, which were used to estimate 2 in-plane spatial gradients for each of the 3 infinitesimal lattice rotations using procedures documented in Ref. [35] and linked to 6 out of 9° of freedom in Nye's dislocation tensor [36].

The GND density presented in this paper is a lower-bound estimation as 6 rotation gradients are used to recover 33 dislocation types for α-Ti: 3 <a> screw and 6 <c+a> screw; 3 <a> edge on basal plane; 3 <a> edge on first order prismatic plane; 6 <a> edge on first order pyramidal plane; 12 <c+a > edge on first order pyramidal plane [37]. In this GND analysis, there are more dislocation types than constraints from lattice curvature and so solution of the resulting equations is ambiguous. We proceed to make a lower bound estimate of GND densities using a standard linear

Table 1
Chemical composition of the as received Grade 1 commercially pure titanium.

Element	Fe	O_2	N_2	C	Ti
Composition	0.35 wt%	700 ppm	35 ppm	0.01 wt%	Balance