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Local stress field induced by twinning in a metastable β titanium alloy

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Abstract. A crystal plasticity based finite element model incorporating deformation twinning is applied in 3D to simulate the stress field around a twin lamella in a metastable β titanium alloy. Compared with conventional 2D simulations, the stress field determined by the 3D simulation shows better agreement with that measured experimentally using high resolution electron backscattered diffraction. Reasons leading to the different results in 2D and 3D simulations are discussed. It is also discussed in which circumstances 2D simulation is sufficient, and in which 3D is necessary.

1. Introduction

Titanium (Ti) alloys have many unique properties, such as low density, and high corrosion resistance, which makes them suitable for many engineering applications. However, the traditional α Ti or dual-phase Ti alloys have either low strength or low ductility, which limits their usage. Recently, several metastable β Ti alloys have been designed to exhibit both high strength and ductility thanks to the enhanced work hardening ability arising from simultaneous TRIP (TTransformation Induced Plasticity) and TWIP (TWinning Induced Plasticity) effects [1, 2].

Twinning plays an important role during deformation of metastable β Ti alloys. Deformation twinning imposes local strains, which must be accommodated by neighboring grains. This will thus lead to local stress concentration, which significantly affects the microscopic plastic yielding under both monotonic and cyclic deformation. Experimentally, the local stresses can be determined using high resolution electron backscattered diffraction (HREBSD) [3], and the stress field around twins has been measured for a tensile deformed Zircaloy-2 sample [4]. Stresses around twins depend on many factors, including the twin shear strain, the morphology of the twin, the orientations of the parent and twin grains, and the orientations of the neighboring grains. To understand the measured stresses, and the influence of various parameters, it is necessary to build a crystal plasticity model that incorporates twinning. In a series of studies by Kumar et al. [5, 6, 7], a crystal plasticity model with a prescribed twin domain is used to simulate the stress field around a twin lamella for metals with hexagonal close-packed (hcp) structure. They found that the stresses depended on twin thickness, the orientations of the neighboring grains, and the elastic and plastic anisotropy. Twinning and stresses around twins have not been



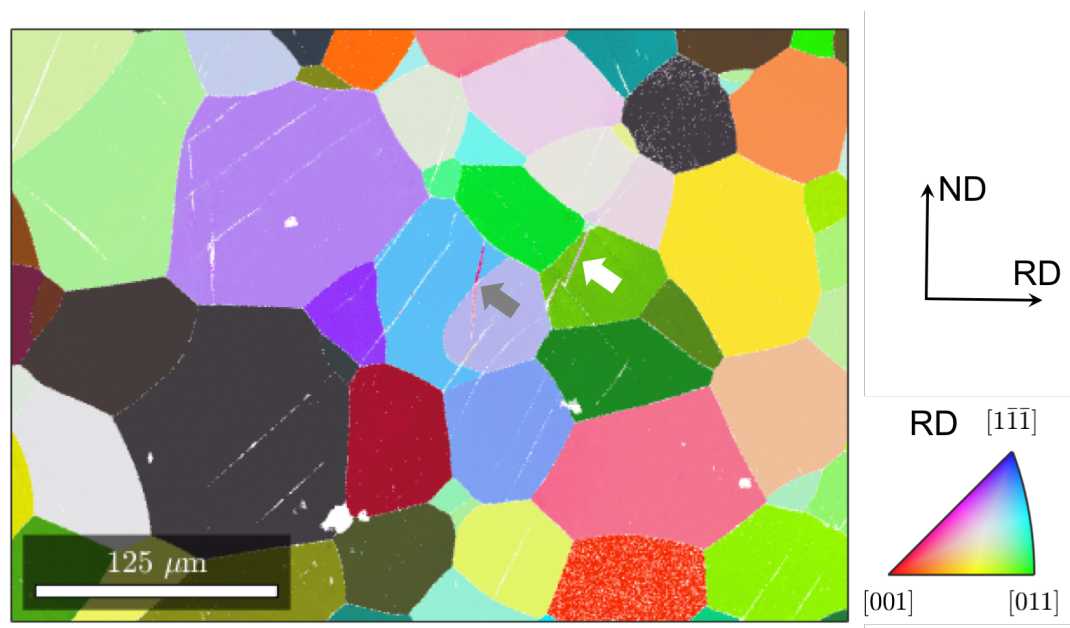


Figure 1. Orientation map showing the microstructure of the longitudinal section after 1% elongation. The tensile direction is horizontal. The colors represent grain orientations. White points are un-indexed points, and the white lines in the figure are likely to be the martensitic laths. The two arrows mark $\{332\} \langle 113 \rangle$ twins.

investigated for metastable β Ti, which has body centered cubic symmetry. Models for a hcp structure (e.g. [5, 8, 9, 10]) cannot be directly applied to metastable β Ti. Moreover, most of the models reported in the literature consider 2D twins or quasi-2D twins with twins extending across the entire thickness, and real 3D simulations incorporating twinning are still rare.

The objective of this work is to build a model that helps understanding of stresses around twins in metastable β Ti. We first construct a 3D crystal plasticity finite element model (CPFEM) that allows consideration of the twin shear strain. This model is then applied to simulate stress fields around a deformation twin in a metastable β Ti alloy. The simulation results are compared with experimental measurements using HREBSD. As a comparison, a 2D finite element (FE) simulation is also conducted, in order to understand in which circumstances 2D simulation is sufficient, and in which 3D is necessary. In the end, we discuss further improvements needed for the model.

2. Experimental results

The material considered in this work is a binary Ti-12 wt% Mo alloy. The ingot was first rolled at room temperature to a thickness reduction of 95%, and then annealed at 1173 K for 15 min and water quenched to obtain a single β phase fully recrystallized microstructure. This single β phase material was used as the starting material for further tensile deformation. The initial grain size was around 50 μm .

Uniaxial tensile deformation was applied along the previous rolling direction (RD). Figure 1 shows the microstructure obtained on the longitudinal section using EBSD after 1% elongation. After applying 1% elongation, twins were developed in a few grains, as marked by the two arrows in figure 1. The activated twinning system in this alloy is $\{332\} \langle 113 \rangle$, according to the orientation relationship of the twins and their parent grains. Apart from twins, in figure 1, white lines/lamellae with similar thicknesses as twins present in many grains. They are not indexed

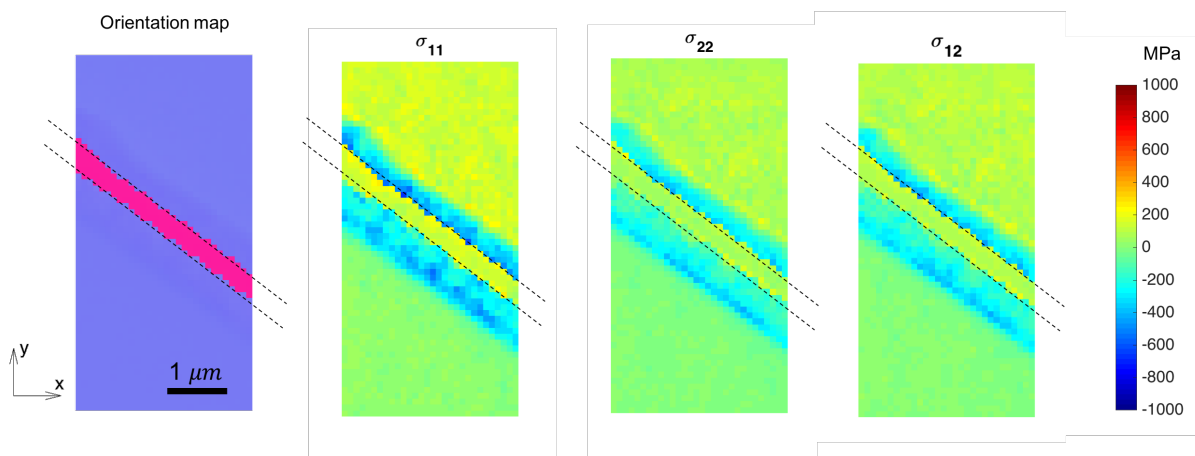


Figure 2. Stress field around a twin measured using HREBSD. The twin is marked by two parallel dashed lines. The stresses are transformed to a coordinate system where direction 1 is the twin shear direction $\vec{b}$ and direction 2 is the normal direction of the twin plane $\vec{n}$. The orientation map is colored according to the crystallographic orientation of the x axis.

in the EBSD measurements. These white lines are likely to be α'' martensite laths. Martensite laths have been observed using transmission electron microscopy in the same material after a similar tensile strain [2]. The α'' phase is not considered when indexing the EBSD patterns, and this is why they appear as un-indexed lines in the EBSD map. At this initial stage of deformation, both martensite transformation and $\{332\}\langle 113 \rangle$ twinning contribute to plastic deformation. This is consistent with the observations in other metastable β Ti alloys [11, 12].

In the sample elongated by 1%, one grain with a twin was selected for HREBSD measurement (not shown in figure 1). The elastic strains and stresses around the twin lamella were determined using HREBSD, as shown in figure 2. The stresses are transformed to a coordinate system where direction 1 is the twin shear direction $\vec{b}$ and direction 2 is the normal direction of the twin plane $\vec{n}$. In the parent grain around the twin, compressive normal stresses along $\vec{b}$ (σ_{11}) are found, and normal stresses along $\vec{n}$ (σ_{22}) are also compressive, but weaker than σ_{11} . Negative shear stresses σ_{12} are found around the twin. Details of the HREBSD measurements can be found elsewhere [3, 13, 14, 15].

3. Model description

A 3D mesh containing 27 Voronoi grains is constructed with a volume of $1 \times 1 \times 1$. The geometry of the polycrystal structure is shown in figure 3a. Periodic boundary conditions are applied. A twin domain is prescribed inside one grain. The twin domain is defined as a plate with a thickness of 0.1, and the twin plate extends through the entire grain. The twin domain represents 3.35% of the grain volume. The twin is visible in a 2D section perpendicular to the macroscopic z direction (see figure 3b). The parent grain and the twin are assigned orientations the same as those measured by HREBSD. The twin interfaces correspond to the $\{332\}$ plane shared by the parent and the twin orientations. In the 2D section shown in figure 3b, the twin has the same inclination as the experimentally characterized section (figure 2), and this 2D section will be used to compare with the experimental results. The mesh is refined around the twin domain to better capture stresses around the twin. All the other grains are assigned random orientations. A 2D geometry is obtained using the 2D section shown in figure 3b. With this treatment, it is possible to compare 2D simulations with 3D ones viewed in the same section, so that grains have the same shape. However, it has to be noted that in 2D simulations, each grain is considered

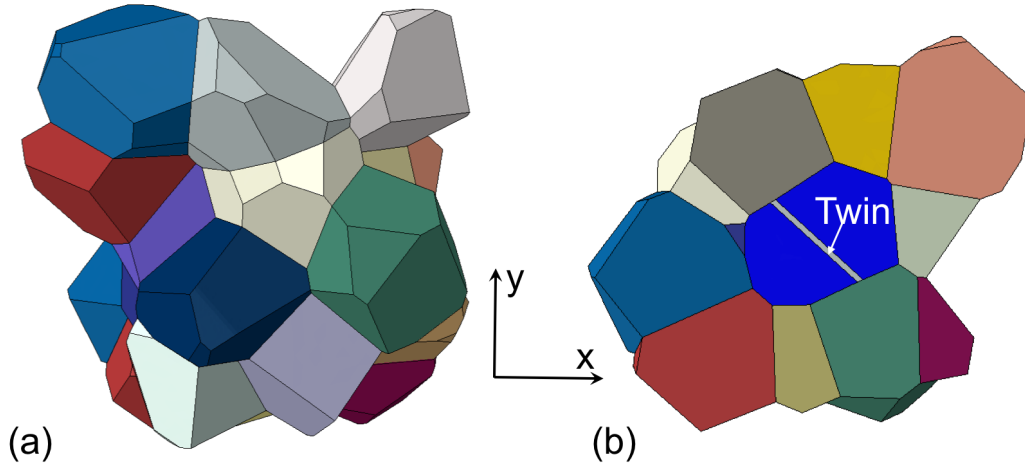


Figure 3. Representation of grains used in the study. (a) The initial 3D polycrystal structure with periodic boundary conditions. (b) A 2D section of the 3D geometry showing the prescribed twin in one grain. This section is also used for the 2D simulation for comparison.

to be a columnar grain along the z direction. The twin lamella is thus perpendicular to the simulated surface in the 2D simulation. The orientations of the parent grain and the twin for the 2D simulation are recalculated to make the $\{332\}$ twin plane normal and the $\{113\}$ twin shear direction on the simulated surface. We consider the 2D mesh elements as plane strain elements, i.e. ϵ_{zz} is the same for all elements in the 2D simulation.

A user material subroutine (UMAT) based on [16] is developed to incorporate twinning. At each time increment, we calculate the elastic and plastic strain increment as:

$$\Delta\epsilon = \Delta\epsilon^{el} + \Delta\epsilon^{pl} + \Delta\epsilon^{tw} \quad (1)$$

where $\Delta\epsilon$ is the total strain increment from the finite element (FE) solver, $\Delta\epsilon^{el}$ is the elastic strain increment, $\Delta\epsilon^{pl}$ is the plastic strain increment due to dislocation slip, and $\Delta\epsilon^{tw}$ is the twin shear strain. $\Delta\epsilon^{tw}$ is zero except for the twin domain during the process of twin formation. The rate of the plastic strain $\dot{\epsilon}^{pl}$ is calculated as:

$$\dot{\epsilon}^{pl} = \sum_k \mu^{(k)} \dot{\gamma}^{(k)}, \mu^{(k)} = \text{sym}(\vec{b}^{(k)} \otimes \vec{n}^{(k)}) \quad (2)$$

where $\mu^{(k)}$ is the symmetric part of the Schmid tensor for the slip system k , $\dot{\gamma}^{(k)}$ is the slip rate on the slip system k , $\vec{b}^{(k)}$ and $\vec{n}^{(k)}$ are the slip direction and the normal of the slip system k . A rate dependent equation is used to calculate the slip rates:

$$\dot{\gamma}^{(k)} = \dot{\gamma}_0 \left| \frac{\tau^{(k)}}{\tau_c^{(k)}} \right|^{1/m} \text{sign}(\tau^{(k)}) \quad (3)$$

where $\dot{\gamma}_0$ and m are two constants, representing the reference slip rate and the sensitivity exponent, respectively. $\tau^{(k)}$ and $\tau_c^{(k)}$ are the resolved shear stress on the slip system k and the critical resolved shear stress (CRSS) of this slip system, respectively. τ_c increases due to strain hardening. The Swift hardening law is used in the present study, and we assume an

identical τ_c for all the slip systems:

$$\tau_c = \tau_{c0} \left(1 + \frac{\Gamma_{tot}}{\Gamma_0}\right)^n, \Gamma_{tot} = \int_0^t \sum_k |\dot{\gamma}^{(k)}| dt \quad (4)$$

where τ_{c0} , Γ_0 and n are material parameters. In this work, the values for τ_{c0} , Γ_0 and n are assumed to be 50 MPa, 0.15 and 0.203. These values are not fine-tuned to match the experimental tensile curve. The present work shows therefore only qualitative results.

The twin shear strain is applied incrementally as a local transformation until the characteristic twin shear strain of the $\{332\} \langle 113 \rangle$ twinning, 0.3536, is fully applied into the twin domain:

$$\Delta\gamma^{tw} = \frac{0.3536}{t_{tw}} \Delta t, \Delta\epsilon^{tw} = \mu^{tw} \Delta\gamma^{tw} \quad (5)$$

where t_{tw} is the total time used for applying the twin shear strain, assumed to be 1 s, Δt is the time increment defined by the FE solver, and μ^{tw} is the Schmid tensor for the prescribed twin variant.

The simulation is performed in two steps as follows:

- Uniaxial tensile deformation along the x direction to 1% elongation. Except for the twin domain, plastic deformation is achieved through dislocation slip in 12 $\{110\} \langle 111 \rangle$ slip systems and 12 $\{112\} \langle 111 \rangle$ slip systems. These 24 slip systems are assumed to have the same CRSS. For the twin domain, $\Delta\epsilon^{tw}$ is imposed in this step.
- Macroscopic elastic unloading, and partial elastic unloading to account for zero out-of-plane stress at the free surface of the sample.

4. Simulation results and discussion

Results of the 2D simulation are shown in figure 4a. The stresses have been transformed to a coordinate system defined by the twin shear direction $\vec{b}$ and the twin normal $\vec{n}$. Stresses from the 2D simulation are similar to those reported in literature [5, 10]. For σ_{11} , a typical butterfly pattern is observed, and σ_{22} is relatively small. For σ_{12} , negative shear stresses, i.e. along the inverse direction of the twin shear direction, are observed inside and around the twin. σ_{12} is one of the most important parameters determining the propagation and thickening of a twin. When a twin forms, σ_{12} is expected to be lower than before twinning both inside and in the vicinity of the twin, as the present simulation shows. The decrease of σ_{12} is termed backstress [5]. Results from the 2D simulation are, however, not in agreement with the HREBSD measurements shown in figure 2. Simulated stresses from the 3D simulation are shown in figure 4b in the same plane as the 2D simulation. Compared with the 2D results, the 3D results have better agreement with experiments, especially for σ_{11} .

Differences between the 2D and 3D simulation results are firstly due to the fact that the twin measured by HREBSD is highly inclined with respect to the observation plane. Figure 5 illustrates the inclination of the twin in 3D. The plane in blue corresponds to the observation plane for the HREBSD measurement, as well as the plane shown in figure 4. The twin plane $\vec{n}$ is inclined 36° with respect to the observation plane. The twin shear direction $\vec{b}$ is not on the observation plane either, but forms an angle of 54° to the observation plane. When a 2D simulation is used, $\vec{n}$ and $\vec{b}$ should be in the simulated plane, because components of ϵ^{tw} out of plane cannot be considered in 2D simulations. This explains why the 2D simulation and the experimental results are significantly different. For many hcp materials, a strong fiber texture is present in the initial material, for which it is possible to find a 2D section where most of the twins have $\vec{b}$ and $\vec{n}$ more or less in the plane. For these situations, a 2D simulation may give satisfactory agreement with experiments (e.g. [4]), whereas a 3D model is needed to simulate inclined twins and/or twin shear out of the plane in more general cases.

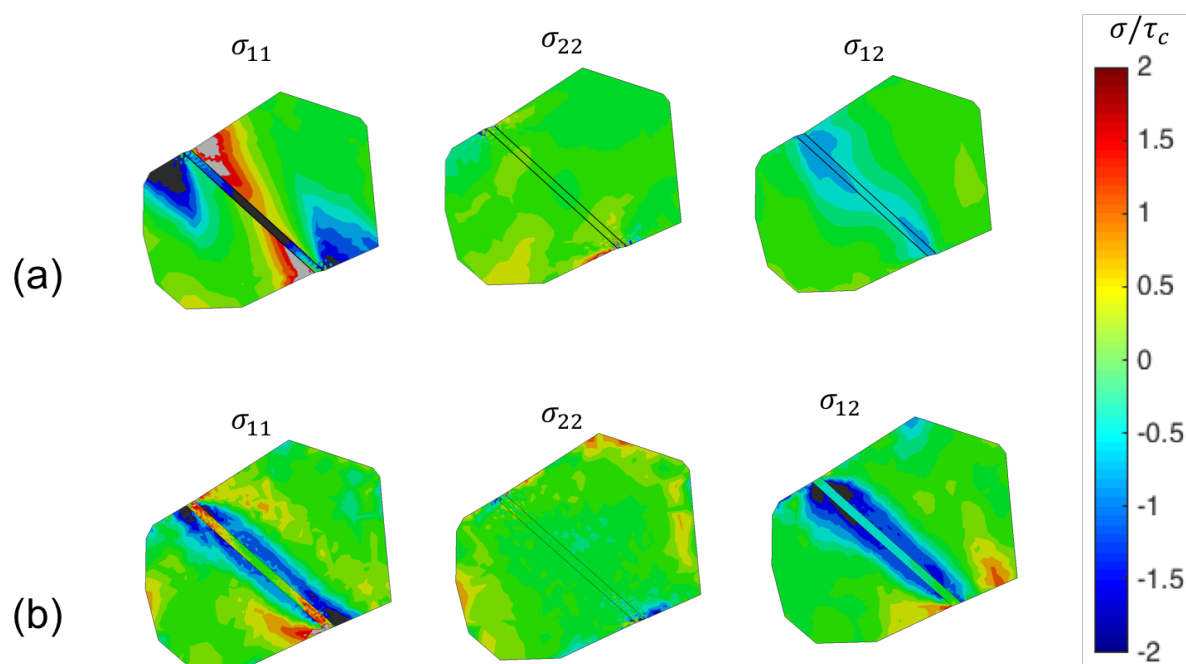


Figure 4. 2D (a) and 3D (b) simulations of the stress field around the twin. For the 3D simulation, the same 2D section as the 2D simulation is shown. The stresses are transformed to a coordinate system where direction 1 is the twin shear direction $\vec{b}$ and direction 2 is the normal direction of the twin plane $\vec{n}$ used for the simulations. Notice that $\vec{b}$ and $\vec{n}$ are on the simulated plane for the 2D simulation, whereas that $\vec{b}$ and $\vec{n}$ correspond to those observed experimentally for the 3D simulation.

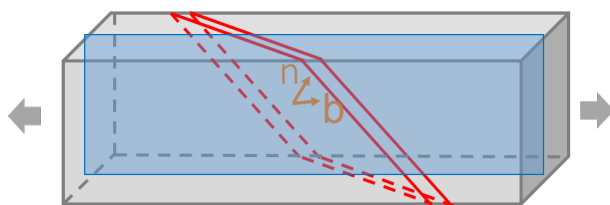


Figure 5. Sketch showing the inclination of the twin plane and twin shear direction for the grain shown in figure 2.

With the 3D model, it is also observed that stresses around the twin show through-thickness variations. Figure 6 shows the variation of σ_{11} in three sections parallel to each other. Figure 6b is approximately at the center of the grain, which is also shown in figure 4b. At the center of the grain, compressive σ_{11} values are found near both sides of the twin. Figures 6a and c are sections close to the edge of the grain, where the compressive σ_{11} at one side of the twin changes to tensile stresses. This change can be related to the influence of neighboring grains. In 2D simulations, only 2 neighboring grains more or less perpendicular to $\vec{b}$ can be considered, whereas in 3D, all neighbors are considered, including those at the lateral side of a twin plate.

The 3D simulation results shown in figure 4b agree qualitatively with the measurements. To get quantitative agreement, improvement of the model is needed. First, the hardening law needs to be fine-tuned. Second, except for the twin regions, it is considered that dislocation slip is the only mode for plastic deformation, however, according to the experimental results, martensitic

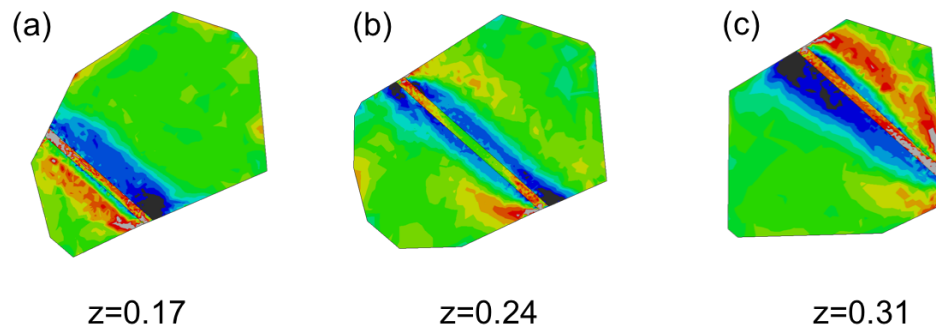


Figure 6. Variation of σ_{11} around the twin in three parallel sections according to the 3D simulation.

transformation and twinning occur simultaneously with dislocation slip. It is therefore necessary to consider the effects of martensitic transformation and twinning in neighboring grains, as well as in the parent grain. These effects will be taken into account in future work.

5. Conclusion

A 3D crystal plasticity finite element model is constructed and it is demonstrated that this model is able to capture the stress field around a mechanical twin. Conventional 2D simulations only give reliable results when the twin is perpendicular to the 2D plane and the twin shear direction is also in the 2D plane. For all the other cases, a 3D model is needed to achieve satisfactory simulations.

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References

- [1] Marteleur M, Sun F, Gloriant T, Vermaut P, Jacques P J and Prima F 2012 *Scripta Materialia* **66** 749–752
- [2] Sun F, Zhang J, Marteleur M, Gloriant T, Vermaut P, Laillé D, Castany P, Curfs C, Jacques P and Prima F 2013 *Acta Materialia* **61** 6406–6417
- [3] Wilkinson A J, Meaden G and Dingley D J 2006 *Ultramicroscopy* **106** 307–313
- [4] Abdolvand H and Wilkinson A J 2016 *International Journal of Plasticity* **84** 160–182
- [5] Kumar M A, Kanjarla A, Niezgoda S, Lebensohn R and Tomé C 2015 *Acta Materialia* **84** 349–358
- [6] Kumar M A, Beyerlein I J and Tomé C N 2016 *Acta Materialia* **116** 143–154
- [7] Kumar M A, Beyerlein I J, McCabe R J and Tome C N 2016 *Nature Communications* **7** 13826
- [8] Abdolvand H and Wilkinson A J 2016 *Acta Materialia* **105** 219–231
- [9] Barnett M R, Stanford N, Ghaderi A and Siska F 2013 *Acta Materialia* **61** 7859–7867
- [10] Zhang R Y, Daymond M R and Holt R A 2008 *Materials Science and Engineering: A* **473** 139–146
- [11] Lai M, Tazan C C and Raabe D 2016 *Acta Materialia* **111** 173–186
- [12] Ahmed M, Wexler D, Casillas G, Savvakini D G and Pereloma E V 2016 *Acta Materialia* **104** 190–200
- [13] Alkorta J 2013 *Ultramicroscopy* **131** 33–38
- [14] Marteleur M 2017 *On the plasticity mechanisms of β metastable Ti alloys, towards enhanced work hardening* Ph.D. thesis UCL-Université Catholique de Louvain
- [15] Alkorta J, Marteleur M, and Jacques P J 2017 *Ultramicroscopy* doi:10.1016/j.ultramicro.2017.06.015
- [16] Dancette S, Delannay L, Renard K, Melchior M and Jacques P 2012 *Acta Materialia* **60** 2135–2145