Local stress fields induced by twinning in β-metastable titanium alloys

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Abstract. A 3D crystal plasticity finite element model incorporating deformation twinning is constructed. This model is applied to simulate the stress fields around a twin lamella in a β-metastable titanium alloy. The stress fields determined by the 3D simulation show good agreement with those measured experimentally using high resolution electron backscattered diffraction (HREBSD).

Introduction

Among different families of titanium alloys, β-stabilized Ti alloys have attracted a lot of attention during the last years. However, these alloys generally suffer from lack of work hardening, which limits their ductility. Recently, several β-metastable Ti grades have been designed to exhibit simultaneous TRIP (TRansformation Induced Plasticity) and TWIP (TWinning Induced Plasticity) effects [1,2]. It has been demonstrated that the work hardening capacity of the as-quenched β phase is improved when stress-induced α" martensitic laths and deformation twins appear in the course of deformation, forming obstacles to dislocation glide [3].

Deformation twinning imposes local strains, which must be accommodated by neighboring grains. Twinning will thus lead to local stress concentration, which significantly affects the mechanical behavior of the material. The local stresses can be determined using HREBSD [4,5]. In this work, a 3D crystal plasticity finite element model (CPFEM) is constructed. This model is applied to the Ti alloy, in order to understand formation of local stress fields in the vicinity of deformation twins.

Experimental results

A binary Ti-12 wt% Mo alloy was investigated [3]. The ingot was first rolled at room temperature to a thickness reduction of 95%, followed by annealing at 1173K for 30 min. A fully recrystallized microstructure with entirely β titanium was obtained, and the grain size was around 50 μm. Uniaxial tensile deformation was then applied along the previous rolling direction.

After applying only 1% tensile strain, twinning was already observed in some grains. As the tensile strain increased, twinning occurred in more grains, and the twin density inside individual grains also increased. The activated twinning system in this alloy is {332}<113>, as determined from the twin and matrix orientations measured by EBSD, which is different from the conventional {112}<111> twinning for body centered cubic metals. The elastic strains and stresses around a twin were determined using HREBSD, and the results are shown in Fig. 7.15 in [6] (submitted for publication).

Crystal plasticity modelling

A 3D mesh containing 27 grains was constructed for the simulation. The geometry of the polycrystal structure is shown in Fig. 1a. Periodic boundary conditions were applied. Crystallographic orientations were assigned to each grain according to the experimentally measured texture. A twin domain is prescribed inside one grain, which is defined by two parallel interfaces (Fig.1b). The parent grain and the twin were assigned the parent and twin orientations measured by HREBSD, respectively. The normal direction of the twin interface corresponds to the {332} plane shared by the parent and the twin orientations. The mesh was refined around the twin domain. As a comparison, a 2D polycrystal structure was obtained using a 2D cut of the 3D structure, from which a 2D mesh was constructed.

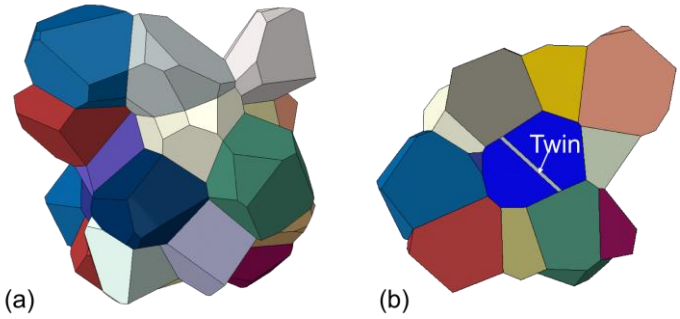

Fig. 1. Representation of grains used in the study. (a) The initial 3D polycrystal structure with periodic boundary conditions. (b) A 2D cut of the 3D mesh showing the precribed twin in one grain. This section is also used for 2D simulation for comparison

The simulation was performed in two steps as follows:

1. Initial uniaxial tensile deformation along the x direction to a strain of 1%. Except for the twin domain, plastic deformation is achieved through dislocation slip, which was simulated using a crystal plasticity subroutine [7]. For the twin domain, an extra shear strain of $\sqrt{3}/4$ was imposed gradually during the tensile loading. During this process, local plastic accommodation occurred around the twin.
2. Elastic unloading of the free surface to mimic the state of the sample for HR-EBSD measurement.

Simulation results

The 2D simulation results show the typical butterfly pattern (Fig. 2). However, this is significantly different from the experimental results in [6]. The 3D simulation provides a much better agreement with experiments. The failure of 2D simulation is because the experimentally measured twin is highly inclined to the observation plane and the twin shear direction is also out of the observation plane. For this situation, 3D simulation is needed to investigate the stress fields around the twin.

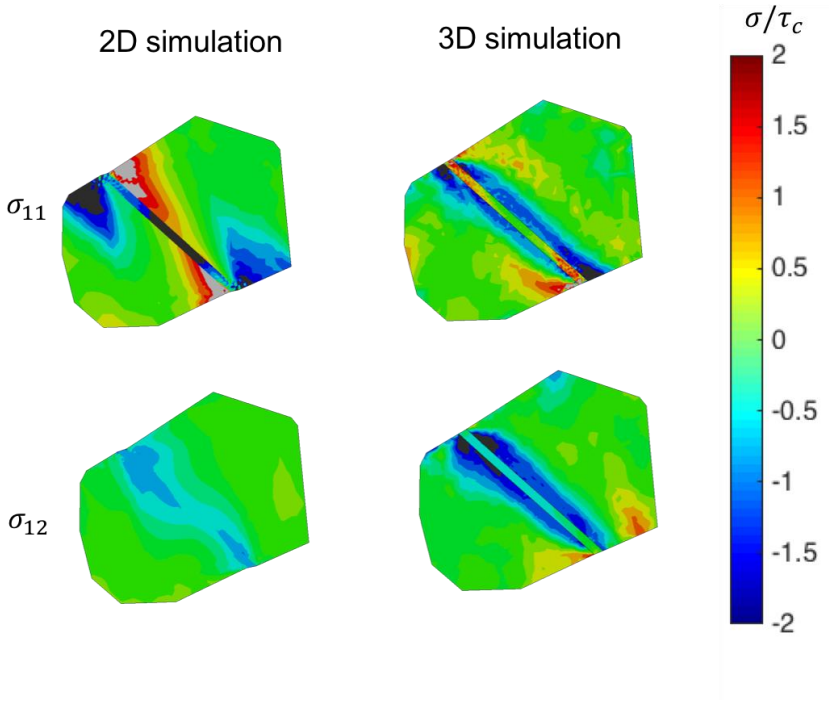

Fig. 2. 2D and 3D simulations of the stress fields around the twin. The stresses are transformed in a coordinate system, where direction 1 is the twin shear direction and direction 2 is the normal direction of the twin plane. For the 3D simulation, the same 2D plane as the 2D simulation is shown.

Conclusions

A 3D CPFEM model is constructed and is demonstrated to be able to capture the stress fields around mechanical twins. The conventional 2D simulation only works 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, the 3D model is needed to give a satisfactory simulation.

References

[1] M. Marterleur et al. Scripta Mater. Vol 66 (2012), p. 749-752
[2] F. Sun et al. Scripta Mater. Vol 94 (2015), p.17-20
[3] F. Sun et al. Acta Mater. Vol 61 (2013), p.6406-6417
[4] A.J. Wilkinson et al. Ultramicroscopy Vol 106 (2006), p.307-313
[5] N. Isasti et al. JOM Vol 69 (2016), p.215-223
[6] M. Marteleur, PhD thesis, Université catholique de Louvain, (2017)
[7] L. Delannay et al. Int.J.Plasticity Vol 22 (2006), p.1879-1898