Materials & Design 83 (2015) 327–343

Contents lists available at ScienceDirect

Materials & Design

journal homepage: www.elsevier.com/locate/matdes

Modelling twinning evolution during plastic deformation in hexagonal close-packed metals

Enrique I. Galindo-Nava

Department of Materials Science and Metallurgy, University of Cambridge, 27 Charles Babbage Rd, Cambridge CB3 0FS, UK

ARTICLE INFO

Article history:
Received 2 January 2015
Revised 10 April 2015
Accepted 1 June 2015
Available online 19 June 2015

Keywords:
Twinning
Modelling
Grain boundaries
Magnesium
Titanium
Crystal plasticity

ABSTRACT

A new model describing the twin size and volume fraction evolution at the grain level is proposed. An evolution equation for the mean twin length on individual grains is expressed in terms of the local grain structure. This includes characterising the grain size and orientation distributions in the deformed specimen. Additionally, the twin volume fraction is predicted by computing the collective twin volume increments on each grain, if the grain structure is known. A twin nucleation-rate equation is proposed; it depends on dislocation activity, and the local twin and grain orientations. The model is applied to describe twinning behaviour in Be, Hf, Mg, Ti and Zr for various loading and texture conditions, including Y addition effects in MgY alloys. Twinning evolution is compared in Mg holding unimodal and bimodal grain size distributions.

1. Introduction

Understanding twinning behaviour is essential for improving the mechanical properties and formability in hexagonal close-packed (HCP) metals [1]. Deformation twinning is activated at the grain level due to the low number of slip systems being insufficient to accommodate strain incompatibilities [2]. Twinning and dislocation activity are highly anisotropic, leading to considerable variations in mechanical and texture evolution under dissimilar loading conditions.

Twinning behaviour shows distinctive variations with grain size [3,4]. For instance, the shear stress required for slip and twin activation increases as the grain size decreases [5,3,6]. Ghaderi and Barnett [7] have shown that the twin volume fraction in Ti can increase from 3% to 25% if the mean grain size increases from 18 to 204 μm; similar results were found by Barnett et al. in a Mg alloy [4]. Tsai and Chang [8] have also observed strong grain size dependence of compressive twinning evolution in AZ31. The twin length is also limited by the grain size [3]. Additionally, Capolungo et al. [9] performed a statistical analysis in Zr for correlating the grain misorientation, size and Schmid factor effects on twinning. They found that the twins with highest Schmid factor have the highest probability of activation and the grains aligned to the loading direction display a higher twin density. This implies that the grain structure also affects twinning activity, via local grain orientations. Additionally, modern thermomechanical processing routes for grain refinement, such as equal-channel angular pressing (ECAP), introduce complex grain structures, such as bimodal grain size distributions [10], and increasing the complexity in understanding twinning behaviour during deformation.

A number of modelling approaches have been proposed for describing twinning and texture evolution with strain, as well as the macroscopic flow stress response. For instance, crystal plasticity introduces anisotropic deformation gradients on the various slip and twin planes [11–13]. Constitutive relations are employed for the resolved shear stress to activate a specific slip or twin mode, a lattice rotation tensor is introduced to account for local reorientations, and the grain size effects are introduced via adding a Hall–Petch term in the resolved shear stress for slip/twinning. The twin volume fraction evolution is simply defined as the ratio between the shear increments of the active twin mode and the characteristic twin shear [14,15]; no information on the twin size and number behaviour is introduced. A viscoplastic self-consistent (VPSC) formulation has been employed by several authors to describe the relative dislocation and twinning activity and predicting the macroscopic flow stress and texture evolution [16–18]; twinning behaviour is treated in the same fashion as in crystal plasticity. Further discussion on these approaches and additional models can be found elsewhere [19,20]. Models including grain size effects on twinning evolution have not been explored in detail, despite twinning being a process occurring at the grain level and displaying strong interrelations [7,4,21,8]. Beyerlein and Tomé [22] have

E-mail address: eg375@cam.ac.uk

http://dx.doi.org/10.1016/j.matdes.2015.06.025
0264-1275/

proposed a probabilistic twin nucleation model at grain boundaries for HCP metas; it is based on estimating the probability for a grain-boundary dislocation to dissociate into partials and nucleate a twin. This model has been integrated by Beyerlein et al. [23] into a crystal plasticity constitutive framework for describing twinning evolution during straining. Although they introduce grain size effects in the twin nucleation rate, their predictions of the twin volume fraction evolution are insensitive to grain size variations; they also concluded that $\{10\bar{1}2\}$ twins do not follow a Hall–Petch law. This implies that by only adding a Hall–Petch term in the resolved shear stress for twinning is insufficient for capturing the grain size effects. Niezgoda et al. [24] have also proposed a stochastic model for twin nucleation in Zr; it is based on linking the probability of twin nucleation with the stress build-up at grain boundaries. A random fluctuating stress term is added to the stress increments to account for the random nature of twin nucleation; no grain size effects were considered. These results suggest describing twinning evolution at the grain level is required to further understand its variations with the initial grain structure and processing conditions [25]. This will also allow us to improve the predictive capabilities of current modelling techniques by also including a complete twinning characterisation in terms of the initial microstructure.

The objective of this work is to define a theoretical framework for describing twinning evolution (mean size, number and volume fraction) with strain in HCP metals. This methodology aims in describing twinning on individual grains and reproducing their collective behaviour if the grain structure is known. This requires: (1) characterising the grain size and orientation (via the Schmid factor) distributions in the deformed specimen (Section 2); this allows us to construct a grain ensemble in the specimen that will determine twin behaviour. (2) Postulating equations for the mean twin size (length and thickness) and nucleation rate in terms of the grain size and local orientations (Section 3); the nucleation rate incorporates dislocation activity effects. (3) Finally, the twin size evolution equations on individual grains can be combined with the grain ensemble for obtaining the twin volume fraction in the specimen. The model results are applied to Be, Ti, Hf, Mg and its alloys, and Zr for several deformation conditions in Section 4; the role of Y additions in the twinning behaviour in MgY alloys is discussed. A summary on the model features and additional model applications are shown in Section 5. The effect on twinning evolution in Mg holding a bimodal grain structure is also explored. Concluding remarks are presented in Section 6. This work is limited to study microstructure evolution with plastic strain, where the evolution equations are assumed to be valid above the yield point. The stress levels then lie above the critical resolved shear stress of the respective active slip modes on each material. This assumption is consistent with the findings by Ghaderi and Barnett [7], where they observed in the plastic region similar stress dependence on the twin number per unit area in Mg and Ti. This implies that similar evolution laws are held in these materials in the plastic regime; material-related effects are introduced in the twin nucleation rate and aspect ratio. Uniaxial compression/tension are considered in this work; these conditions impose the level of macroscopic strain ε by fixing a constant strain rate. This implies that describing twinning evolution with ε is equivalent to describing twinning evolution with applied stress σ, as these parameters are uniquely related in the plastic region. For simplicity in the calculations, fixed dislocation density with strain will be assumed, and it is only affected by temperature, strain rate, grain size and orientation variations.

2. Twinning activation: grain size and orientation distributions

Describing twinning evolution in polycrystalline materials requires characterising the grain structure and local orientation distributions. These are represented by the grain size, which can be obtained by means of the mean intercept method, and Schmid factor distributions. Twins with the highest Schmid factor are more likely to be activated [26], whereas twin nucleation and growth can increase in coarser grains due to lower dislocation densities [27–29] and higher stress concentrations at grain boundaries [3,24].

Twinning evolution in various HCP metals is explored in this work; the experimental data were obtained from the literature. Table 1 shows the denomination employed in this work and deformation conditions of these materials; D stands for the mean grain size; In the case of Be, the grain size was reported to be lower than 50 μm; $D = 30$ μm was considered for the model calculations. No solid solution effects in the twinning behaviour are considered in AZ31; this is to simplify the model calculations, as the twin volume fraction variations between this alloy and pure Mg are small [30]. A similar case applies for MgY alloys, where solid solution effects are considered to affect the texture and activation rate of additional slip systems. IPC and TTC stand for uniaxial in-plane and trough-thickness compression, respectively, i.e. compression parallel and traverse to the rolling direction, respectively; Ten. stands for uniaxial tension parallel to the rolling direction. A typical rolling texture consists of strong basal fibres along the normal direction of rolling. Almost every experimental result under study displays strong basal texture from previous thermomechanical processing [31]; most of the experimental textures lie 20° within the ideal rolling texture (basal poles 20° from the normal direction). This is further discussed in Section 2.2.

2.1. System under consideration

The system under study consists of a specimen undergoing uniaxial deformation. The specimen contains N_g grains of different size D_k, with $k = 1, \ldots, N_g$, and mean value $D; N_g$ depends upon the specimen's volume. Different twin activity occurs on each grain (depending on its local activation). The activation of two twin modes on each grain is considered only. For a given macroscopic strain ε, a grain k of size D_k contains N_k^t and N_k^c twins of mode t and c, respectively. In order to account for the planar nature of twins, it is assumed that the twin depth instantaneously expands in one direction throughout the grain once it is nucleated, i.e. the twin depth equals D_k. Describing the expansion rate of the twin length and thickness is only needed. If a twin aspect ratio is assumed constant with strain, the twin length and thickness will expand at the same rate; this is further explored in Section 3. The t-mode twins have length $L_{k,j}^t$, thickness $w_{k,j}^t$ and Schmid factor m_k^t, where $j = 1, \ldots, N_k^t$; a similar case occurs for c-mode twins with parameters: $L_{k,j}^c, w_{k,j}^c$ and m_k^c, where $j = 1, \ldots, N_k^c$. It is assumed that the initial grain orientation is constant in the grain interiors. Fig. 1(a) shows a schematic representation of this system: the black prisms delineate the grain boundaries (D_k), the hexagonal prisms represent the relative orientation on each grain (m_k^t and m_k^c), the blue (solid) and red (dashed) rectangles represent the t- and c-mode twins ($\{L_{k,j}^t, w_{k,j}^t\}_{j=1}^{N_k^t}$ and $\{L_{k,j}^c, w_{k,j}^c\}_{j=1}^{N_k^c}$), respectively; twins of rectangular shape are assumed, and the depth of each twin lies orthogonal to the figure to simplify the analysis. It is considered that c-mode (secondary) twins active within the t-twins. Three deformation conditions are considered: compression parallel to the rolling direction, i.e. in-plane compression (IPC), compression normal to the rolling direction, i.e. through-thickness compression (TTC), and uniaxial tension. Fig. 1(b)–(d) shows the schematic representation on the twinning behaviour for these conditions. The rolling direction lies parallel to the vertical axis; tensile and compressive twins are represented by the blue and red rectangles, respectively. Twinning activity is high in grains oriented parallel to the loading direction (high Schmid factor), whereas it decreases in grains oriented traverse to the loading direction