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Numerical analysis of twin thickening process in magnesium alloys

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ABSTRACT

A finite element study of the stress field evolution around the $\{10\bar{1}2\}$ tensile twin of different thickness in magnesium alloy is performed. The system is represented by the 2D models of one and three elastic elliptical inclusions with different aspect ratios surrounded by the plastic matrix. Anisotropic elasticity and crystal plasticity theory are used to describe the material behavior. Numerical results for single inclusion overestimate the initial stress for the stable twin aspect ratio by a factor of two compared to the experimental results. Multiple inclusions case obtains values closer to the experimental ones. Therefore it is concluded that the process of twin thickening cannot be solved within the analysis of the single inclusion and an interaction between twins in the same and neighboring grains plays a crucial role during the twin thickening process.

1. Introduction

Twining is an important deformation mechanism in HCP metals [1–5]. Its presence is linked with the limited number of easily activated slip systems. The process of twinning is usually divided into three stages: nucleation, propagation and thickening. Nucleation is a localized phenomenon based on the interaction between grain boundaries and dislocations [6,7]. Twin propagation is a rapid increase in twin diameter that follows nucleation. It terminates once a twin impinges upon the boundaries of its parent grain or another obstacle. Twin propagation is accompanied by the relaxation of stresses inside the grain. Therefore, it is supposed that stress relaxation is a driving force for twinning [8,9]. The last stage is a twin thickening where the twin grows in thickness. It is assumed that this occurs until a stable twin aspect ratio is attained. The aspect ratio is thus expected to vary with applied stress. Ghaderi and Barnett [10,11] have measured twin aspect ratio with respect to the average applied twin shear stress for compression tests on an extruded magnesium AZ31 alloy. The results are shown in Fig. 1 for different grain sizes. The average applied twin shear stress is defined as: $\tau_i = k \cdot \sigma$, where k is the twin Schmid factor and σ is the applied stress. There is a clear trend in the increase of twin aspect ratio with initial stress. Eshelby type analysis has been applied to the problem by a number of works [12–14]. This analysis determines the stresses inside an elliptical inclusion that undergoes an internal shear transformation. The elliptical inclusion has a particular advantage as it produces a uniform back stress field for an elastic solution and it also closely resembles the real twin shape. This kind of solution allows one to establish direct relations between the aspect ratio and the back stress. However, the solutions based on the elastic theory underestimates the stable twin aspect ratios by an order of magnitude. Therefore it is clear that plasticity induced in the twin vicinity plays a crucial role in achieving the local equilibrium. There are several numerical studies that have investigated stress fields around individual twins in plastic media. Zhang et al. [15,16] performed 2D and 3D FE simulations of lamellar twin inside an elastic-plastic media and proved that there are stress relaxation and state of minimal energy for given twin thickness. Barnett et al. [17] performed similar simulations for elliptical twin and proved the relation between the twin aspect ratio and initial stress for zero average stress inside the twin. The study showed the significance of plasticity on the back stress relaxation, but the predictions of the stable twin aspect ratios were still at least two times smaller than the experimentally measured ones. Kumar et al. [18] have used the crystal plasticity FFT based model to simulate a lamellar twin inside a matrix composed of several grains with different orientations. They found that stresses are non-uniformly distributed inside twins due to the effect of the plastic relaxation. The orientation of the neighboring grain was found to have only a minor effect on the stresses inside the twin.

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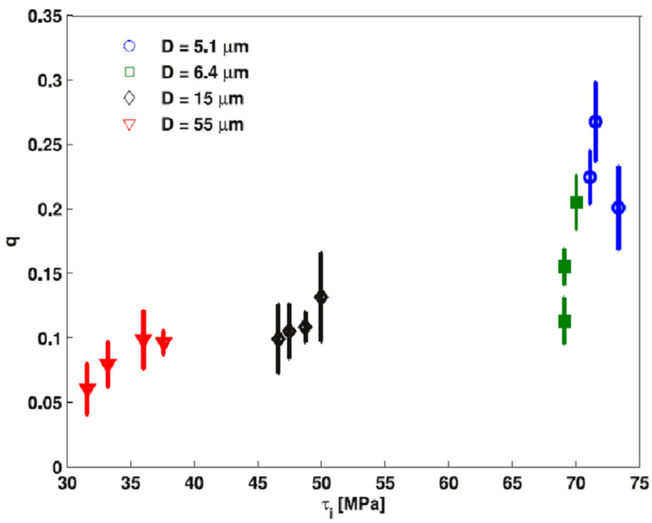

Fig. 1. The relation between stable twin aspect ratio and applied shear stress during compression test of AZ 31 alloy with different grain size [10]. The applied shear stress is defined as: $\tau_i = k \cdot \sigma$, where k is the twin Schmid factor and σ is the applied stress.

Experiments show that interactions between twins can play a crucial role in twin nucleation, growth, and thickening. It was observed that a number of twins in grain increases with increasing grain size [19–22]. It is also observed that twins create band structures which suggest that there is a strong interaction between twins across grain boundaries [23]. Kumar et al. [24] performed a numerical study of interactions between parallel lamellar twins in one grain and proves that stress fields induced by twins influence their spacing and therefore a number of twins within one grain.

The present study simulates an elliptical twin inside a constraining matrix using an FE crystal plasticity model. The main goals are to investigate the stress field around the elliptical twin with different aspect ratios and compare numerically predicted values of initial stress for stable twins with experimental observations. An interaction of twins across the grain boundary is also analyzed. The process of twin thickening inside the grain is described upon an analysis of the results. The next section is dedicated to the description of FE model and constitutive behavior. Results are described next and this is followed by a discussion of the twin thickening process. The last chapter summarizes the main results.

2. Simulations

The system is modeled as a 2D elliptical inclusion inside a matrix. The basic scheme with boundary conditions is shown in Fig. 2. A central grain is surrounded by four neighboring grains. In our case, all neighboring grains have the same orientation so the division is illustrative. An initial stress is imposed as a pressure on the vertical edges in the direction of the global X-axis. The dashed line square represents a boundary inside the system, the sides of which are constrained to remain straight and parallel during deformation. These two conditions provide stress and kinematic boundary conditions. The whole system is protected against rigid body movement by fixed nodes in the centers of the frame edges (illustrated by the black dots in Fig. 2). The elliptical inclusion is inclined to the global X-axis by 46.84° which corresponds to a $\{10\bar{1}2\}$ tensile twin in an ideally oriented Mg crystal being extended along the c-axis. The local coordinate system of the twin is defined so that the 1-axis is parallel to the major axis of the ellipse and the 2-axis is in the direction of the minor axis. Four aspect ratios are taken into

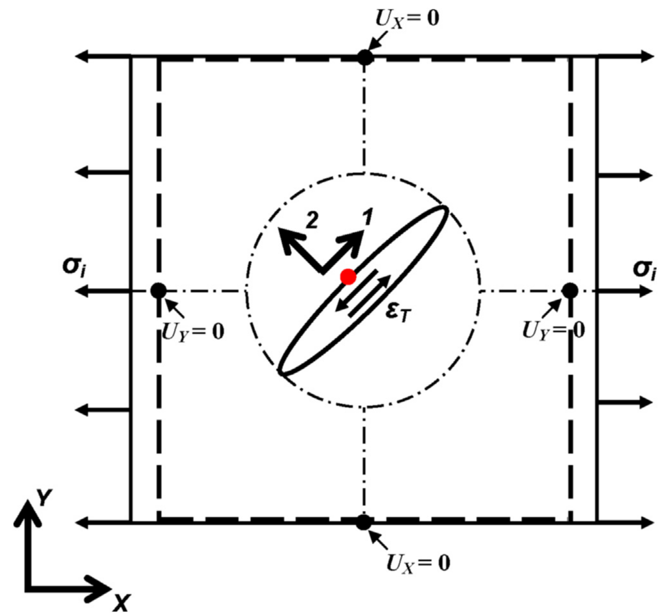

Fig. 2. Schematic of the simulated system with prescribed boundary conditions and loading. (not in scale). Dashed line defines the frame that remains straight and parallel during simulations. Dash-dotted line shows the division of the domain on individual grains. Red spot at the grain boundary indicates the location that is used to extract stress values. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

account: 0.05 (1/20), 0.067 (1/15), 0.1 (1/10) and 0.2 (1/5). All of these values lie within the experimentally observed range.

The FEM simulations were performed using the Z-set code [25] with 2.5D eight-node quadratic elements. The mesh is 2D but the calculation of constitutive behavior accounts also for out of plane slip systems. Plane strain conditions are prescribed in the out of plane direction.

The size of the simulated system is expressed in arbitrary units as the model does not include any internal length scale. Matrix is a square of 100 × 100 units and the inclusion has a major axis 26 units long. The mesh density is increased in the central part around the inclusion because this is an area of stress concentration. The typical size of an element in this region is 0.06 units^2 which is sufficient according to a mesh density study.

Loading of the system is imposed in two steps. The first step is used to apply an external load of a given level. This is performed by an application of stress at the external vertical edges. This stress is held constant during the second step. An internal shear in the inclusion is introduced by a pseudo-thermal deformation. An anisotropic expansion coefficient is defined in the twin coordinates. An artificial increase of temperature then induces the desired twinning shear (0.13 for $\{10\bar{1}2\}$ tensile twin in magnesium).

Material behavior of the matrix is modeled within the framework of crystal plasticity. The theory is based on decomposition of the deformation gradient into elastic and plastic parts [26,27]:

$$\mathbf{F} = \mathbf{F^e F^p} \tag{1}$$

where the plastic part is related to the slip occurring in slip systems characterized by slip direction ($\mathrm{m^s}$) and normal to the slip plane ($\mathrm{n^s}$). It can be written as:

$$\dot{\mathbf{F}}^{\mathbf{p}} \mathbf{F}^{\mathbf{p}-1} = \sum_{s=1}^{n} \dot{\gamma}^s \mathbf{m^s} \otimes \mathbf{n^s}. \tag{2}$$