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Simulation of deformation twins and their interactions with cracks

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ABSTRACT

A discrete dislocation model was used to simulate residual stress fields close to deformation twins in stainless steels. Dislocation pairs were distributed along an initially elliptical twin boundary and an iterative scheme used to allow the dislocations to relax towards positions where the internal shear stresses were below a friction stress. The relaxed twin shape was close to elliptical but the flanks were flatter and the twin tips where the grain boundaries are situated were somewhat blunted compared to an ellipse. A dislocation-based boundary element model was then used to assess the interaction between the stress field from such twins and a crack. The stress field near the tip of the crack was characterized in terms of mode I and mode II stress intensity factors. The effects of twin width, length, orientation and distance from the crack tip on the strength of the interaction were studied. Wider, shorter twins were found to induce the largest stress intensity at the crack tip when close to the crack tip and aligned perpendicular to the crack plane. The influence of a pair of deformation twins does not significantly exceed the influence of a single deformation twin.

1. Introduction

Slip and twinning are the major deformation modes which enable a crystalline solid to generate a permanent shape change under the action of an applied stress. An extensive review on deformation twinning has been given by Christian and Mahajan [1]. Considerably more attention has been paid to understanding slip than twinning but there is currently interest in twinning. The classical definition of twinning requires that the twin and matrix lattices are related by either a reflection in some plane or by a rotation of 180° about some axis [1]. In many cases especially for the FCC, HCP and BCC metals both of these conditions are met and such twins are termed compound twins. Deformation twins can form by a homogeneous simple shear of the parent lattice. Deformation twinning has been observed in FCC, BCC and HCP metals and the characteristic shear strains can be quite large. The large lattice rotation between a twin and the parent lattice makes deformation twinning have a significant impact on both the intensity and nature of deformation textures [2,3]. Deformation twins often take up a lenticular shape in order to best accommodate the large shear strain while minimizing strain energy generated within the surrounding matrix [1].

In the FCC metals deformation twinning is perhaps most studied in steels where a class of austenitic alloys known as TWIP (twinning induced plasticity) steels have been developed primarily for the automotive industry e.g. [4–6]. In the austenitic stainless steels there is also evidence of intense twin-like deformation bands that form in increasing number during cold deformation [7–10] and are characterized by the classic 60° rotation about ⟨1 1 1⟩ compared to the matrix grain. There is some evidence that significant plastic deformation is required before these twins are observed and the threshold strain is dependent on the alloy composition [7–11]. These deformation twin bands are of considerable technological importance and are currently of particular interest within the nuclear industry because they have been found to be present in alloys that have shown susceptibility to intergranular stress corrosion cracking (SCC) in the cold worked state. In these alloys the SCC cracks mostly follow grain boundaries which have been oxidized and embrittled by the environmental exposure (hydrogenated water at moderate ~300 °C temperatures) prior to cracking. Segregation during sensitization through either thermal exposure in service or accelerated heat treatment before laboratory tests and irradiation damage may worsen the situation but neither are necessary. This is of very significant concern because steels such as 304 had until relatively recently been largely considered immune to SCC in these environments [9]. Detailed TEM work by Lozano-Perez et al. [9] showed that deformation twins intersecting a free surface are preferred SCC nucleation sites while crack tips growing along grain boundaries branch into intersecting twin-like deformation bands which are preferentially oxidised.

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Deformation twinning has been modeled using a variety of approaches including molecular dynamics simulation [12–15], dislocation [16], disclination dipole [17] and finite element [18,19] modeling. The dislocation modeling approach is of interest here as it allows us to combine modeling of the twin with dislocation modeling of the crack. Mitchell and Hirth [16] gave an elegant model using a continuous density distribution of infinitesimal partial dislocations within a double-ended dislocation pile-up to represent the deformation twin. An analytical solution in which dislocations were at equilibrium was found for the density distribution and shape of the deformation twin via Hilbert transformations. The shape of an isolated twin in their 2 dimensional analysis was found to be an ellipse to first approximation though higher order terms show that twin tips are blunter with increasing stress while the twin boundary is populated with edge dislocations, while higher stress tends to sharpen the twin tip for the screw case.

Dislocation mechanics has a more extensive history in the modeling of cracks and fracture. The seminal work by Billby Cotterell and Swinden [20,21] found equilibrium solutions for continuous density distributions of infinitesimal dislocation arrays representing the crack and associated plastic zone. A second type of solution to this problem in which dislocation densities are allowed to increase at the far end of the plastic zone which is blocked by a microstructural feature has found considerable use in modeling short fatigue crack propagation [22–24]. However, more complex geometries and loading cases have required a move to discrete dislocation treatments and numerical simulation rather than analytical solutions [25–34].

The question we seek to address in this paper is whether or not localized stresses near the tips of deformation twins seen in cold worked austenitic stainless steels could provide significant enhancement of the mechanical driving force for intergranular cracks and thus, in part, contribute to the recently observed susceptibility to stress corrosion cracking. To this end we develop a discrete dislocation version of the Mitchell and Hirth [16] model of deformation twins using arrays of edge dislocations which are allowed to relax to an equilibrium configuration. Stresses from the deformation twin are then used to load a dislocation-based boundary element model of a crack, which is assumed to be growing along a straight section of grain boundary at which the twin has terminated on one side of the boundary. The effects of the size, proximity and inclination of the deformation twin on the stress intensity factors (modes I and II) induced at the crack tip are investigated. For ease of computation we work within an elastically isotropic medium. We also assume that the ideal twinning shear for $\langle 1\,1\,2\rangle\{11\bar{1}\}$ twins in FCC crystals is present and does not relax through dislocation mediated plasticity and that the twin shape is not perturbed by the presence of the crack. These assumptions make our calculations an upperbound assessment of the stress intensity that could be generated by the deformation twin.

2. Methodology

2.1. Simulation of deformation twins

To simulate twins, we start from an elliptical shape with partial dislocations positioned along the elliptical twin boundary as proposed in [16] (see Fig. 1). For an ellipse centred at the origin with its major axis along the x'-direction partial dislocations in the right hand half of the ellipse have positive Burgers vector while those at positions mirrored across the y'-axis have negative Burgers vector. The Burgers vectors are of 1/6 a[1 1 2] type (i.e. the x'-axis is parallel to [1 1 2]) with magnitude $b = a/\sqrt{6}$. The twin is on the $(11\bar{1})$ plane (i.e. the y'-axis is along $[11\bar{1}]$) with the partial

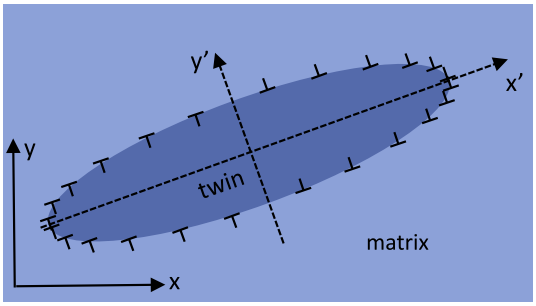

Fig. 1. Discrete dislocation array representation of a twin.

dislocations on planes separated along the y'-axis by $a/\sqrt{3}$. The characteristic twinning shear γ is then given by b/d (where d is the spacing of slip planes along the y'-axis) and is $1/\sqrt{2}$ for the FCC system.

In order to find a relaxed twin shape an elliptical starting geometry was chosen which is known to be a reasonably good approximation. The twin was then divided up into a number of slip planes spaced much further apart in the simulation than the $(11\bar{1})$ planes in the crystal. To keep the required twinning shear of $1/\sqrt{2}$ for our chosen material the magnitude of the Burgers vector for all dislocation partials at the boundary of the twin are changed in proportion to the plane spacing.

The shear stress generated by all the partial dislocations positioned on the twin boundary is then calculated at the dislocation positions. Dislocations are then moved according to their shear stress. If the shear stress is higher than a fixed critical shear stress (or friction stress) + τ_c, the dislocation is moved outward, away from the centre of the ellipse. The distance of movement was set at one quarter of the distance from the current position of the dislocation to that of the neighboring dislocation (which is further outward). The movement was constrained to be along the x'-direction i.e. along a horizontal plane (constant y'). Dislocations are not permitted to move beyond the original two ends of the twin which are considered pinned by impenetrable grain boundaries. If the shear stress at a dislocation position is below $-\tau_c$ it is moved toward the centre. Again the distance between the dislocation location and the neighboring dislocation (closer to centre) is calculated and the dislocation is allowed to move one quarter of that distance toward $x' = 0$, again with y' constant. Once dislocations at $x' = 0$ start to pile-up, distances between dislocations of the two twin halves on the same planes are calculated and dislocation pairs are allowed to eliminate once their separation is smaller than 1 nm (at which point the mutual interaction causes stresses in excess of 1 GPa).

Using the approach of moving dislocation partials along horizontal planes according to their shear stresses does not result in a twin shape with zero shear stresses along the twin boundary (calculated at the positions of dislocations). Therefore, a friction stress τ_c has to be introduced as mentioned earlier to define a maximum and minimum shear stress. If the shear stress at a dislocation position is within the range $-\tau_c$ to $+\tau_c$ then the dislocation at that position does not move. Once a relaxed twin shape is obtained a coordinate transformation is conducted and the twin is turned to allow the deformation twin to be placed in front of the crack tip.

2.2. Simulation of crack opening and stress field

For the simulation of crack propagation a dislocation-based boundary element model BEM approach was developed as had previously been used by Riemelmoser et al., Nowell et al. and Schick et al. [25–28,30]. The most important principles of the modeling