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The effects of twins on the large strain deformation and fracture of hexagonal close packed crystalline materials

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ABSTRACT

We investigated how twin modes in hexagonal close packed materials can affect large inelastic strain behavior and fracture. We considered the two twin mode systems of $(11\bar{2}1)[\bar{1}\bar{1}26]$ and (0001) $[\bar{1}\bar{1}20]$ in zircaloy-2, with each mode having 24 unique twin systems. We then incorporated these twin and parent slip systems with a dislocation-density crystalline plasticity, a non-linear finite-element, and fracture framework that accounts for crack nucleation and propagation. We investigated how these twin modes affect the interrelated effects of crack nucleation and propagation, dislocation density and inelastic slip evolution, stress accumulation, and lattice rotation. The predictions indicate that twin modes significantly affect local deformation and fracture behavior, and, therefore, are essential for the accurate representation of behavior at different physical scales in heterogeneous crystalline hexagonal close packed systems.

1. Introduction

Hexagonal close packed crystalline (h.c.p.) based alloys have extensive applications for high temperature and strength functionalities. This is due to a combination of desirable mechanical strength, high corrosion resistance, and strong creep resistance [1–4]. Twinning is a dominant deformation mechanism in h.c.p. materials, and it can significantly affect behavior, such as fracture, strength, and ductility, at different scales [5–18]. Kaschner and Tome [19] have proposed a dislocation barrier model, where tensile and compressive twins impede the propagation of dislocations and other twins in zirconium, and they concluded that twins play a dominant role in affecting the overall hardening of h.c.p. crystalline systems. In contrast to face centered cubic (f.c.c.) and body centered cubic (b.c.c.) materials, which have a limited numbers of twinning systems, there are at least seven twinning modes in h.c.p. materials [20]. Twinning dislocations can also propagate more easily as they have short Burgers vectors, which clearly indicates that twinning is a dominant mechanism for accommodating plastic deformation along the c-axis of h.c.p. crystals [21].

Furthermore, in h.c.p. crystalline materials, there is a material competition between slip and twins. As noted by Wang et al. [22], plastic deformation in h.c.p. materials is due to both slip and twinning, and twinning adds significant strengthening and ductility. When twinning occurs, the parent crystal is sheared to a new orientation determined by the operating twinning system. The crystallographic relationship between parent and twins can be uniquely represented by a correspondence matrix as shown by Niewczas [23]. The correspondence matrix can be used to transform the parent slip systems to twin systems under different twinning modes, and this provides a framework to relate the twin systems to the parent matrix.

A number of modeling approaches have been used for investigating twinning and texture evolution. Beyerlein and Tome [24] have proposed a probabilistic twin nucleation model at grain boundaries (GBs) within a crystal plasticity formulation for h.c.p metals; it is based on estimating the probability for a grain boundary dislocation to dissociate into partials that nucleate into a twin. This model has also been extended by Beyerlein et al. [25] into a crystal plasticity constitutive framework for twin nucleation and growth. Although they introduced grain size effects in the twin nucleation rate, their predictions of the twin volume fraction evolution are insensitive to grain size variations. Moreover, Lebensohn and Tome developed the VPSC model [26] to simulate the mechanical properties of materials, including texture evolution in zircaloys [13]. Knezevic et al. [27] used crystal plasticity finite element models, based on 2D and 3D polycrystalline microstructures, to understand 3D topological effects on microstructural

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deformation. Furthermore, Niezgoda et al. have proposed a stochastic model for twin nucleation in Zr [21]; it is based on linking the probability of twin nucleation with normal stress accumulation at the GBs. A random fluctuating stress term is added to the stress increments to account for the random nature of twin nucleation. Kalidindi [28] proposed a different scheme, which was applied with a crystal plasticity Taylor based approach. In this approach, the grains are subdivided into virtual matrix and twin domains upon the activation of twinning. The constitutive response at the matrix and twin domain are all based on a Taylor approximation. This approach has been employed with some success for a variety of material for h.c.p. metals, such as titanium [29], and magnesium [1]. Notably, the calculations are performed in a relaxed (referential) configuration in which the misorientation between the twinned and untwined parent domains are fixed during deformation. This avoids unnecessary twin proliferation and, yet, permits the possibility that the parent and twin domains may not maintain their specific twin misorientation relationship as deformation evolves.

The effects of twinning on fracture have not been investigated for zircaloys within the framework of accounting of how large inelastic strain behavior, dislocation-density evolution, twin orientations and modes and parent orientation affect crack nucleation and propagation. Hence, in this paper, we introduce an approach that we have previously used and validated in Ref. [5] for pure h.c.p. systems, and we couple that approach with the twin modes normally associated with zirconium alloys [23]. We use these new twin systems and parent slip systems in h.c.p. materials with a dislocation-density crystalline plasticity formulation, and a fracture approach that accounts for crack nucleation and propagation within a nonlinear finite-element framework. We then investigated how these new twin systems can affect crack nucleation and propagation, dislocation density and inelastic slip evolution, stress accumulation, and lattice rotation in h.c.p. zircaloys. This paper is organized as follows: the multiple slip crystalline plasticity formulation and derivation of dislocation-density evolution equations and mobile and immobile dislocation-density evolution are presented in Section 2; the twinning systems in zircaloys are introduced in Section 3; the computational approach, and microstructural failure method are outlined in Section 4; the results with fracture and without fracture are presented and discussed in Section 5; a summary of the results and conclusions are given in Section 6.

2. Multiple-slip crystal plasticity dislocation-density based formulation

In this section, the multiple-slip crystal plasticity rate-dependent constitutive formulation and the derivation of the mobile and immobile dislocation-densities are briefly outlined. The dislocation-density crystal plasticity constitutive framework used in this study is based on the formulation developed by Zikry and Wu [30,31] and Shanthraj and Zikry [28]. It is assumed that the velocity gradient is decomposed into a symmetric deformation rate tensor, D_{ij}, and an anti-symmetric spin tensor W_{ij}. D_{ij} and W_{ij} can then be additively decomposed into elastic and inelastic components [32]. Following the method of, Pratheek [33], it is assumed that, for a given deformed state of the material, the total dislocation-density, $\rho^{(\alpha)}$, can be additively decomposed into a mobile and an immobile dislocation-density, $\rho_m^{(\alpha)}$ and $\rho_{im}^{(\alpha)}$. During an increment of strain on a slip system, a mobile dislocation-density rate is generated and an immobile dislocation-density rate is annihilated. Furthermore, the mobile and immobile dislocation-density rates can be coupled through the formation and destruction of junctions as the stored immobile dislocations act as obstacles for evolving mobile dislocations.

The evolution equations for mobile and immobile dislocation densities, can now be obtained by considering the generation, interaction, immobilization, and annihilation of dislocation densities as

$$\frac{d\rho_m^\alpha}{dt} = |\dot{\gamma}^\alpha|\left(\frac{g_{sour}^\alpha}{b^2}\left(\frac{\rho_{im}^\alpha}{\rho_m^\alpha}\right) - g_{mnter}^\alpha - \rho_m^\alpha - \frac{g_{immob-}^\alpha}{b}\sqrt{\rho_{im}^\alpha}\right), \tag{1}$$

$$\frac{d\rho_{im}^\alpha}{dt} = |\dot{\gamma}^\alpha|\left(g_{mnter+}^\alpha\rho_m^\alpha + \frac{g_{immob+}^\alpha}{b}\sqrt{\rho_{im}^\alpha} - g_{recov}^\alpha\rho_{im}^\alpha\right), \tag{2}$$

where $\dot{\gamma}^\alpha$ is the slip rate on slip-system α, g_{sour} is the coefficient pertaining to an increase in the mobile dislocation-density due to dislocation sources, $\dot{\rho}_{generation}^{(\alpha)}$, g_{mnter} is the coefficient related to the trapping of mobile dislocations due to forest intersections, cross-slip around obstacles, or dislocation interactions, $\dot{\rho}_{interaction}^{(\alpha)}$, g_{recov} is a coefficient related to the rearrangement and annihilation of immobile dislocations which is related to $\dot{\rho}_{annihilation}^{(\alpha)}$, and g_{immob} are coefficients related to the immobilization of mobile dislocations which is also shown in $\dot{\rho}_{interaction}^{(\alpha)}$. These coefficients, which have been nondimensionalized, are summarized in Table 1 where f_0, and φ are geometric parameters. H_0 is the reference activation enthalpy, and ρ_s is the saturation density. It should be noted that these coefficients are functions of the immobile and mobile densities, and hence are updated as a function of the deformation mode.

A power law relation for the slip-rate, $\dot{\gamma}^\alpha$ characterize the rate-dependent constitutive description on each slip system as

$$\dot{\gamma}^{(\alpha)} = \dot{\gamma}_{ref}^{(\alpha)}\left[\frac{\tau^{(\alpha)}}{\tau_{ref}^{(\alpha)}}\right]\left[\frac{|\tau^{(\alpha)}|}{\tau_{ref}^{(\alpha)}}\right]^{\left(\frac{1}{m}-1\right)}, \tag{3}$$

where $''^{(\#)}_{ref}$ is the reference shear strain-rate which corresponds to a reference shear stress $\tau_{ref}^{(\alpha)}$, and m is the rate sensitivity parameter. $\tau^{(\alpha)}$ is the resolved shear stress on slip system α. The reference stress used is a modification of widely used classical forms [34] that relate reference stress to immobile dislocation-density ρ_{im} as

$$\tau_{ref}^{(\alpha)} = \left(\tau_y^{(\alpha)} + G\sum_{\beta=1}^{nss} b^{(\beta)}\sqrt{a_{\alpha\beta}\rho_{im}^{(\beta)}}\right)\left(\frac{T}{T_0}\right)^{-\xi}, \tag{4}$$

where $\tau_y^{(\alpha)}$ is the static yield stress on slip system α, G is the shear

Table 1
g coefficients.

g Coefficients	Expression
g_{sour}^α	$b^\alpha\varphi\sum_\beta\sqrt{\rho_{im}^\beta}$
g_{mnter-}^α	$l_c f_0\sum_\beta\sqrt{a_{\alpha\beta}}\left[\frac{\rho_m^\beta}{\rho_m^\alpha b^\alpha} + \frac{\dot{\gamma}^\beta}{\dot{\gamma}^\alpha b^\beta}\right]$
g_{immob-}^α	$\frac{l_c f_0}{\sqrt{\rho_{im}^\alpha}}\sum_\beta\sqrt{a_{\alpha\beta}}\rho_{im}^\beta$
g_{mnter+}^α	$\frac{l_c f_0}{\dot{\gamma}^\alpha\rho_m^\alpha}\sum_{\beta,\gamma} n_\alpha^{\beta\gamma}\sqrt{a_{\beta\gamma}}\left[\frac{\rho_m^\gamma\dot{\gamma}^\beta}{b^\beta} + \frac{\rho_m^\beta\dot{\gamma}^\gamma}{b^\gamma}\right]$
g_{immob+}^α	$\frac{l_c f_0}{\dot{\gamma}^\alpha\sqrt{\rho_{im}^\alpha}}\sum_\beta n_\alpha^{\beta\gamma}\sqrt{a_{\beta\gamma}}\rho_{im}^\gamma\dot{\gamma}^\beta$
g_{recov}^α	$\frac{l_c f_0}{\dot{\gamma}^\alpha}\left(\sum_\beta\sqrt{a_{\alpha\beta}}\frac{\dot{\gamma}^\beta}{b^\beta}\right)e^{\left(\frac{-H_0\left(1-\sqrt{\frac{\rho_{im}^\alpha}{\rho_s}}\right)}{kT}\right)}$