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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 $(11\bar{2})$ and (0001) 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.

Keywords: H.C.P. crystals, twins, fracture, dislocation-densities, orientation effects

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

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4 systems to twin systems under different twinning modes, and this provides a framework
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6 to relate the twin systems to the parent matrix.
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9 A number of modeling approaches have been used for investigating twinning and
10 texture evolution. Beyerlein and Tome [24] have proposed a probabilistic twin
11 nucleation model at grain boundaries (GBs) within a crystal plasticity formulation for
12 h.c.p metals; it is based on estimating the probability for a grain boundary dislocation to
13 dissociate into partials that nucleate into a twin. This model has also been extended by
14 Beyerlein et al. [25] into a crystal plasticity constitutive framework for twin nucleation
15 and growth. Although they introduced grain size effects in the twin nucleation rate, their
16 predictions of the twin volume fraction evolution are insensitive to grain size variations.
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18 Moreover, Lebensohn and Tome developed the VPSC model [26] to simulate the
19 mechanical properties of materials, including texture evolution in zircalloys [13].
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22 Knezevic et al. [27] used crystal plasticity finite element models, based on 2D and 3D
23 polycrystalline microstructures, to understand 3D topological effects on microstructural
24 deformation. Furthermore, Niezgoda et al. have proposed a stochastic model for twin
25 nucleation in Zr [21]; it is based on linking the probability of twin nucleation with normal
26 stress accumulation at the GBs. A random fluctuating stress term is added to the stress
27 increments to account for the random nature of twin nucleation. Kalidindi [28] proposed
28 a different scheme, which was applied with a crystal plasticity Taylor based approach. In
29 this approach, the grains are subdivided into virtual matrix and twin domains upon the
30 activation of twinning. The constitutive response at the matrix and twin domain are all
31 based on a Taylor approximation. This approach has been employed with some success
32 for a variety of material for h.c.p. metals, such as titanium, [29] and magnesium [1].
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4 Notably, the calculations are performed in a relaxed (referential) configuration in which
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6 the misorientation between the twinned and untwined parent domains are fixed during
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8 deformation. This avoids unnecessary twin proliferation and, yet, permits the possibility
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10 that the parent and twin domains may not maintain their specific twin misorientation
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12 relationship as deformation evolves.
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16 The effects of twinning on fracture have not been investigated for zircalloys within
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18 the framework of accounting of how large inelastic strain behavior, dislocation-density
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20 evolution, twin orientations and modes and parent orientation affect crack nucleation and
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22 propagation. Hence, in this paper, we introduce an approach that we have previously
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24 used and validated in [5] for pure h.c.p. systems, and we couple that approach with the
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26 twin modes normally associated with zirconium alloys [23]. We use these new twin
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28 systems and parent slip systems in h.c.p. materials with a dislocation-density crystalline
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30 plasticity formulation, and a fracture approach that accounts for crack nucleation and
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32 propagation within a nonlinear finite-element framework. We then investigated how
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34 these new twin systems can affect crack nucleation and propagation, dislocation density
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36 and inelastic slip evolution, stress accumulation, and lattice rotation in h.c.p. zircalloys.
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38 This paper is organized as follows: the multiple slip crystalline plasticity formulation and
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40 derivation of dislocation-density evolution equations and mobile and immobile
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42 dislocation-density evolution are presented in Section 2; the twinning systems in
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44 zircalloys are introduced in Section 3; the computational approach, and microstructural
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46 failure method are outlined in Section 4; the results with fracture and without fracture are
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48 presented and discussed in Section 5; a summary of the results and conclusions are given
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50 in Section 6.
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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, $\rho^{(a)}$, can be additively decomposed into a mobile and an immobile dislocation-density, $\rho_m^{(a)}$ and $\rho_{im}^{(a)}$. 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

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

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

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_{minter} 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.

Table 1. g coefficients

g Coefficients	Expression
g_{sour}^{β}	$b^{\beta} j \dot{a} \sqrt{r_{im}^{\beta}}$
$g_{minter-}^{\beta}$	$l_c f_0 \sum_{\beta} \sqrt{a_{\alpha\beta}} \left[\frac{\rho_m^{\beta}}{\rho_m^{\alpha} b^{\alpha}} + \frac{\dot{\gamma}^{\beta}}{\dot{\gamma}^{\alpha} b^{\beta}} \right]$
g_{immob-}^{β}	$\frac{l_c f_0}{\sqrt{\rho_{im}^{\alpha}}} \sum_{\beta} \sqrt{a_{\alpha\beta}} \rho_{im}^{\beta}$
$g_{minter+}^{\beta}$	$\frac{l_c f_0}{\dot{\gamma}^{\alpha} \rho_m^{\alpha}} \sum_{\beta, \gamma} n_{\alpha}^{\beta\gamma} \sqrt{a_{\beta\gamma}} \left[\frac{\rho_m^{\gamma} \dot{\gamma}^{\beta}}{b^{\beta}} + \frac{\rho_m^{\beta} \dot{\gamma}^{\gamma}}{b^{\gamma}} \right]$
g_{immob+}^{β}	

	$\frac{l_c f_0}{\dot{\gamma}^\alpha \sqrt{\rho_{im}^\alpha}} \sum_{\beta} n_{\alpha}^{\beta\gamma} \sqrt{a_{\beta\gamma}} \rho_{im}^\gamma \dot{\gamma}^\beta$
$g_{ref}^{(a)}$	$\frac{l_c f_0}{\dot{\gamma}^\alpha} \left(\sum_{\beta} \sqrt{a_{\alpha\beta}} \frac{\dot{\gamma}^\beta}{b^\beta} \right) e^{\left(\frac{-H_0 \left(1 - \sqrt{\frac{\rho_{im}^\alpha}{\rho_s}} \right)}{kT} \right)}$

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

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

where $\dot{\gamma}_{ref}^{(\#)}$ is the reference shear strain-rate which corresponds to a reference shear stress $\tau_{ref}^{(a)}$, and m is the rate sensitivity parameter. $\tau^{(a)}$ 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

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

where $\tau_y^{(a)}$ is the static yield stress on slip system α , G is the shear modulus, nss is the number of slip systems, $b^{(b)}$ is the magnitude of the Burgers vector, and a_{ab} are Taylor coefficients, which are related to the strength of interactions between slip-systems

(Devincre et al. [35]; Kubin et al. [36,37]), T is the temperature, T_0 is the reference temperature, and ξ is the thermal softening exponent.

3. TWIN SYSTEMS IN ZIRCALOYS

H.C.P. materials and alloys deform by slip and twinning, but due to a limited number of slip modes imposed by the h.c.p. lattice, twinning is an essential mechanism pertaining to the behavior of zircaloys [12]. When twinning occurs, the parent crystal is sheared to a new orientation by the operating twinning mode. By using Niewczas's method [23], we obtained the sheared parent slip systems for Zr and the tensile loading conditions for twinning deformation [11,38,39] (Table 2).

Table 2: Transformation of parent slip system to slip system for the twin Zr with $c/a = 1.594$, twinning mode $(11\bar{2}1)$ $[\bar{1}\bar{1}26]$ and twinning shear = 0.627353.

		Parent slip system		Twin slip system	
Twin mode 1		$(11\bar{2}1)$	$[\bar{1}\bar{1}26]$	$(11\bar{2}1)$	$[\bar{1}\bar{1}2\bar{6}]$
Twin mode 2		(0001)	$[\bar{1}\bar{1}20]$	$(000\bar{1})$	$[\bar{1}\bar{1}20]$
1	Basal	(0001)	$[2\bar{1}\bar{1}0]$	$(000\bar{1})$	$[\bar{1}2\bar{1}0]$
2		(0001)	$[\bar{1}2\bar{1}0]$	$(000\bar{1})$	$[2\bar{1}\bar{1}0]$
3		(0001)	$[\bar{1}\bar{1}20]$	$(000\bar{1})$	$[\bar{1}\bar{1}20]$
4		$(10\bar{1}0)$	$[\bar{1}2\bar{1}0]$	$(01\bar{1}\bar{1})$	$[2\bar{1}\bar{1}0]$
5	Prismatic	$(0\bar{1}10)$	$[2\bar{1}\bar{1}0]$	$(\bar{1}01\bar{1})$	$[\bar{1}2\bar{1}0]$
6		$(\bar{1}100)$	$[\bar{1}\bar{1}20]$	$(\bar{1}\bar{1}00)$	$[\bar{1}\bar{1}20]$
7		$(10\bar{1}1)$	$[\bar{1}2\bar{1}0]$	$(01\bar{1}0)$	$[2\bar{1}\bar{1}0]$
8	Pyramidal <a>	$(0\bar{1}11)$	$[2\bar{1}\bar{1}0]$	$(\bar{1}01\bar{2})$	$[\bar{1}2\bar{1}0]$
9		$(\bar{1}101)$	$[\bar{1}\bar{1}20]$	$(\bar{1}\bar{1}0\bar{1})$	$[\bar{1}\bar{1}20]$
10		$(\bar{1}011)$	$[\bar{1}2\bar{1}0]$	$(0\bar{1}\bar{1}2)$	$[2\bar{1}\bar{1}0]$
11		$(0\bar{1}\bar{1}1)$	$[2\bar{1}\bar{1}0]$	$(10\bar{1}0)$	$[\bar{1}2\bar{1}0]$
12	Pyramidal <c+a>	$(\bar{1}\bar{1}01)$	$[\bar{1}\bar{1}20]$	$(\bar{1}\bar{1}0\bar{1})$	$[\bar{1}\bar{1}20]$
13		$(10\bar{1}1)$	$[\bar{1}\bar{1}23]$	$(01\bar{1}0)$	$[000\bar{1}]$
14		$(10\bar{1}1)$	$[\bar{2}\bar{1}13]$	$(01\bar{1}0)$	$[2\bar{1}\bar{1}\bar{3}]$
15		$(0\bar{1}11)$	$[\bar{1}\bar{1}23]$	$(\bar{1}01\bar{2})$	$[224\bar{3}]$
16		$(0\bar{1}11)$	$[\bar{1}2\bar{1}3]$	$(\bar{1}01\bar{2})$	$[10\bar{1}\bar{1}]$
17		$(\bar{1}\bar{1}01)$	$[2\bar{1}\bar{1}3]$	$(\bar{1}\bar{1}0\bar{1})$	$[01\bar{1}\bar{1}]$
18		$(\bar{1}\bar{1}01)$	$[\bar{1}2\bar{1}3]$	$(\bar{1}\bar{1}0\bar{1})$	$[\bar{1}2\bar{1}\bar{3}]$
19		$(\bar{1}011)$	$[2\bar{1}\bar{1}3]$	$(0\bar{1}\bar{1}2)$	$[01\bar{1}\bar{1}]$
20		$(\bar{1}011)$	$[\bar{1}\bar{1}23]$	$(0\bar{1}\bar{1}2)$	$[224\bar{3}]$
21		$(0\bar{1}\bar{1}1)$	$[\bar{1}\bar{1}23]$	$(10\bar{1}0)$	$[000\bar{1}]$
22		$(0\bar{1}\bar{1}1)$	$[\bar{1}2\bar{1}3]$	$(10\bar{1}0)$	$[\bar{1}2\bar{1}\bar{3}]$
23		$(\bar{1}\bar{1}01)$	$[\bar{2}\bar{1}13]$	$(\bar{1}\bar{1}0\bar{1})$	$[2\bar{1}\bar{1}\bar{3}]$
24		$(\bar{1}\bar{1}01)$	$[\bar{1}2\bar{1}3]$	$(\bar{1}\bar{1}0\bar{1})$	$[10\bar{1}\bar{1}]$

4. COMPUTATIONAL APPROACH

The total deformation rate tensor D_{ij} and the plastic deformation rate tensor D_{ij}^p , are needed to update the material stress state. The method used here is that developed by Zikry [30] for rate-dependent crystalline plasticity formulations, and only a brief outline will be presented here. For quasi-static deformations, an implicit FE method with BFGS (Broyden, Fletcher, Goldfarb, and Shanno) iteration is used to obtain the total deformation rate tensor D_{ij} . To overcome numerical instabilities associated with stiffness a hybrid explicit-implicit method is used to obtain the plastic deformation rate tensor D_{ij}^p . Numerical stiffness can be encountered when due to different rate changes along slip systems, slip-rates, resolved shear-stresses, and dislocation-densities can vary widely. An explicit central difference finite element method is used to obtain the total deformation rate tensor, D_{ij} . To solve for the plastic deformation rate tensor, D_{ij}^p , the time derivative of the resolved shear-stress is used together with the objective stress rate, and the assumption that the elastic modulus tensor is isotropic, to obtain the following system of coupled nonlinear differential equations for each active slip-system:

$$\dot{\tau}^{(\alpha)} = 2\mu \left(P_{ij}^{(\alpha)} D_{ij} - P_{ij}^{(\alpha)} \left[\sum_{\beta=1}^{24} P_{ij}^{(\beta)} \dot{\gamma}_{ref}^{(\beta)} \left(\frac{\tau^{(\beta)}}{\tau_{ref}} \right)^{\frac{1}{m}} \right] \right) \quad (5)$$

To overcome numerical instabilities associated with stiffness, a hybrid explicit-implicit method is used to obtain the plastic deformation rate tensor. This hybrid numerical scheme is also used to update the evolutionary equations for the mobile and immobile densities.

4.1. Microstructural failure criterion and numerical implementation of overlapping element method

The inherent fracture mode in h.c.p. zircaloy systems would be cleavage fracture on the basal $\{1000\}_{\kappa'}$ planes [40]. To account for this as a microstructural failure criterion, the orientation of the cleavage planes for each variant in the global coordinate system is obtained by applying the series of transformations as

$$\mathbf{n}_{\text{cleave}} = [\mathbf{T}_1] \mathbf{n}_{\text{cleave}, \kappa'}, \quad (6)$$

where $[\mathbf{T}]_1$, relates the parent h.c.p. Euler grain orientation to the global coordinates.

The global orientation of the cleavage planes in the current configuration is then obtained by updating, at every time-step, the lattice rotations as $\dot{\mathbf{n}}_{\text{cleave}} = \mathbf{W}^* \mathbf{n}_{\text{cleave}}$. The normal component of the traction acting on each cleavage plane has a direct influence on fracture along that plane [40,41]. Therefore, the maximum normal component of the traction on cleavage planes is monitored and compared with a critical fracture stress σ_{frac} to determine failure. The failure criterion is then given by

$$t_{\text{cleave}} > \sigma_{\text{frac}}, \quad (7)$$

where $t_{\text{cleave}} = \max_{(0001), \text{planes}} \langle \mathbf{n}_{\text{cleave}}^T [\boldsymbol{\sigma}] \mathbf{n}_{\text{cleave}} \rangle$.

For the fracture analysis, we followed the approach of Wu and Zikry [42] and Hansbo and Hansbo [43], and consider one element with a crack defined implicitly by $f(\mathbf{X})=0$. This divides the element domain into two subdomains with areas A_{e1} and A_{e2} .

The direction of crack propagation would be along the most favorable cleavage plane [44,45]. Adding phantom nodes on top of the existing nodes, the original cracked element is replaced by two overlapping elements. The two overlapping elements do not share nodes, and therefore can have independent displacement fields. For each overlapping element, only the subdomain with area A_{e1} or A_{e2} , corresponding to one of the two subdomains for the original cracked element, is considered as active. Details for implementation of overlapping element method are given in Wu and Zikry [42].

5. Results and Discussion

The multiple-slip dislocation-density-based crystal plasticity formulation, and the overlap fracture method were used to investigate the microstructural failure behavior of Zircaloy-2 [46]. The parent h.c.p. zircaloy-2 grains and the h.c.p. twin grains are assumed to have random low angle GB misorientations, where the maximum misorientation was assumed to be less than 5° . In this study, 40 parent Zircaloy-2 grains and 46 twin grains (10% volume fraction) were oriented based on the loading plane (0001) and a loading direction of $[2\bar{1}\bar{1}0]$. A convergent plane strain mesh of 16,177 elements was used with a model size of 5mm $\times$ 8mm, and a displacement load is applied for a quasi-static nominal strain rate with a fixed bottom edge (Fig. 1).

Fig. 1. Computational and microstructural model

The material properties assumed for the constituent crystals are representative of zicaloy-2 (Table 3) [46,47], and the three deformation h.c.p. slip system modes are assumed as potentially active; prismatic, basal, and pyramidal for both parent and twin systems (Table 2).

Table 3: Properties of Zircaloy-2

$E(\text{GPa})$	Young's Modulus	180
ν	Poisson's ratio	0.34
$\sigma_y(\text{MPa})$	Static yield stress	250
m	Rate sensitivity coeff.	20
$\dot{\gamma} (s^{-1})$	Shear strain rate	1×10^{-4}

The effects of the twin systems can be clearly seen by the local behavior through spatial contours (Fig. 2). At a nominal strain of 10%, the most active immobile slip system in parent grains corresponded to the pyramidal system $(0\bar{1}11) [\bar{1}2\bar{1}3]$, and the maximum normalized (the immobile densities are normalized by the initial immobile densities) value was 600,000. The most active immobile slip system in the twin grains was the pyramidal $(1\bar{1}0\bar{1}) [\bar{1}2\bar{1}3]$ system, and its maximum normalized value was 70,000, which occurred at the interfaces of the twin grains and the zircaloy parent material. As these results indicate (Fig. 2), the matrix deformation affects twin deformation and morphology. This is due to the extensive dislocation-density matrix activity near the twin boundaries, which impinges on the twins. Furthermore, there was significant twin lattice rotation in these regions. The maximum lattice rotation within the twin systems was 30° (Fig. 3a). At a nominal strain of 10%, the high dislocation-densities resulted in the accumulation of shear slip both within the matrix and the twins (Fig. 3b), and the maximum accumulated plastic slip was approximately 0.7. The normalized normal stress (normalized with the static yield stress) is shown in Figure 4 at a nominal strain of 10%, and the maximum normalized value was 5 within one of the twins. These results indicate that the twins both strengthened the aggregate and increased ductility, which is significantly different than the behavior of pure zircaloys [46,47]. This is consistent with experimental observations [11,12,48-52] of zircaloy-2 aggregates that indicate that twinning structures are both sources of ductility and strengthening.

We then compared the change of pyramidal immobile dislocation density activity along the interface between parent and twin grains. The dislocation density activity in parent and twin grains are significantly different from each other. For the parent slip

system, we have a minimum dislocation density activity inside the twin grains (Fig. 5), when the most active dislocation density activity is a maximum inside the twin grains, we have minimal activity within the parent grains (Fig. 6). This difference in slip and dislocation-density activity indicates that interfacial gradients (Fig. 5-6) would develop between twins and parent, and this results in higher ductility of the crystalline system.

Fig. 2. Immobile dislocation density activity (a) pyramidal parent slip system $(0\bar{1}11)$ $[\bar{1}2\bar{1}3]$ (b) pyramidal twin slip system $(1\bar{1}0\bar{1})$ $[\bar{1}2\bar{1}3]$

Fig. 3. (a) Lattice rotation (b) shear slip at 8% nominal strain

Fig. 4. Normalized normal stress with yield stress value at 8% nominal strain

Fig. 5. Immobile dislocation density activity for pyramidal $(0\bar{1}11)$ $[\bar{1}2\bar{1}3]$ parent slip-system

Fig. 6. Immobile dislocation density activity for pyramidal $(1\bar{1}0\bar{1})$ $[\bar{1}2\bar{1}3]$ twin slip system

5.1 FRACTURE OF ZIRCALOYS

To investigate fracture in zircaloy aggregates, we introduced an edge crack in the model (Figure 2) with a crack length, a , of a/w of 0.1 where w is the width of the model and a is the length of the crack. The most active immobile dislocation density slip systems were the same as the case without fracture for both twin and parent grains. The crack propagated in a planar manner, and this can be due to the low angle GB misorientations between grains [47]. Furthermore, due to the different slip systems between the parent and the twins, which results in slip, dislocation density, and stress incompatibilities. There were higher normal stresses within the twins; these higher stresses act as obstacles to the propagating crack, and the crack deviated around the twins (Figs. 7 a-b). The twins also added more ductility to the system as shown in Figures 8 (a-c) at different nominal strains of 2%, 3% and 8%. The higher ductility associated with twins has been observed experimentally [53,54]. The evolution of crack propagation is shown in Figs. 9 (a-d) for different nominal strains, and as seen the crack propagates around the twins, and this is also consistent with experimental observations [55,56]. Because of high stresses and low mobile and immobile dislocation density activity on the basal planes, crack nucleation and propagation occurs on the basal planes, which is consistent with experimental observations [57]. We used the basal plane as the cleavage plane since fracture would occur in that plane, because there is minimum dislocation density activity along that strengthening plane.

Fig. 7. Immobile dislocation density activity (a) pyramidal parent slip system $(0\bar{1}11)$ $[\bar{1}2\bar{1}3]$ (b) pyramidal twin slip system $(1\bar{1}0\bar{1})$ $[\bar{1}2\bar{1}3]$

Fig. 8. Shear slip (a) at 2% nominal strain (b) at 3% nominal strain (c) at 8% nominal strain

Fig. 9. Normalized normal stress (a) at 1% nominal strain (b) at 2% nominal strain (c) at 3% nominal strain (d) at 7% nominal strain

6. Conclusion

We have introduced a dislocation density based multiple slip crystal plasticity formulation that accounts for the behavior of parent and twin systems, and we investigated the effects of twin and parent grains for an aggregate with and without fracture. We introduced 24 unique twin systems based on two specific twin modes of $(11\bar{2}1)[\bar{1}\bar{1}26]$ and $(0001)[\bar{1}\bar{1}20]$. The twins significantly affected local behavior, in aggregates without cracks, such as shear slip accumulation, dislocation-density evolution, lattice rotation, thermal and stress growth. Higher mobile and immobile dislocation density activity occurs on prismatic and pyramidal planes, and lower dislocation density activity occurs on the basal planes for both the twins and the parent.

The twins resulted in higher strength, ductility and the activation of different slip systems and orientations than those of the parent zircaloy, and they resulted in interfacial mismatches with the matrix. These interfacial incompatibilities resulted in higher stresses and ductilities, and this significantly affected crack nucleation and propagation in that the twin systems acted as barriers in the path of the propagating cracks. The predictions also indicated that cracking will be on the basal planes, which is consistent with experimental observations [57] related to the failure of zircalloys. This study underscores the need to accurately physically represent twin modes and parent interactions and orientations to better understand local deformation and fracture behavior for large strain inelastic deformations.

ACKNOWLEDGEMENTS

Support from the Consortium for Advanced Simulation of Light Water Reactors
an Energy Innovation Hub for Modeling and Simulation of Nuclear Reactors under U.S.
Department of Energy Contract No. DE-AC05-00OR227 is gratefully acknowledged.

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Graphical Abstract – One of the objectives of this paper is to investigate how dislocation density incompatibilities between twins and the parent matrix affects crack growth. The figure below show how the maximum dislocation occur on different planes for the twin and the matrix. The Immobile dislocation density activity is for the pyramidal $(11\bar{0}1)$ $[\bar{1}2\bar{1}3]$ twin slip system.