MULTI-SCALE MODELING AND EXPERIMENTAL STUDY OF DEFORMATION TWINNING IN HEXAGONAL CLOSE-PACKED MATERIALS

by

Hamidreza Abdolvand

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Queen’s University
Kingston, Ontario, Canada

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Abstract

Zirconium and its alloys have been extensively used in both heavy and light water nuclear reactors. Like other Hexagonal Close-Packed (HCP) materials, e.g., magnesium, zirconium alloys develop different textures during manufacturing process which result in highly anisotropic materials with different responses under different loading conditions. Slip and twinning are two major deformation mechanisms during plastic deformation of zirconium. This dissertation uses various experimental techniques and a crystal plasticity scheme in the finite element framework to study deformation mechanisms in HCP materials with an emphasis on twinning in Zircaloy-2. The current study is presented as a manuscript format dissertation comprised of four manuscript chapters. After a literature review in Chapter 2, Chapter 3 reports steps in developing a crystal plasticity finite element user material subroutine for modeling deformation in Zircaloy-2 at room temperature. It is shown in Chapter 3 that the developed rate dependent equations are capable of capturing evolution of key features, e.g., texture, lattice strains, and twin volume fractions, during deformation by twinning and slip. Chapter 4 reports various assumptions and approaches in modeling twinning where results are compared against neutron diffraction measurements from the literature. It is shown in Chapter 4 that the predominant twin reorientation scheme can explain texture development more precisely than the other schemes discussed. Chapter 5 and 6 are two connected chapters where in the first one the formation of twins is studied statistically and in the second one, local inception and propagation of twins is studied. Numerical results of these two chapters are compared with 2D electron backscattered diffraction measurements, both carried out by the author and from the literature. Results from these two connected chapters emphasize the important role of grain boundary geometry and stress concentration sites on twin nucleation and growth. The four manuscript chapters are followed by summarizing conclusions and suggestions for future work in Chapter 7.
Co-Authorship

This dissertation is presented in a manuscript format dissertation, with manuscript chapter based accepted or submitted journal articles. These manuscript chapters were based on the following journal publications:

Chapter 3


Chapter 4


Chapter 5


Chapter 6


The work conducted in this dissertation is my own, with co-authors acting primarily in an advisory capacity. I have included the twinning mode of deformation into a subroutine and developed all of the pre- and post- processors for data analysis. Also, I performed all SEM/EBSD
experimental studies presented in Chapter 6. Co-authors have made the following contributions to the publications above:

Modeling Advisement

M. R. Daymond and C. Mareau

Experimental Planning/Assistance

M. R. Daymond

Self Consistent Simulations (for Chapter 3)

C. Mareau
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It is a pleasure to thank those who made this thesis possible: Dr. Charles Mareau for all of his assistance in developing the CPFE code and answering my endless questions. Your guidance was invaluable; Professor Bradley Diak for being patient in training me to use the SEM/EBSD facilities; Professor Rick Holt for sharing his knowledge of Zircaloy-2; Mohammad Sattari, Marta Majkut, Greg Allen, and Matthew Kerr for their assistance in performing the experimental parts of this thesis and all of the Nuclear Materials Research Group members at Queen’s University for the useful discussions I have had with them. I would also like to acknowledge the financial support of NSERC, COG, OPG, and Nu-Tech Precision Metals under the Industrial Research Chair Program in Nuclear Materials at Queen’s University.

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To my family
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<tbody>
<tr>
<td>BC</td>
<td>Boundary Condition</td>
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<tr>
<td>CE</td>
<td>Continuity Equation</td>
</tr>
<tr>
<td>CF</td>
<td>Concentration Factor</td>
</tr>
<tr>
<td>Comp</td>
<td>Compression</td>
</tr>
<tr>
<td>CP</td>
<td>Crystal Plasticity</td>
</tr>
<tr>
<td>CPFE</td>
<td>Crystal Plasticity Finite Element</td>
</tr>
<tr>
<td>CPFEM</td>
<td>Crystal Plasticity Finite Element Modeling</td>
</tr>
<tr>
<td>CRSS</td>
<td>Critical Resolved Shear Stress</td>
</tr>
<tr>
<td>EBSD</td>
<td>Electron BackScattered Diffraction</td>
</tr>
<tr>
<td>EPSC</td>
<td>Elastic Plastic Self Consistent</td>
</tr>
<tr>
<td>err</td>
<td>Error</td>
</tr>
<tr>
<td>ES</td>
<td>Equal Stress</td>
</tr>
<tr>
<td>Exp</td>
<td>Experiment</td>
</tr>
<tr>
<td>FCC</td>
<td>Face Centered Cubic</td>
</tr>
<tr>
<td>FE</td>
<td>Finite Element</td>
</tr>
<tr>
<td>FIF</td>
<td>Finite Initial Fraction</td>
</tr>
<tr>
<td>GBM</td>
<td>Grain Boundaries Misorientation</td>
</tr>
<tr>
<td>GSF</td>
<td>Geometrical Schmid Factor</td>
</tr>
<tr>
<td>HCP</td>
<td>Hexagonal Close-Packed</td>
</tr>
<tr>
<td>IP</td>
<td>Integration Point</td>
</tr>
<tr>
<td>IPC</td>
<td>In Plane Compression</td>
</tr>
<tr>
<td>LSF</td>
<td>Local Schmid Factor</td>
</tr>
</tbody>
</table>
MAD  Mean Angular Deviation
MT   Multiple Twin
ND   Normal Direction
NE   Number of Element
PBC  Periodic Boundary Condition
PTR  Predominant Twinning Reorientation
RD   Rolling Direction
RSS  Resolved Shear Stress
SC   Self Consistent
SF   Schmid Factor
SOE  Subset Of Element
TD   Transverse Direction
Ten  Tension
TIS  Twin Inception Site
TOF  Time of Flight
TVF  Twin Volume Fraction
TVFRE Twin Volume Fraction Rate Effect
UMAT User MATerial
F    Deformation gradient
F^e  Elastic part of deformation gradient
F^p  Plastic part of deformation gradient
L    Velocity gradient
L^e  Elastic part of velocity gradient
L^p  Plastic part of velocity gradient
D    Strain rate tensor
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D^e$</td>
<td>Elastic part of strain rate</td>
</tr>
<tr>
<td>$D^p$</td>
<td>Plastic part of strain rate</td>
</tr>
<tr>
<td>$\Omega$</td>
<td>Spin rate tensor</td>
</tr>
<tr>
<td>$\Omega^e$</td>
<td>Elastic part of spin rate</td>
</tr>
<tr>
<td>$\Omega^p$</td>
<td>Plastic part of spin rate</td>
</tr>
<tr>
<td>$m^\alpha$</td>
<td>Slip direction of the slip system $\alpha$</td>
</tr>
<tr>
<td>$n^\alpha$</td>
<td>Normal to the slip plane $\alpha$</td>
</tr>
<tr>
<td>$S^\alpha$</td>
<td>Schmid tensor</td>
</tr>
<tr>
<td>$P^\alpha$</td>
<td>Symmetric part of the Schmid tensor</td>
</tr>
<tr>
<td>$W^\alpha$</td>
<td>Skew symmetric part of the Schmid tensor</td>
</tr>
<tr>
<td>$\Psi$</td>
<td>Kirchoff stress tensor</td>
</tr>
<tr>
<td>$J$</td>
<td>Jacobian (volume ratio)</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>Cauchy stress tensor</td>
</tr>
<tr>
<td>$I$</td>
<td>Identity tensor</td>
</tr>
<tr>
<td>$\delta_{ij}$</td>
<td>Kronocker delta</td>
</tr>
<tr>
<td>$\varepsilon$</td>
<td>Strain tensor</td>
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<tr>
<td>$\varepsilon^e$</td>
<td>Elastic strain</td>
</tr>
<tr>
<td>$\varepsilon^p$</td>
<td>Plastic strain</td>
</tr>
<tr>
<td>$\gamma^\alpha$</td>
<td>Shear strain on the slip/twin system $\alpha$</td>
</tr>
<tr>
<td>$\mathcal{L}$</td>
<td>Elastic modulus</td>
</tr>
<tr>
<td>$\tau^\alpha$</td>
<td>Resolved shear stress on the slip/twin system $\alpha$</td>
</tr>
<tr>
<td>$g^\alpha$</td>
<td>Current strength of the slip/twin system $\alpha$</td>
</tr>
<tr>
<td>$g_0^\alpha$</td>
<td>Critical resolved shear stress of the slip/twin system $\alpha$</td>
</tr>
<tr>
<td>$g_0^\alpha + g_1^\alpha$</td>
<td>Final back-extrapolated CRSS of the slip/twin system $\alpha$</td>
</tr>
</tbody>
</table>
$\theta^\alpha_0$ Initial hardening rate of the slip/twin system $\alpha$

$\theta^\alpha_1$ Asymptotic hardening rate of the slip/twin system $\alpha$

$\Gamma$ Accumulated plastic shear

$f^\beta$ Twin volume fraction resulted from activity of the $\beta^{th}$ twin system

$q_{\alpha\beta}$ A parameter describes interaction between slip/twin system $\alpha$ and $\beta$

$h_{\alpha\beta}$ A parameter describes interaction between slip/twin system $\alpha$ and $\beta$ and is a function of the introduced hardening law
Chapter 1

Introduction

1.1 Zirconium in the nuclear industry

Zirconium and its alloys have been widely used in the nuclear industry due to their low neutron capture cross-section, good corrosion resistance in hot water, and reasonable mechanical properties [1, 2]. Nuclear reactors operating in Canada use the CANDU (CANada Deuterium Uranium) design. In the CANDU design, the whole fuel channels are inside a vessel called calandria filled with D$_2$O as the moderator. The outermost tube of the fuel channel is called calandria tube which is made of Zircaloy-2, the material that is studied in this research. Inside a calandria tube is the pressure tube, made of Zr-2.5Nb, where heavy water passes through fuel bundles, made of Zircaloy-4, to generate high pressure steam for power generation. Zircaloy-2 have also been used for pressure tubes in early CANDU reactors [3, 4], and for fuel cladding. The nominal composition of Zircaloy-2 is 1.2-1.7 wt% Sn, 0.07-0.2 wt% Fe, 0.05-0.15 wt% Cr, 0.03-0.08 wt% Ni, 1400 wt ppm Oxygen [5].

Deformation in the calandria tube can be divided into three categories: axial elongation due to thermal expansion, ovality from external pressure applied by the moderator, and creep sag due to carrying part of fuel channel weight [6]. Understanding the deformation mechanism in Zircaloy-2 is crucial for having an estimation of in-reactor response of calandria tubes under the aforementioned loading conditions.
1.2 Deformation mechanism in zirconium alloys

Zirconium alloys can be generally divided into two categories: single phase alloys, e.g. Zircaloy-2 with $\alpha$-Zr, and dual phase alloys, e.g. Zr-2.5Nb with $\alpha/\beta$-Zr. With a Hexagonal Close-Packed (HCP) crystal structure, $\alpha$-Zr deforms plastically by contribution of both plastic slip and tensile twinning at room temperature. Slip in polycrystals can happen by movement of dislocations on a specific plane, also called the slip plane, in a specific direction, also called the slip direction. Plastic relaxation due to twinning, a rapid change in the orientation of part of a grain, could be also considered as pseudo slip [7], i.e. there exists a twin plane and twinning direction for accommodating plastic relaxation due to twinning. Fig. 1-1. shows the different slip and twinning systems observed in a Zr single crystal. Generally, in $\alpha$-zirconium, prism planes $\{1 \bar{1} 0 0\}$ are the easiest systems to be activated in $\langle 1 1 \bar{2} 0 \rangle$ direction, also called $\langle a \rangle$ direction, and slip on basal planes $\{0 0 0 2\}$ in the same direction has also been observed. A slip system with the same component in the $\langle 0 0 0 1 \rangle$ direction, also called $\langle c \rangle$, has been observed only under constraint and at high deformation temperatures [8]. The corresponding slip mode is slip that occurs on first or second order pyramidal planes $\{1 0 \bar{1} 1\}$ or $\{1 \bar{2} 1 1\}$ in $\langle c+a \rangle$ directions $\langle 1 1 \bar{2} 3 \rangle$. At room temperature, for stress along the c-axis, the twinning mechanism $\{1 \bar{1} 0 2\} < 1 0 \bar{1} 1 >$ is easily activated ($\{1 1 \bar{2} 1\} < 1 1 \bar{2} 3 >$ slip also contributes to the elongation along the c-direction but it is more difficult to activate) which results in some hard grains reorienting around 85 degrees [9]. It has been shown that at room temperature, basal $\langle 1 \bar{2} 1 0 \rangle$, prism $\langle 1 \bar{2} 1 0 \rangle$, pyramidal $\langle 1 1 \bar{2} 3 \rangle$, and tensile twinning $\langle \bar{1} 0 1 1 \rangle$ systems can explain the plastic deformation in Zircaloy-2 properly [10, 11].
1.3 This research

1.3.1 Motivation
Hydrogen uptake in zirconium components is a potential life-limiting mechanism for both pressure tubes and fuel cladding in CANDU reactors. The presence of hydrogen degrades mechanical properties of these components as the solubility of hydrogen in zirconium is low and brittle hydride phases form [4]. In pressure tubes, corrosion slowly occurs at the zirconium/heavy water interface and some of the deuterium/hydrogen released is absorbed into the zirconium pressure tube. This is a potential issue when reactors are taken off-line and cooled to ambient
temperature, as the solubility of hydrogen decreases with decreasing temperature and hydrides form in the material. Pressure tube cracking can occur by a thermally assisted slow cracking mechanism termed Delayed Hydride Cracking (DHC), where hydrides form at stress concentrations and repeated fracture of these hydrides leads to failure (<100wt-ppm hydrogen) [12]. It is experimentally observed that at a crack tip, many twins can form [13] which can potentially influence crack propagation process and the stress conditions at the crack tip.

With the aim of modeling and better understanding stress concentrations and eventually crack propagation in zirconium alloys, and to study the interaction between crack and surrounding grains at the crack tip, a Crystal Plasticity Finite Element (CPFE) code has been developed in this research. The ultimate aim of the current undergoing project is to use the developed CPFE code to study phenomena related to cracks in zirconium alloys which can lead to a better surveillance analysis of in core components of CANDU nuclear reactors.

1.3.2 Objectives

This research aims to develop a CPFE code to study elastic and plastic deformation of HCP materials under different loading conditions. The objectives of the research are:

1. To develop a user material finite element code to study behavior of HCP materials both at macro-scale and micro-scale.
2. To study plastic deformation by twinning using various experimental techniques.
3. To study internal stress development, texture evolution, and load sharing between aggregates of HCP polycrystals.
4. To understand limits and advantages of using CPFE in modeling twin inception and propagation.
1.3.3 Guide to the thesis

As noted in the previous section, a manuscript format will be used to present the research in this dissertation. For this reason, the introduction to this dissertation (Chapter 1) is intentionally kept short, as each part of the work is individually introduced. The literature review (Chapter 2) is a summary of all of the literature reviews presented in the other chapters, some extra related works are also discussed. Chapter 3 presents a published International Journal of Plasticity paper [14] covering a study of modeling average behavior of families of grains, which is a typical output of a neutron diffraction experiment. In-situ neutron diffraction experiments were carried out by Xu et al. [10, 11] to study lattice strains and texture evolution of Zircaloy-2 are used to validate the developed CPFE code in this section. Chapter 4 presents a published Acta Materialia paper [15] covering different assumptions that can be made in the CPFE code to model twinning as well as to capture relaxation due to twinning. Previously published in-situ neutron diffraction data on MgAZ31 [16] and on Zircaloy-2 [10] are used for this purpose. Chapter 5 and 6 presents two connected papers submitted in the Journal of the Mechanics and Physics of Solids covering our study on nucleation and propagation of twins in CPFE. The Electron BackScattered Diffraction (EBSD) technique is used to measure grain orientations in Zircaloy-2 before and after straining. Measured grain maps are imported into the FE solver and modeled to study local effect, e.g. grain-grain interactions, on twin nucleation and propagation. A statistical study of twin inception is also carried out by comparing results of 3D modeling with experimental results presented in Capolungo et al. [17]. Chapter 7 then reviews the work, draws conclusions from across the chapters and suggests further avenues of exploration. In the appendix mathematical details of the code is presented.
Reference List


Chapter 2

Literature Review

The experimental work in this dissertation uses diffraction techniques, e.g. neutron and electron backscattered, to study the mechanical response of HCP polycrystals under different loading conditions. Therefore, this review is composed of two parts, the first focuses on the experimental techniques and the second reviews application of crystal plasticity in modeling material behavior.

2.1 Experimental studies

Deformation in polycrystalline materials under a specific loading condition is a function of various parameters such as material crystal structure, elastic and plastic properties of the material single crystal, grain size and shape, and the orientation distribution of grains. In a single crystal, atoms have a regular arrangement in the crystal structure by which many of crystal properties, e.g. being isotropic or anisotropic, can be explained. For instance, due to having different distances between atoms in an HCP crystal structure, different responses will be achieved if an HCP single crystal deforms along the c-axis or the a-axis of the crystal. The individual crystals, or grains, are domains with continuous lattice orientation and vary widely in size, with $10^{-7}$ to $10^{-3}$m being a typical range [1]. Each grain has an orientation which can be expressed by a rotation matrix to convert from global coordinates to crystal local coordinates. Depending on the shape of the sample or processing of the material, the global coordinate often coincides with that of the sample. For instance, in a rolled plate, the axes of the sample (global) coordinate can be identified as the Rolling Direction (RD), Transverse Direction (TD), and Normal Direction (ND). Three
Euler angles ($\varphi_1$, $\varphi$, $\varphi_2$) can identify the rotation matrix for converting sample coordinates to crystal coordinates. Grains in a polycrystal, as a result of the manufacturing process, may be oriented in a specific direction; the distribution of crystallographic orientation of grains is called texture.

In the following sections, the methods that are used in this dissertation for characterizing material response under different conditions are explained.

### 2.1.1 Neutron diffraction

In this section, some of the key features of measuring elastic strains and texture in polycrystalline materials using neutron diffraction are explained, mostly based on references [2-6].

In contrast to conventional X-ray or synchrotron X-ray where the depth of penetration is just a few micrometers or millimeters, respectively, thermal neutrons, i.e. neutrons with wavelengths close to lattice spacing, can penetrate up to several centimeters in most engineering materials. Hence, a bigger gauge volume or a higher number of grains can contribute to the inspected property hence high quality statistics of the property of the material can be obtained. The principle of neutron diffraction is similar to other diffraction methods and is based on the Bragg’s law [7]:

$$n\lambda = 2dsin\theta$$  \hspace{1cm} (2-1)

where $\lambda$ is wavelength, $d$ is the plane spacing, $\theta$ is half of the diffraction angle, and $n$ is the order of diffraction. In Fig. 2-1 a schematic of diffraction by planes of atoms are shown.
Load sharing between aggregates of a polycrystalline material can directly influence the macroscopic behavior of the material under a specific loading condition. Lattice strain, the elastic strain inside a group of grains that satisfy the Bragg condition for an incident beam, can be used to monitor load sharing inside the material. The lattice strain and texture measurements used in chapters three and four of this dissertation were partially carried out (by F. Xu) at the National Research Universal (NRU) reactor at Chalk River, Canada, and partially at the Engin-X beam line, ISIS, Rutherford Appleton Laboratory, UK.

Lattice strain measurements at NRU are carried out using a single constant wavelength of thermal neutrons (Fig. 2-2). The incident beam is collimated by sŏller slits, then passes through an aperture defining its width and is diffracted by the polycrystalline sample with a take-off angle of $2\theta$; then the diffracted beam passes through another aperture, is collimated by another set of sŏller slits and finally reaches the detector [4]. Only grains in the gauge volume, identified by the two apertures, and satisfying the Bragg condition can be detected. Depending on the average size of the grains, normally from hundreds to thousands of them contribute to the lattice strain measurement and therefore good statistics for internal strain evolution will be obtained. In Fig. 2-2 a schematic of the lattice strain measurement at NRU is shown.
Lattice strain can be determined by changes of in plane-spacing or diffraction angle as follows [2]:

$$\varepsilon_{hkl} = \frac{d_{hkl} - d_{ref}}{d_{ref}} = \frac{\sin \theta_{ref}}{\sin \theta_{hkl}} - 1$$

(2-2)

where "hkl" is the diffracting plane, and "ref" refers to the reference sample or state, which is normally the unloaded sample. Data in this kind of experiment are usually gathered in the form of neutron counts as a function of diffraction angle where a Gaussian curve can be used to fit to the data. The center of this fit represents the average diffraction angle ($2\theta$) satisfying Brag law and a shift in the estimated center reflects the changes in the lattice spacing. The angle can be converted then to plane spacing using Bragg’s law (Eq. 2-1) and to the lattice strain using Eq. 2-2. The whole in situ set up is placed on a rotating frame that allows the measurement of lattice strain in the either the loading direction or one of the Poisson directions.

On the Time Of Flight (TOF) neutron beam line Engin-X [8], a “white” incident beam that contains a continuous spectrum of wavelength is used (Fig. 2-3). In general, the pulsed beam is collimated to impinge on a specimen, and is then diffracted towards a detector at a pre-selected
The time of neutron flight from the moderator to a detector is proportional to the neutron wavelength, which is proportional to the lattice spacing of the diffracting plane in the specimen [4]. By measuring the changes in the time of flight, one measures the changes in the plane spacing, i.e. lattice strain using following equation:

\[
\varepsilon_{hkl} = \frac{d_{hkl} - d_{\text{ref}}}{d_{\text{ref}}} = \frac{\lambda_{hkl} - \lambda_{\text{ref}}}{\lambda_{\text{ref}}}
\]

\[
= \frac{t_{hkl} - t_{\text{ref}}}{t_{\text{ref}}}
\]

(2-3)

A schematic of the test set up at Engin-X is shown in Fig. 2-3. At Engin-X the white beam is collimated by slits and then passes through adjustable aperture to define the gauge volume, before reaching the specimen; then the diffracted beam passes through a radial collimator and reaches a bank of detectors. There are two detector banks perpendicular to the incident beam each covering a range of angles [8]. Lattice strains can be measured in the similar way explained for single wavelength measurement and using Eq. 2-3. Samples can be mounted at 45 degrees with respect to the incident beam to measure lattice strains parallel and perpendicular to the loading direction at the same time.

Fig. 2-3. Schematic set-up for time of flight measurement for Engin-X at ISIS [4].
Texture measurement is carried out at NRU using single wavelength (monochromatic) thermal neutrons, where the sample is completely bathed in the neutron beam. In this texture measurement, the specimen is mounted in an Eulerian cradle schematically shown in Fig. 2-4a, in order to be rotated through \( \chi \) (zenith angle, \( 0^\circ-90^\circ \)) and \( \eta \) (azimuth angle, \( 0^\circ-360^\circ \)). A spectrometer is also required to attain the desired diffraction angles for measuring a set of pole figures (i.e. each pole figure corresponds to one diffraction angle). In the measurement, the sample is firstly rotated to a \( \chi \) angle, then rotated through \( \eta \) from \( 0^\circ-360^\circ \) in a step size of typically \( 5^\circ \); at each step, the diffraction intensity is recorded. Then the sample is rotated to the next \( \chi \) angle, with a step size of typically \( 5^\circ \), and again the sample is rotated through \( \eta \) while the intensity is measured. This process is repeated until \( \chi \) is scanned from \( 0^\circ \) to \( 90^\circ \). In this manner, all the sample directions (one after another in a step size of typically \( 5^\circ \) through \( \chi \)) are brought into the diffraction direction, i.e. the scattering vector. Thus, the intensity of one diffraction peak is measured along ‘all’ the sample directions. The sampling grid is shown schematically in Fig. 2-4b. The whole procedure is repeated for measurement of each pole figure with a different diffraction angle [3].
2.1.2 Electron Back Scattered Diffraction

The Electron Back Scatter Diffraction (EBSD) technique is used (by the author) to measure orientation map of grains and map them into the developed crystal plasticity finite element code. In this section some key features of the EBSD technique are mentioned. More details can be found elsewhere [3, 9].

Electron Back Scatter Diffraction, when employed as an additional characterization technique within a Scanning Electron Microscope (SEM), enables individual grain orientations, local texture, point-to-point orientation correlations, and phase identification and distributions to be determined routinely on the surfaces of bulk polycrystals [9]. In contrast to neutron diffraction, where no information about shape, location, or orientation of each individual grain exists, with EBSD all of the mentioned information can be extracted from the surface of polycrystalline materials. The first observation of a diffraction pattern in backscattering mode was reported in 1928 by Nishikawa and Kikuchi [10] in the same volume where transmission electron
microscopy (TEM) Kikuchi patterns were discussed. This technique was discussed in detail by Alam et al. [11] and later investigated by Venables et al. [12, 13].

When an electron beam hits the surface of a tilted sample (typically tilted ~70°), due to elastic interaction between the incident beam and planes of atoms, Kikuchi patterns can be formed on the phosphor screen. When more than one Kikuchi band is generated (as shown in Fig. 2-5), knowing the angle between the bands as well as the bands’ width can lead to determination of the grain orientation.

![A sample Kikuchi band of α-Zr.](image)

**Fig. 2-5. A sample Kikuchi band of α-Zr.**

Nowadays the whole orientation map by EBSD can be performed automatically once the sample is set-up. Depending on the step size used for scanning the electron beam relative to the grain size, the orientation of many points within each grain can be determined. Due to local crystal imperfections or dislocation accumulation, orientation variation always exists inside each grain, though a unique orientation can be assigned to each grain by averaging over all of the orientations using the following equation [14-16]:

```
[Equation]
```
where \( q \) represent orientation in quaternion space and can be calculated from the orientation matrix \( (g) \) using following equation [3]:

\[
\vec{r} = \begin{bmatrix} r_1 \\ r_2 \\ r_3 \end{bmatrix} = \begin{bmatrix} g_{23} - g_{32} \\ g_{31} - g_{13} \\ g_{12} - g_{21} \end{bmatrix}, \quad \omega = \cos^{-1} \frac{g:1 - 1}{2} \tag{2-5}
\]

where \( I \) is the two dimensional identity tensor. Each dislocation or crystal imperfection within the body of a crystal has a stress field associated with it which causes the crystal to deviate from the perfect one. Since diffracted electrons will slightly deviate from Bragg’s condition, deviation from perfect crystal reduces the quality of the captured Kikuchi patterns and makes the indexing process difficult. Hence, with more plastic deformation, dislocation density increases and Kikuchi pattern quality reduces. Also, elastic deformation changes lattice spacing and consequently changes the bands’ width in the Kikuchi pattern. Deviation from standard lattice spacing of undeformed crystals available in the library of the automatic indexing programs (such as the HKL program that is used in this research) is another reason for inability to index acquired patterns at higher plastic deformations. The quality of indexing process at each point is given by a parameter termed the Mean Angular Deviation (MAD) that reflects how close the indexed pattern is to the internal available library. Normally a MAD < 1 is considered acceptable for EBSD indexing.

### 2.2 Crystal plasticity

The overall deformation of polycrystal materials is influenced by the properties and morphology of each single crystal and how these combine at different length scales. The crystal plasticity class
of constitutive models can be used to model deformation and texture evolution of polycrystals, taking into account the effects and interactions of each grain or families of grains. This constitutive model is based on decomposing the deformation into an elastic stretching of the crystal lattice and permanent deformation due to twinning and slip, i.e. motion of dislocations through the lattice. The main application of the constitutive equations is to model rotations of individual grains in a polycrystal, and account for texture evolution during plastic deformation and its consequences in terms of anisotropy of the material as well as strength evolution (hardening) in the elements of the polycrystal. The concept of crystal plasticity was shaped by contributions of Taylor, Schmid and their coworkers [17, 18] after early qualitative observations of slip in aluminum. Different assumptions have been suggested to calculate the deformation/rotation of each grain; for instance, Taylor proposed that internal grains experience the same strain as the applied one [19]. This theory is also called “full constraint theory” which results in a stress upper bound calculation. In this context each grain will experience different stress conditions; consequently, force equilibrium is not satisfied between grains. In contrast to the Taylor upper bound theory, Sachs [20] assumed that each grain experiences the same stress state as the one applied and worked out the lower bound; however, in this case, compatibility equations are not satisfied. A more realistic interaction between grains is given in the Self Consistent (SC) framework [21, 22] where interaction between adjacent grains is replaced by simplified interaction of a grain with an average effective medium. In the SC framework, the true interaction between a grain and its surrounding neighbours is replaced by the interaction of the grain with a medium that represents all of the other grains. The most realistic representation of interaction between grains can be achieved in the finite element framework where both equilibrium and compatibility equations can be solved, in the weak form, simultaneously. More
recently, a formulation to compute local response of polycrystals based on fast Fourier transform algorithm is proposed in which exact solution to the equilibrium equations can be determined [23-25].

The Kinematic theory for mechanics of crystals, in the current research, was initially proposed by Hill [26], Rice [27], and Rice and Hill [28]; these equations, later, were rewritten in the format that can be implemented into the finite element framework by Asaro and coworkers [29-32]. In the kinematic equations it is assumed that the total deformation in a polycrystal can be divided into elastic and plastic parts (shown in Fig. 2-6) in which the former causes lattice stretching and rotation, and the latter causes shear in the crystal by movement of dislocation on specific plane, also called the slip plane, and in a specific direction, also called the slip direction.

![Fig. 2-6. Kinematics of elastic-plastic deformation of crystalline solid deforming by crystallographic slip][32].

Multiple slip systems (at most five systems) can contribute in the total plastic deformation of a polycrystal where shear on each of the slip system can be calculated considering two different approaches. In the first approach, also called the rate independent approach, Taylor assumed that between all of the possible combination of slips systems, the set that minimizes plastic work rate
contribute to the deformation [19]. A solution to the Taylor assumption could in potential be more than one set of systems, which causes the so-called “Taylor ambiguity” where by choosing different sets of slip systems, different texture evolution can be estimated. Alternatively, the energy assumption of Taylor was solved by Bishop and Hill [33, 34] where the maximum work principle determines the deviatoric stress vector for a prescribed strain.

In the second approach, a visco-plastic strain rate sensitivity [31, 35] is used where shear can happen in all of the slip systems. In this context, which is also called the rate dependent scheme and is the one used in the current research, the value of the shear is a function of the ratio of the resolved shear stress on each slip system and the current strength of the system [31, 35, 36]. The strength of the system can also evolve with the shear on each system; different models have been proposed for modeling each slip system evolution where each has advantages and disadvantageous over the other. For instance, Pierce et al. [30] proposed a model in which strength of each slip system correlates with secant hyperbolic of the total shear on all of the system; although the Peirce model is simple, Bauschinger effects cannot be captured in this model. Alternate models, e.g. Bassani and Wu [37], are needed if Bauschinger effects are of interest. In this research an extended Voce hardening rule [38] is used where the strength of each slip system is proportional to the total accumulated shear on all of the systems (Γ) as follows:

\[
\tau^\alpha = \tau_0^\alpha + (\tau_1^\alpha + \theta_1^\alpha \Gamma) \left(1 - \exp \left(-\frac{\theta \Gamma}{\tau_1^\alpha}\right)\right)
\]

(2-6)

where \(\tau^\alpha\) is the strength of the system \(\alpha\), \(\tau_0^\alpha\) is the critical resolved shear stress of the system \(\alpha\); the relationship between all of the parameters for a slip system is shown in Fig. 2-7. This is a phenomenological hardening law that has been used successfully in many prior models e.g. [38-40].
2.3 Deformation mechanism in zirconium

As stated previously, α-zirconium (Zr) has the HCP crystallographic structure. Zr has anisotropic thermal, elastic, and plastic properties, both at the single crystal and polycrystal levels. The thermal expansion coefficients along the a- and c-axes have been reported to be in the ranges of $5 < \alpha_a < 5.7 \times 10^{-6} \text{ K}^{-1}$ and $7.5 < \alpha_c < 12 \times 10^{-6} \text{ K}^{-1}$, respectively [41]. Nominal stress-free lattice spacings at room temperature in the a- and c-axes are 3.23118 Å and 5.14634 Å, respectively, and the c/a ratio is 1.59271 [42]. The elastic constants of single crystal Zr at room temperature are $C_{11}=143.5$, $C_{22}=143.5$, $C_{33}=164.9$, $C_{44}=C_{55}=32.1$, $C_{66}=35.5$, $C_{12}=72.5$, and $C_{13}=C_{23}=65.4$, all values given in GPa [42]. Along the c-axis, the Young’s modulus is 125 GPa, which is the maximum, and along the a-axis, it is 99 GPa [4].
Fig. 2-8. Different (a) slip and (b) twinning system that can be active in Zr [43].

Depending on the temperature and loading condition different slip or twinning system can be responsible for plastic deformation in Zr. The primary deformation mode in α-Zr single crystal is slip on \{1 0 1 0\} prism planes with a Burgers vector of \(\frac{1}{3}(1 1 \bar{2} 0)\), or prism <a> slip (slip/twin systems are shown in Fig 2-8). Prism slip in Zr single crystal has been observed at 77K, 300K, 575K and 1075K [44, 45]; it is the easiest slip mechanism to activate at all temperatures [46]. Basal <a> slip \{0 0 0 1\}(1 1 \bar{2} 0) in the single crystal has been detected at temperatures higher than 850K in grains unfavourably oriented for prism slip [46]. <c+a> slip along \{1 1 \bar{2} 3\} has been observed only under deformation with certain constraints or at high temperatures. The slip plane was determined as \{1 0 1 0\} by Akhtar [46], and \{1 1 \bar{2} 1\} by Tenckhoff [43]. Four twin planes were found to be active in a single crystal, i.e. \{1 1 \bar{2} 1\}, \{1 1 \bar{2} 2\}, \{1 1 \bar{2} 3\}, and \{1 0 1 2\} by Rapperport [44, 45]. \{1 1 \bar{2} 1\} twins were present at all the test temperatures (77K to 1075K), with \{1 1 \bar{1} 2\}, \{1 1 \bar{2} 2\} and \{1 1 \bar{2} 3\} appearing in a deceasing order of importance. During tensile testing of single crystal Zr, at 77K the predominant twinning was on the plane \{1 1 \bar{2} 1\}.
While at 295K, it was on \(\{1 0 \overline{1} 2\}\) [47]. During compression, below 800K the twinning plane was \(\{1 1 \overline{2} 2\}\), while above 800K it was \(\{1 0 \overline{1} 1\}\) [4, 48]. Both the CRSS and hardening of a slip system are a function of alloying elements, grain size, microstructure (e.g. dislocation pile-ups), temperature and deformation history, hence, the ratio between CRSSs for the activation of the deformation systems in Zr alloys is different from what it is presented in Table 2-1. For instance, in Zircaloy-2 the ratio between CRSS of prism, pyramidal \(<c+a>\), and tensile twinning for tension along RD is 1:1.82:1.91, or for industrial grade Zr under uniaxial tension along RD is 1:1.6:2.

**Table 2-1. CRSS for slip modes in single crystal Zr (MPa) [4]**

<table>
<thead>
<tr>
<th>Material</th>
<th>Temperature</th>
<th>Prism slip</th>
<th>Basal slip</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>High purity reactor grade crystal Zr bar</td>
<td>77</td>
<td>10.0</td>
<td>&gt;41</td>
<td></td>
</tr>
<tr>
<td></td>
<td>300</td>
<td>6.5</td>
<td>&gt;24</td>
<td>[44, 45]</td>
</tr>
<tr>
<td></td>
<td>575</td>
<td>2.0</td>
<td>&gt;12</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1075</td>
<td>0.2</td>
<td>&gt;5</td>
<td></td>
</tr>
<tr>
<td>99.8-99.99 wt% Zr (\frac{140 \text{ ppm O}}{1200 \text{ ppm O}})</td>
<td>300</td>
<td>(\frac{3.8 - 6.1}{53.2})</td>
<td>(\frac{13.2 - 25}{138 - 1678})</td>
<td>[49]</td>
</tr>
</tbody>
</table>

### 2.4 Deformation twinning

A general deformation in polycrystals needs five independent slip systems to be active at the same time. In HCP crystals, deformation along the c-axis of the crystal can be accommodated either by one of the pyramidal systems or by tensile twinning. In contrast to plastic slip, which occurs gradually by movement of dislocations on slip plane in slip direction as well as crystal reorientation toward easy glide direction, twinning causes a swift reorientation in part of a grain.
at the inception, with gradual thickening and growth of the twin with continued plastic deformation. Fig. 2-9 shows a collection of mechanical twins in a Zircaloy-2 sample after 3% straining.

The whole twinning process can be divided into four stages. In the first stage, which will be called nucleation, twinning related dislocations accumulate where the twin zone is considered an embryo that may or may not lead to a successful twin [50]. In the second stage, dislocations related to twinning reach a critical value that can trigger a twin to form; in the third stage, called propagation, twins form with a needle shape, typically crossing an entire grain, and in the fourth stage, called propagation, the propagated twin thickens. The conditions for the nucleation of twins have been discussed in great detail. Elementary considerations of the homogeneous nucleation of twins under stress [51] involve the elastic strain energy of the constrained transformation [21], the changes in the Helmholtz free energy of the partially stressed lattice, the interface energy, and the work done by the prevailing stress state [52]. All such analyses show that under the usual levels of applied stresses, the free energy of activation for homogeneous twin nucleation is unattainably large. This leads to the conclusion that twin nucleation requires a high local stress concentration (by a factor of 20–50), pre-existing embryos, and/or special heterogeneities such as pole sources [53, 54] to circumvent the need for nucleation. As a result of these generally acknowledged difficulties, the reported measurements of critical resolved shear stresses for twinning show a very large scatter [54]. During the formation and early growth of a mechanical twin, the twin assumes a lenticular shape that minimizes the elastic strain energy of transformation [21, 51], which, however, severely concentrates shear at the tip, ahead of the twin. As a result, in crystals with high plastic slip resistance, under uniform levels of stress, twins propagate with a near-sonic
velocity [55], but under very non-uniform stresses, such as in surface indentations, they can spread quasi-statically, and fully reverse when the stress is removed [52, 56].

![Distribution of twins in Zircaloy-2 sample after 3% straining in ND direction](image)

**Fig. 2-9. Distribution of twins in Zircaloy-2 sample after 3% straining in ND direction (basal plane normals are mostly parallel to ND)**

### 2.4.1 Modeling and experimental study of deformation twinning

Most of the references of this section are discussed in detail in chapters 3-6, in this section an overview over the key points from them will be presented.

Twin formation and the subsequent rapid change in crystallographic orientation result in a significant change in texture as well as hardening of polycrystals. During plastic deformation by both slip and twinning the total deformation gradient in polycrystals can be decomposed into elastic and plastic parts, similar to the slip base plastic deformation, in which the plastic part of the deformation gradient, in contrast to slip, crystallographic reorientation exists. Fig. 2-10 shows how the total deformation gradient can be decomposed.
Although twin formation is a rapid process at the inception stage, the effect of twin relaxation, which happens both at inception stage and during twin propagation, has been modeled as pseudo-slip where twin relaxation happens on the twin plane in twin direction [57-60]. Twin volume fraction (f) correlates with the amount of shear on the twin system and a reference shear which is a characteristic of the material. For texture evolution, a preliminary assumption in accounting for the swift crystallographic rotation due to twinning was proposed by Van Houtte [61] in which a random grain, chosen based on the “Monte Carlo” approach, is selected and the whole grain is reoriented. This method has subsequently been implemented in many numerical simulations, along with approaches to improve on the same basic assumption. To name a few, Tomé et al. [58] showed that it is necessary to consider a large number of grain orientations to obtain reasonable results using Van Houtte’s assumptions directly; instead, it was proposed to reorient a grain with respect to the most active twinning system, the so-called Predominant Twinning Reorientation (PTR) scheme. Lebensohn and Tomé proposed a volume fraction transfer scheme in which Euler space was divided into cells, where instead of keeping grain volume constant while changing orientation, the volume fraction assigned to each cell evolved [62]. The neutron diffraction
technique has been used extensively to monitor texture evolution during deforming polycrystal [6, 58, 60, 61] and checking the validity of the afore-mentioned methods.

For twin inception, lattice strains measurement during twinning have revealed significant stress gradients between twin and parent grain, observed in both magnesium [63] as well as zirconium alloys [5, 39, 64]. The mechanism of the relaxation is still not well understood. Clausen et al. [63] have proposed that back stresses resulting by constraints imposed by neighboring grains can cause the observed relaxation right at the twin inception. Three dimensional synchrotron X-ray studies has revealed that twins at nucleation have totally different stresses than their parent grain and equilibrium conditions [65, 66] are not satisfied at the twin boundary [67]. Statistical studies of twins have revealed that twins can nucleate in grains with both a high tendency and a low tendency for twinning, where the probability of having twins increases with tendency of the grain to twin [68, 69]. It is shown in the current research that local stresses caused by neighboring grain can cause high fluctuations in local stresses and initiate twin in grains with a nominally low tendency for twinning.

One of the challenges in the modeling as well as experimental study of twinning is the interactions between a twin and other twins as well as pre-existing dislocations in the parent grain [70, 71]. These interactions influence the work hardening of the sample by changing the mean free path of dislocations. Several models have been proposed for taking into account these phenomena; for instance, Proust et al. [72] proposed that slip, in twins, can happen just in the systems that are nearly parallel to the twin plane (effectively due to Hall-Petch hardening effects though not explicitly included) and suggested a composite model for the hardening rule. This model was then modified in order to consider the effect of detwinning [73]. Also, Salem et al.
proposed another hardening model for formally considering twin size (Hall-Petch) effect as well as the changes in the mean free path of dislocations.

In terms of modeling, two different approaches have been used in parallel to study different aspects of twin formation. In the first and predominant one, crystal plasticity equations are applied within a Self Consistent (SC) framework. The SC approach uses Eshelby [21] theory, an inclusion in a homogenous medium, to study macroscopic and to some extend microscopic deformations in crystals. This approach initially was used by Tomé and Lebensohn [75] in modeling twins in anisotropic materials. Some of the modifications that have been made to this approach includes first considering the effects of large deformation [76], and also the effects of grain boundaries and neighboring effects on twin inception [77, 78]. In the second approach, crystal plasticity equations are implemented in the finite element framework; texture evolution was studied by Kalidindi [57] using an FE approach where a new time integration scheme was suggested. In Kalidindi’s work, instead of using the volume transfer scheme introduced by Lebensohn and Tomé [62] and generating another crystal (the twin) in the parent grain, both twin and parent grain orientation were calculated based in the reference crystal configuration (i.e., this is mathematically efficient as extra equations are not needed to be solved for both parent and twin). This formulation was successful in modeling texture development in the two case studies carried out on FCC and an HCP polycrystals. Staroselsky and Anand [59, 60] proposed a rate dependent approach to simulate plastic deformation of AZ31B magnesium alloy where the plastic part of the deformation gradient was modified to account for sliding at grain boundaries. In Staroselsky and Anand’s work [59, 60] “a grain boundary layer” with small volume fraction is considered to deform with a simple isotropic plasticity type flow rule, while the rest of the crystal deform according to crystal plasticity. The primary purpose of introducing the isotropic plasticity
term is to bound the stress levels (at the grain boundaries) in their numerical calculations; Plastic deformation in AM30 magnesium alloy under different loading paths was also studied by Lévesque et al. [79] in the FE framework. More recently, Izadbakhsh et al. [80, 81] proposed a new constitutive model to account for primary and secondary twinning; their model was used to study plastic deformation in magnesium. Works by both Lévesque et al. [79] and Izadbakhsh et al. [80, 81] have emphasized determining the forming limit diagram of magnesium alloys and they used similar large deformation formulations in their mathematical modeling where in Izadbakhsh et al. [80, 81] primary and double twins were considered to have contribution to the material deformation.

2.4.2 Other studies of twinning

At a lower length scale, effects of various parameters on twin formation have been studied within atomistic modeling frameworks. Understanding the interaction between dislocations with twin/parent grain boundaries are the key topic in these studies. In terms of interaction between dislocations and Twin Boundaries (TB) four different possibilities (as shown in Fig. 2-11) exist [82]: a) direct transmission (Fig. 2-11a), i.e. cross-slip; b) direct transmission including an incorporation along the twin boundary (Fig. 2-11b) c) indirect transmission including residual dislocations in the twin boundary where the incident and outgoing slip systems do not possess a same line direction (Fig. 2-11c), and can be dissociated into a two step processes of incident dislocation incorporation, followed by nucleation of an outgoing dislocation from the twin; and d) complete blockage and no transmission – where the dislocation is incorporated in the TB only (Fig. 2-11d) [82]. During the interaction process, residual dislocations remain at the boundary and additional local stress concentrations are generated at the intersection site. When numerous twin-
slip and twin-twin interactions occur in a polycrystal, the deformation behavior is reflected with additional work hardening [82, 83]. Through atomistic simulations, slip transition through various types of \(\langle 110\rangle\) tilts and \(\langle 111\rangle\) twists grain boundaries were studied by Sangid et al. [83] where it was shown that there exists a direct correlation between the magnitude of the residual Burgers vector and the energy barrier for slip transmission at the coherent twin boundary. Engineering twin boundaries at the nanometer scale is regarded as an effective approach to achieve high strength while maintaining a substantial work-hardening ability. The effects of twin thickness, grain size as well as strain rate on the work-hardening behavior of polycrystalline pure Cu with nanoscale twins are analyzed by Lu et al. [84]. Also, the effect of twin spacing and temperature on the deformation behavior of nanotwinned magnesium is investigated by Song and Li [85] using molecular dynamics simulation. Serra and Bacon [86] showed that plastic slip is not transferred from one crystal to the other with a residual dislocation left at the interface; instead, the matrix dislocation decomposes into interfacial defects. Hence matrix slip dislocations can become a new source of twinning dislocations; these then produce twin growth when the appropriate stress is applied to the crystal. Studies of nucleation mechanisms of deformation twins within an atomistic simulation framework showed that, in HCP metals, a stable twin nucleus consists of multiple atomic layers [87, 88]. Further, a molecular dynamics study by Wang et al. [78] showed that low angle tilt boundaries contain a uniform array of large misfit grain boundary dislocations that when exposed to a local stress concentration, the grain boundary dislocations dissociate into small number of twin partial dislocations which then coalesce into a single twin nucleus.
Fig. 2-11. Different possibilities in which Twin Boundary (TB) can act as barrier to dislocation. (a) dislocation transmission by a cross slip process, (b) dislocation transmission involving an incorporation along the twin boundary at the same line intersection, (c) dislocation transmission involving an incorporation along the twin boundary with a different line of intersection, and (d) dislocation blockage after incorporation [82].

In addition to the mentioned non-destructive tests (neutron, x-ray or electron diffraction), acoustic emission technique has been used as a method for study twin nucleation and propagation [89-95]. In contrast to neutron diffraction technique where the order of data measurement for each time step is of several minutes, in the acoustic emission technique many data can be collected in a few milliseconds; by taking advantage over the collection speed, recently, Muránsky et al. [89] have been able to distinguish twin nucleation from twin propagation using acoustic signals while the whole twin deformation process was studied by an in-situ neutron diffraction study. Test set-up of this experiment is shown in Fig. 2-12a. By this experiment, it is shown that yielding and immediate post-yielding plasticity in compression along the extrusion direction of ZM20 Mg alloys is governed primarily by twin nucleation, whereas plasticity at higher strains is presumably
governed by twin growth and dislocation slip. It is further shown that, in the fine-grained alloy, collaborative twin nucleation in many grains dominates yielding, whereas twin nucleation in the coarse-grained alloy is progressive and occurs over a larger strain range. This test also showed that twins in the coarse-grained alloy are nucleated less relaxed with respect to surrounding polycrystalline aggregate than those in the fine-grained alloy. Máthis et al. [94] has also shown that a correlation exists between acoustic signals and the deformation process in AM60 magnesium alloy. This technique is then applied for investigating three magnesium alloys, AM60, AM50 and AM20 by Máthis et al. [93]. The acoustic emission results and optical micrographs showed an important role of twinning during plastic deformation up to 200 °C and a change of deformation mechanism above this temperature. Acoustic emission is also used to quantitatively investigate the effects of grain size and strain rate on twinning behavior of pure magnesium during compression where an exponential relation was determined between twinning relaxation and the cumulative acoustic emission counts [95].

Fig. 2-12: Application of neutron diffraction along acoustic emission (AE) technique in an in-situ test used for studying twinning [89]
Reference List


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Chapter 3

Incorporation of twinning into a crystal plasticity finite element model: evolution of lattice strains and texture in Zircaloy-2

A crystal plasticity finite element code is developed to model lattice strains and texture evolution of HCP crystals. The code is implemented to model elastic and plastic deformation considering slip and twinning based plastic deformation. The model accounts for twinning reorientation and growth. Twinning, as well as slip, is considered to follow a rate dependent formulation. The results of the simulations are compared to previously published in-situ neutron diffraction data. Experimental results of the evolution of the texture and lattice strains under uniaxial tension/compression loading along the rolling, transverse, and normal direction of a piece of rolled Zircaloy-2 are compared with model predictions. The rate dependent formulation introduced is capable of correctly capturing the influence of slip and twinning deformation on lattice strains as well as texture evolution.

3.1 Introduction

All polycrystalline materials can have grains with a non-random distribution of crystal orientations or texture. The overall deformation of polycrystal materials is influenced by the properties and morphology of each single crystal and how these combine at different length scales. The crystal plasticity class of constitutive models can be used to model deformation and texture evolution of polycrystals, taking into account the effects and interactions of each grain or families of grains. This constitutive model is based on decomposing the deformation into an elastic stretching of the crystal lattice and permanent deformation due to twinning and slip, i.e.
motion of dislocations through the lattice. The concept of crystal plasticity was shaped by contribution of Taylor, Schmid and their coworkers [1, 2] after early qualitative observations of slip in aluminum. Quantitative analysis of slip based plastic deformation is feasible by a number of constitutive models, e.g., that established by Asaro and Needleman [3]. The nature of this formulation is such that a wide variety of modeling can be performed to inspect both local and global behavior of materials. Slip based crystal plasticity has shown noticeable success in, e.g., modeling grain boundary mechanics [4-6], texture evolution [7], yield surfaces of single crystals [8, 9], and surface roughening [10].

The complexity of modeling deformation in hexagonal close packed (HCP) materials originates from the anisotropic single crystal properties and highly textured structure found in most practical HCP materials. In these types of metals, the low number of easy slip systems, their asymmetric distribution, and the strict crystallographic orientation relationships for twinning result in the formation of strong deformation textures (e.g., [11]). A low number of easy slip systems also tends to promote deformation by twinning. In the current study, a dilute zirconium alloy with HCP crystal structure and moderately high tendency to twin is considered as a case study. Zirconium and its alloys are extensively used in various nuclear reactors, both light and heavy water types, for different applications [12]. A complete general understanding of the development of intergranular constraints in Zircaloy-2, the alloy studied here, will allow an improved understanding of the plastic deformation of Zr alloys, and contribute to the prediction of in-reactor deformation of in-core components made by different manufacturing routes.
While slip based plastic deformation has been widely studied, fundamental questions about twinning are still unanswered. For instance, questions such as how twinning initiates or when a grain becomes saturated in terms of accommodating further twinning is still not understood. Nonetheless, deformation twinning has been incorporated, in addition to crystallographic slip, within a crystal plasticity approach. A significant contribution was made by Van Houtte [13] where it was postulated that at the time of twinning initiation, and based on a statistical criterion on the twinning volume fraction, twinning could be accounted for by reorienting the total volume of the twinning grain. Later, Tomé et al. [14] showed that it is necessary to consider a large number of grain orientations to obtain reasonable results using Van Houtte’s assumptions. Another model was proposed by Kalidindi [15] in which twinning was considered as pseudo-slip and plastic slip was considered in both the original grain (parent) and the new-born grain (child); the results were validated by comparing with textures of low stacking fault energy Face Centered Cubic (FCC) and HCP metals. Using similar formulations to Kalidindi’s work, Salem et al. [16] studied the interaction between twinning and slip systems and proposed a hardening law that was successful in modeling α-titanium. The effects of child formation on dislocation mean free path reduction in the parent grain, i.e. Hall-Petch effects, as well as the effects of increase in the child’s size or decrease in hardening rate were considered by implementation of the twinning volume fraction within the hardening description of the material. Staroselsky and Anand [17] developed a rate independent constitutive law for modeling slip and twinning in HCP materials based on Van Houtte’s criteria of reorientation due to twinning in addition to a modified flow rule to account for grain boundary plastic strain accommodation effects. The model was implemented to simulate texture evolution and the average stress-strain curve in magnesium rod and plates.
More recently, the effects of slip and twinning on forming limit diagram of magnesium is studied by Lévesque et al. [18] using a rate dependent scheme.

Besides the crystal plasticity finite element (CPFE) approach, the Self Consistent (SC) approach, in which grains are ellipsoidal inclusions within a homogenous equivalent medium [19], has been extensively used in modeling slip and twinning based deformation of materials. For example, recently Neil et al. [20] included finite strain rigid body rotation in a SC code to capture large strain deformation in copper and stainless steel. The mathematical and experimental approach that was used in this study is similar to that we have followed here. In modeling twinning, relaxation and reorientation due to twinning has been studied by Clausen et al. [21] and the results of SC modeling were compared to the response of Mg AZ31, considering some of the assumptions required to understand the initial stress state within newly formed twins. Magnesium is commonly considered a suitable material for studying the mechanics of twinning as it has high tendency to twin [22]. For example, the hardening evolution during twinning and detwinning has been investigated by Proust et al. [23, 24] using SC approach.

In the current study, we have developed a crystal plasticity finite element code to capture deformation in HCP materials considering slip and twinning as the two major deformation modes. The code is used to simulate deformation of Zircaloy-2 under uniaxial tension/compression tests along Rolling (RD), Transverse (TD) and Normal (ND) Directions relative to a parent plate, and the results are compared with neutron diffraction in situ tests carried out by Xu et al. [25]. The measured average strain-stress curves, lattice strains, texture, and twinning volume fractions are compared with model predictions to validate the code.
3.2 Crystal plasticity modeling

3.2.1 General formulation

In this section, the modeling framework used to determine polycrystalline deformation in which both slip and twinning can occur is briefly summarized. The framework of the current code was initially developed by Huang [26] to capture slip based plastic deformation in FCC polycrystals. In the absence of twinning, material flows through the crystal lattice via dislocation motion, whereas the lattice itself, with the material embedded on it, undergoes elastic deformation and rotations [27]. Then the total velocity gradient (L) in the current state can be written based on the elastic part (F^e) and plastic part (F^p) of the deformation gradient as follows:

\[
L = \hat{F} F^{-1} = \hat{F}^e \ast \hat{F}^{-1} + F^e \hat{F}^p F^p \ast \hat{F} F^{-1} \quad (3-1)
\]

where L can be expressed as

\[
L = D + \Omega = \text{sym}(L) + \text{asym}(L) \quad (3-2)
\]

D and \( \Omega \) are symmetric and asymmetric parts of the velocity gradient and are the symmetric rate of stretching and spin tensors, respectively. D and \( \Omega \) can also be decomposed into elastic parts (D^e, \( \Omega^e \)) and plastic parts (D^p, \( \Omega^p \)). In the presence of twinning, the lattice can rotate not only by elastic rotation, but by twinning. In the presence of slip inside the twinned zone, the plastic part of the velocity gradient can be written as [15]:

\[
F^p = F^p \hat{F}^e F^e \hat{F}^{-1} \quad (3-3)
\]
\[ L^P = \dot{\gamma}^P \dot{f}^P \dot{f}^{-1} = \left( 1 - \sum_{\beta=1}^{N^{tw}} f^\beta \right) \sum_{\alpha=1}^{N^s} S^\alpha \dot{\gamma}^\alpha + \sum_{\beta=1}^{N^{tw}} S^\beta \dot{\gamma}^\beta + \sum_{\alpha=1}^{N^{st}} \left( f^\beta \sum_{\alpha=1}^{N^{st}} S^\alpha \dot{\gamma}^\alpha \right) \]  

where \( \dot{\gamma}^\alpha \) represents shear rate in slip system \( \alpha \), \( f \) is the twin volume fraction of the twinned region, \( \dot{\gamma}^{tw}_0 \) is constant shear strain associated with twinning, \( S^\alpha \) and \( S^\beta \) are Schmid factors of slip and twinning systems respectively. There are three terms in the right hand side of Eq. 3-3, the first term represents the contribution of plastic slip in the untwinned zone (parent), the second term represents twinning and the last term represents slip deformation in the twinned zone (child). \( N^s, N^{tw}, \) and \( N^{st} \) are the number of slip systems in the untwinned zone, number of twinning systems in the untwinned zone, and number of slip systems in the twinned zone, respectively. It is worth noting that in the Eq. 3-3, the effects of twinning volume fraction on accumulated slip inside parent and child are not considered. These terms become significant as twinning plastic deformation, or twinning volume fraction, increases. Hence, in the case of a high twinning volume fraction, such as typically happens during loading of Mg alloys, the absence of these terms can be significant, altering the predicted response of the material.

In our current model, a rate dependent formulation is implemented by which all slip and twinning shear rates can be calculated following Asaro and Needleman [3]:

\[ \dot{\gamma}^\alpha = \dot{\gamma}_0 \left| \frac{\tau^\alpha}{g^\alpha} \right|^n \text{sign} \left( \frac{\tau^\alpha}{g^\alpha} \right) \]  

\[ (3-4) \]

In the above formulation, the rate dependency can be controlled by \( n \); if the material is rate independent, a large value can be chosen (~50), whereas if the material is highly rate dependent, a
typical value of 10 can be used. $\dot{\gamma}_0$ is a reference shear strain rate. $\tau^\alpha$ and $g^\alpha$ are resolved shear stress on the slip or twinning system $\alpha$ and strength of this system, respectively.

The strain rate of the twinning systems is related to twinning volume fraction with the following equation [15]:

$$\dot{\beta}^\beta = \frac{\gamma^\beta}{\gamma_0} , \ f^\beta \geq 0 , \sum_{\beta} f^\beta \leq 1 , \text{if } \tau^\beta > 0$$

$$\dot{\beta}^\beta = 0 \text{ if } \tau^\beta \leq 0$$

(3-5)

The restrictions that are imposed on Eq. 3-5 indicate that twinning volume fraction cannot be negative, the sum of the twinned volume cannot exceed the grain volume itself, and the twinned regions are not allowed to untwin. $\tau^\alpha$ is the resolved shear stress which is a function of imposed stress and Schmid factor [27]:

$$\tau^\alpha = P^\alpha \cdot \Psi$$

(3-6)

where $P^\alpha$ is the symmetric part of the Schmid factor and $\Psi$ is the Kirchoff stress. The Jaumann rate of Kirchoff stress is related to the elastic part of the rate of deformation and elastic tensor as:

$$\Psi^e = \mathcal{L} : D^e \text{ where } \Psi^e = \Psi - \Omega^e \Psi + \Psi \Omega^e$$

(3-7)

The above equation shows how Kirchoff stress evolves in the current configuration; the objective stress rate that is defined in Eq. 3-7 is constructed for an observer attached to the crystal lattice.
Consequently, in this type of formulation, elastic modulus does not need to be updated since the coordinate system is attached to the lattice; instead, the rotation of lattice is considered in the stress calculation and in the determination of rate of deformation by updating the slip plane normal and slip direction [28]:

\[
\begin{align*}
\dot{m}^\alpha &= (D^e + \Omega^e).m^\alpha \\
\dot{n}^\alpha &= -n^\alpha(D^e + \Omega^e)
\end{align*}
\] (3-8)

where \(m^\alpha\) and \(n^\alpha\) are the slip or twinning direction and normal to slip/twinning plane, respectively. These two vectors are taken to be vectors that define the slip/twinning system \(\alpha\) in the reference state but are not, in general, unit vectors; instead they remain orthogonal during the loading process.

The strength of each slip and twining system is assumed to follow an extended Voce hardening:

\[
g^\alpha = g_0^\alpha + (g_1^\alpha + \theta_1^\alpha \Gamma)\left(1 - \exp\left(-\frac{\theta_0^\alpha \Gamma}{g_1^\alpha}\right)\right)
\] (3-9)

where \(g^\alpha\) is Critical Resolved Shear Stress (CRSS), \(g_0^\alpha\) is initial CRSS, \(\Gamma\) is accumulated shear on all slip/twin systems, \(\theta_0^\alpha\) is initial hardening rate, and \(g_1^\alpha\) and \(\theta_1^\alpha\) determine asymptotic characteristic of hardening. The rate of evolution of CRSS, \(\dot{g}^\alpha\), on each slip or twinning system \(\alpha\) is related to the rate of strain as:
\[
\dot{\gamma}^\alpha = \sum_{\beta} h_{\alpha\beta} \dot{\gamma}^\beta
\]

(3-10)

where \( h_{\beta\beta} \) is self hardening and \( h_{\alpha\beta} \) is latent hardening and both are functions of total accumulated shear strain on all slip and twinning systems.

### 3.2.2 Twinning considerations

Fig. 3-1 illustrates a grain with a twinned zone. There are two regions \( \mathcal{H}_1 \) and \( \mathcal{H}_2 \) which are separated by a plane \( \mathcal{P} \) with unit vector \( n^{tw} \). The deformation in each region is homogenous and continuous across the interface. Then, at the macroscopic level, the relationship between deformation gradient of two regions is:

\[
F_2 = SF_1 \text{ where } S = I + \gamma_0^{tw} m^{tw} \otimes n^{tw}
\]

(3-11)

One of the two regions can always be considered as an undistorted reference, and consequently, \( F_1 = I \) (where \( I \) is the identity matrix). There is a formal notation system often used to describe twinning \([29, 30]\) that contains four quantities \( \{K_1, K_2, \eta_1, \eta_2\} \). \( K_1 \) is the interface of the twin, the plane orthogonal to \( n^{tw} \) and is called the first undistorted plane or twinning plane. \( \eta_1 \) is parallel to the direction of shear or \( m^{tw} \). \( K_2 \) is the second undistorted plane and is a unique plane where \( \eta_2 \) lies in and is perpendicular to the intersection of \( K_1 \) and \( K_2 \). The plane containing \( \eta_1, \eta_2 \), and the normals to \( K_1, K_2 \) are the plane of shear (S). It can be shown that a vector parallel to a direction \( \eta_2 \) in S will be of same length after the shear has been applied, if the angle \( \alpha \) that it makes with \( n^{tw} \) is given by \( \gamma_0^{tw} = 2\tan \alpha \). Then, all vectors in \( K_2 \) are unchanged in length, but rotated. Then
the rotation matrix that must be used to convert vectors in the untwinned zone into those in the
twinned zone can be determined by a simple reflection equation:

\[ R^{tw} = 2n^{tw} \otimes n^{tw} - I \]  \hspace{1cm} (3-12)

**Fig. 3-1. Twinned and untwinned zone in a grain**

All of the above equations have been implemented in an implicit finite element code (UMAT)
executed in the ABAQUS environment. The word “implicit” in this context means that all of the
state variables at time \( t + \Delta t \) are calculated consistent with values of all other variables at \( t + \Delta t \).
At the beginning of each time increment, the finite element solver provides the UMAT with some
quantities, such as strain increment \( \Delta \varepsilon \) and time increment \( \Delta t \), then the stress increment and
Jacobian matrix (the variation of stress increment with respect to the variation of strain
increment), must be evaluated based on these variables. Abrupt changes in Jacobian matrix (such
as caused by rotation of the elastic stiffness due to twinning) can cause instability in the program
and hence either smaller time increments will be required, i.e. simulation time will be increased, or after a specific number of iterations the FE solver terminates and simulation will not be completed. Hence, the identification of twinning or creation of a twinned zone must be implemented carefully.

In the currently reported work, handling of the twinned zone is based on the model proposed by Clausen et al. [21], therein implemented within a self-consistent framework. However some modifications relative to Clausen’s implementation have been applied here, as described below. The physical condition for twinning initiation is not well understood and here we have specified a critical volume fraction that must be reached at each Integration Point (IP) to generate a new “child” grain at that IP. Therefore, at each iteration of a time increment, the shear strain on each twinning system is calculated and consequently the total volume fraction of twinning can be determined (Eq. 3-5). Once the value of accumulated shear strain due to twinning reaches a critical value, here it is taken to be that associated with a twin volume fraction of 2%, a new child is generated based on the predominant twinning system. In this case, all of the slip systems in the child are reoriented from the parent based on the most active twinning system using Eq. 3-12. Although there are different methods to identify the state of stress and strain in the new grains, it is considered here that the initial stress in the new child grain is equal to the stress in the parent at the time of creation of the child, and that the resolved shear stress on each slip system is then determined based on the new Schmid factors and stresses. In order to allow for relaxation in the child (i.e. a more gradual strength increase), all of the plastic shear strains on all slip systems are set to that of parent’s slip systems. Also the initial strength of child is set to that of the parent at the given iteration.
Because of crystallographic reorientation and the subsequent change in Schmid factors in the child, the resolved shear stress on some slip systems can exceed the current strength of the slip system. Since a rate dependent formulation is used, this would cause numerical instability. To overcome this numerical instability, it is assumed that just at twin inception, the resolved shear stress must not exceed the current strength, i.e. these systems must be on the yield surface, although in a rate dependent formulation, being on the yield surface is not strictly a constraint.

No secondary twinning is allowed in the child in the model reported here, and the increase in volume fraction of the child is determined from subsequent twinning deformation in the parent. Consequently, the volume fraction of parent decreases and may eventually reach zero while that of child increases until potentially the IP has only the characteristics of a child grain. Since all of these volume increments are gradual, the Jacobian matrix does not change abruptly and a very stable analysis can be obtained. In the current formulation, the deformation gradient in the parent and child are considered to be the same and hence different stresses and Jacobians are calculated for each at the end of each time increment. The stress and Jacobian are then held to be representative for the IP as a whole, are calculated based on volume averaged stresses or Jacobians in the parent and twinned zones, e.g., Eq. 3-13, with a similar equation holding for the Jacobian:

$$\sigma^{\text{new}} = \sigma^{\text{old}} + \Delta \sigma$$

$$\Delta \sigma = \left(1 - \sum_{\beta=1}^{N_{\text{tw}}} f^\beta \right) \Delta \sigma^{\text{parent}} + \sum_{\beta=1}^{N_{\text{tw}}} f^\beta \Delta \sigma^{\beta,\text{child}} + \sum_{\beta=1}^{N_{\text{tw}}} \Delta f^\beta (\sigma^{\beta,\text{child}} - \sigma^{\text{parent}})$$  (3-13)
3.3 Crystal plasticity finite element modeling

3.3.1 The model

Neutron diffraction technique was used to measure texture and lattice strain development of Zircaloy-2. The experimental procedure can be seen elsewhere [25], but in brief, the material used is a piece of warm-rolled plate taken from mid-thickness of Zircaloy-2 plate, a place with uniform texture illustrated in Fig. 3-2. In situ tension/compression tests were performed using the time-of-flight neutron diffraction technique and lattice strains were measured in directions parallel and perpendicular to the loading axis.

![Initial texture of Zircaloy-2](image)

**Fig. 3-2. Initial texture of Zircaloy-2**

The measured texture (discretised to 1872 orientations) was used as the input to the FE code, assigning Number of Elements (NE) of each orientation within the model in proportion to the measured volume fraction of the orientation. Since the exact place/shape of each grain is not directly available from a neutron diffraction experiment, elements of various orientations were
randomly dispersed in a cubic geometry in the FE solver. Each cube is a cluster of elements having the same orientation and represents family of grains having the same orientation.

### 3.3.2 Influence of the clustering elements and size of mesh

A number of parametric studies were conducted to ensure that a sufficient density of elements was used to describe each grain. One interesting example observed during this study is explained here. In this study elements were clustered individually, in pairs, in lines (four elements), in planes and in cubes (e.g. $2 \times 2 \times 2$); it was seen that clustering elements results in a more relaxed response. In an individual cubic element there are eight corners that are potentially locations of stress concentration. If the element is required to yield, these edges are likely where the yielding will initiate. Clustering elements leads to a reduction in the number of corners between elements with different orientations, and hence makes the model plastically harder. On the other hand, a grain will not be able to easily describe the variation of stresses occurring across it if a small number of IPs (elements) are present in the grains. This is usually called geometric hardening ($i.e.$, fewer elements/grain leads to hardening). These two phenomena are competing; the result shown here is to have more relaxation when elements are clustered.

Classically, there are several factors that must be checked to verify the convergence of the results in a FE simulation. In terms of an average strain-stress response, this is quite straightforward, but when lattice strains are evolved, the situation becomes more complicated as the number of IPs associated with a grain orientation appropriate for diffraction depends on the diffraction orientations and varies as the grain lattices rotate. In this study, the validity of convergence results was verified by changing the number of elements used to represent an orientation and the number of IPs per element. Four different cases were tested as follows:
• 20³ C3D20 elements, i.e. 216,000 IPs or approximately 115 IPs per orientation (with the actual number of IPs varying dependent on the given diffraction peak and direction in the sample),
• 22³ C3D20 elements, i.e. 287,496 IPs or ~153 IPs per orientation,
• 24³ C3D20 elements, i.e. 373,248 IPs or ~200 IPs per orientation,
• 26³ C3D20 elements, i.e. 474,552 IPs or ~254 IPs per orientation,

where C3D20 elements are continuum stress/displacement elements for 3D stress analysis having 20 nodes [31]. In terms of average strain-stress results, it was revealed that convergent results were achieved with an even smaller model, i.e. 20³ C3D8 (64,000 IPs). However, in terms of lattice strains, more IPs are needed and 22³ C3D20 or alternatively 36³ C3D8 was required to obtain convergence. Distribution of these elements as blocks of 2x2x2 C3D8 elements with the same orientation was found to give convergent solution for average lattice strains, which can be compared directly with strains determined by diffraction.

3.3.3 Applied boundary conditions
The initiation and propagation of twinning can be potentially significantly affected by Boundary Conditions (BC) since boundaries can show stress concentrations associated with the applied constraints. Several possible approaches were examined to minimize the effects of boundary assumptions. For example, it was determined that three layers of elements used as a boundary layer surrounding the core elements, with material properties identical to the core but not allowing for twinning reorientation, produced good results. The results reported in this paper however reflect the use of Periodic Boundary Conditions (PBC) [32, 33]. The use of PBCs
requires the application of equations on the surface nodes of the modeled elements, which make the block of modeled elements represent a ‘unit cell’, i.e. that repeats indefinitely. These equations are such that opposite surfaces deform in the same manner which result in a continuum of deformation between cells. Two dimensional equations that were used by Kumar et al. [34] are extended in three dimension and are applied to the model. For instance, the following constraints are imposed on surface ABCD and EFGH of Fig. 3-3:

\[ u_i^{ABCD} - u_i^A = u_i^{EFGH} - u_i^E \text{ where } i = x, y, z \quad (3-14) \]

where \( u_i^{ABCD} \) is displacement in the \( i \) direction (\( x, y, \) and \( z \)) of the surface ABCD where corners and lines connecting the corners are not included in this equation. Corner A is fixed in the \( x \) and \( y \)-direction and external displacement for tension/compression along ND is applied at this point. Corner E is fixed in all directions. Similar constraints are imposed on four other surfaces where the master nodes are F and H. Corner F is fixed in \( x \) and \( z \)-directions but is free to move in the \( y \)-direction. Corner H is also fixed in \( y \) and \( z \)-directions and is free to move in the \( x \)-direction. These two corners (F and H) are the places where tension/compression along TD and RD are imposed. Constraints on the connecting lines are such that those lines belonging to the master surfaces move with the master nodes. For instance, constraints that are imposed on line BC are as follows:

\[ u_i^{BC} - u_i^F = u_i^{AD} - u_i^A \text{ where } i = x, y, z \]

\[ u_{x,y,z}^E = u_{x,y}^A = u_{y,z}^H = u_{x,z}^F = 0 \quad (3-15) \]
We note that there was no benefit in terms of time of simulation between PBC and the use of three layers of boundary elements, due to the many additional constraint equations that needed to be solved at each iteration.

![Fig. 3-3. The cube of elements where orientations are assigned (a) before straining (b) after 10% straining y-z view with scale factor of 3](image)

### 3.4 Results and validation

#### 3.4.1 Average strain stress curves

Measured orientations were assigned to a cube with 36×36×36 first-order eight-noded elements (C3D8), i.e. ~200 IPs (ignoring texture weighting) were assigned to each orientation. Elements of each orientation were clustered in the form of cubes with eight elements (2×2×2) to permit some stress variation inside each grain. In the first step of the simulation, the model was cooled down from 898 K to 298 K to include the effects of residual thermal stresses induced in the manufacturing process, which have a significant impact on the generation of internal strains in zirconium [35]. In the second modeling step, 15% uniaxial strain was applied at the specified nodes while temperature was kept constant. Uniaxial tension/compression loads along either ND,
TD and RD were applied at the specified nodes with a macroscopic strain rate of 5.5E-5 s⁻¹ (to correlate with the experimental test).

### Table 3-1. Single crystal properties of Zircaloy-2

<table>
<thead>
<tr>
<th></th>
<th>n</th>
<th>( \dot{\gamma}_0 ) s⁻¹</th>
<th>( g_0 ) GPa</th>
<th>( g_1 ) GPa</th>
<th>( \theta_0 ) GPa</th>
<th>( \theta_1 ) GPa</th>
<th>( h^{\text{ss}} ) (self)</th>
<th>( h^{\text{st}} ) t=Prism</th>
<th>( h^{\text{st}} ) t=Basal</th>
<th>( h^{\text{st}} ) t=Pyramidal</th>
<th>( h^{\text{st}} ) t=Tensile twinning</th>
</tr>
</thead>
<tbody>
<tr>
<td>Prism</td>
<td>20</td>
<td>3.5×10⁻⁴</td>
<td>0.12</td>
<td>0.33</td>
<td>0.01</td>
<td>0</td>
<td>5</td>
<td>5</td>
<td>5</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Basal</td>
<td>20</td>
<td>3.5×10⁻⁴</td>
<td>0.168</td>
<td>0.22</td>
<td>0.05</td>
<td>0</td>
<td>5</td>
<td>1</td>
<td>5</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Pyramidal</td>
<td>20</td>
<td>1.0×10⁻⁴</td>
<td>0.331</td>
<td>0.27</td>
<td>0.62</td>
<td>0.28</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Tensile twinning</td>
<td>20</td>
<td>1.0×10⁻⁴</td>
<td>0.25</td>
<td>0.2</td>
<td>0.05</td>
<td>0</td>
<td>1</td>
<td>5</td>
<td>5</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>

In order to capture proper texture and lattice strain evolution in Zircaloy-2 it is typically considered necessary to include basal \( \langle 1 \bar{2} 1 0 \rangle \), prismatic \( \langle 1 \bar{2} 1 0 \rangle \), and pyramidal \( \langle 1 1 \bar{2} 3 \rangle \) slip deformation along with tensile twinning \( \langle \bar{1} 0 1 1 \rangle \) [36]. These systems are all considered in the modeling here.

The elastic properties of the single crystal assumed to be identical to those of pure Zirconium determined by Fisher and Renken [37]: \( C_{11}=143.5 \) GPa, \( C_{33}=164.9 \) GPa, \( C_{12}=72.5 \) GPa, \( C_{13}=65.4 \) GPa, and \( C_{44}=32.1 \) GPa. The thermal properties that were measured by Xu et al. [35] for this alloy are applied to the model and are: \( \alpha_1=5.3\times10^{-6} \) and \( \alpha_3=10.1\times10^{-6} \) 1/K. The implemented single crystal properties of the plastic modes (critical resolved shear stress, hardening, etc.) were the ones determined by optimizing agreement between a self consistent model [38] to the same experimental results that are discussed here.
It is worth noting that if the same single crystal (slip or twinning system) material properties are used in both SC and CPFE modeling, the results of the latter are plastically softer than that of the former. These softer results arise from the use of sharp edge geometries in the CPFE modeling, i.e. assigning brick or triangular element geometry to the grains, while ellipsoidal or spherical geometries are assigned to the grains within a self consistent modeling. This ellipsoidal geometry leads to a uniform stress state in the grain (Eshelby 1957), i.e. that intragranular fluctuations of the stress and strain fields are not considered. In contrast the angular geometry of CPFE models
results in intragranular stress concentrations that lead to grains being prone to localized yield earlier than would be expected based on SC results (see Section 3.5.1 for further discussion). Here, we have therefore adjusted the initial critical resolved shear stresses to compensate for these geometry effects, while keeping other parameters (e.g., hardening) the same as those determined by the SC model [45]. By comparing CPFE results regarding the relative activity of different slip/twinning systems with that obtained from SC results, it was determined that the CRSS of prismatic, basal, and pyramidal systems needed to be increased roughly by about 20, 5, and 32 percent, respectively compared to the optimized SC results (the CRSS for twinning was not changed) to optimize CPFE agreement with the experimental results. We have not adjusted the other hardening parameters, although one could undoubtedly improve agreement with experiment further somewhat by such a change. Table 3-1 shows the single crystal properties that are used in the FE simulations.

The average stresses and strains at each time step are $\frac{1}{N}\sum \sigma$ where $N$ is total number of elements multiplied by the number of IPs per element and $\sigma$ is the stress at each IP. Generally acceptable results were achieved using the single crystal parameters given above. As illustrated in Fig. 3-4, due to strong texture, different behaviors are observed for loading in different directions relative to the parent plate. For instance, for deformation along ND there are lots of plastically hard grains (i.e. grains with \{0 0 0 2\} plane normal parallel to the loading direction); hence either tensile twinning and/or pyramidal slip must be activated leading to the highest yield stress in tension is observed in this direction. In contrast deformation along RD needs basal and prismatic slip systems to be activated and hence the minimum yield stress is observed in this direction. The difference between yield points of Ten./Comp. along RD and TD is due to difference in
population of \{0 \, 0 \, 0 \, 2\} planes in these two directions with more in TD than RD. It can be seen that the CRSSs of the single crystals have been well determined as the yield points (i.e. inflections) of the individual lattice strain curves, which are controlled by CRSSs of different slip/twin systems, are well captured in all six directions. However, while the curvature that follows yielding is captured in some directions, i.e. Comp. RD, Comp. TD, and Ten. ND, it is not well captured in the other three loading directions. This curvature is controlled by the load transfer between grain families that are undergoing different levels of plastic deformation and hence by the values of \(\theta_0, \theta_1\) used in the Voce hardening [39], and also by the power law coefficients (Eq. 3-4). For instance, the overestimation of strains seen after yielding in the Ten. RD is because of the assigned values to the \(\theta_0\) and \(\theta_1\) for the prismatic and basal systems. On the other hand, an underestimation of the curvature associated with yield is observed in the Comp. ND where the curvature is also affected by the \(\theta_0\) and \(\theta_1\) of the prismatic and basal systems. Changing the values of \(\theta_0\) and \(\theta_1\) could improve the prediction of behavior in these two directions, but will then change the predictions in the other directions as well. This difficulty in matching all aspects of such a large data set firstly demonstrates the strong constraints placed on polycrystal models by matching measurements taken in multiple orientations on a given sample. Secondly it suggests that a more complex, perhaps dislocation based model is needed to describe the hardening behavior – especially the interaction between different slip systems and between slip systems and twinning – which is only crudely described by the hardening matrix approach used here.
3.4.2 Texture evolution

In Fig. 3-5, calculated textures using CPFEM are compared to measured ones. The model qualitatively and quantitatively captured the main features of the pole figures, i.e. the positions of the maximum and minimum concentrations of the texture components and changes associated with twinning. Interestingly, in comparing to SC modeling of texture [36] the maximum and minimum of texture is significantly better captured by FE modeling than SC modeling which could be related to more realistic representation of compatibility equations in the FE modeling, i.e. the inclusion of grain neighborhood interaction effects, and to a better description of the intragranular fluctuations in crystallographic orientation. A more quantitative comparison between experimental and CPFE results for textures could be represented by checking texture coefficients or fibres; this is a potential method that is not followed here.
Fig. 3-5. Texture of Zircaloy-2 for loading along different directions: comparison between modeling (CPFEM) and experiments (Exp).
In Comp. ND, Fig. 3-5, more basal normals are grouped close to ND than for the initial texture, but in general the basal normal distribution around ND does not change significantly since basal slip reorients basal normals toward ND while pyramidal slip does the opposite. Twinning deformation is not very active in this case and twinning volume fraction (Fig. 3-6) at the end of the loading is less than 2%. While negligible twinning is observed in Comp. ND, more than 20% of the initial grain volume is twinned in Tension along ND. Because of the more difficult deformation along TD during tension along ND, the basal distribution around ND spreads more towards TD than towards RD as a result of basal slip. It is also observed that residual stresses have considerable effects on texture calculation. Ignoring the initial thermal stresses in the modeling would result in missing some poles, especially in Tens. ND, and missing some inflections in the lattice strain curves (discussed below).

Tension and compression along TD also activate tensile twinning; however, twinning volume fractions are much less than Ten. ND. The activity of tensile twinning results in appearance of basal normals near TD in Comp. TD.
Fig. 3-6. Twinning volume fractions. Comparison between a elastic-plastic self consistent (EPSC) model [38] and CPFE results : a) tension tests; b) compression tests.

While Comp. RD activates twinning, negligible twinning occurs in Ten. RD. this is clearly evident in Fig 3-6. Most of the deformation is accommodated by basal slip in Ten. RD which results in expansion of basal normals in the ND-TD plane and contraction of those in the ND-RD plane.

In general agreement between the model and experiment for texture predictions is good; worst agreement (though still reasonable) is achieved for the Comp. ND test. In this orientation <c+a> slip will be heavily active. Despite multiple attempts focusing on this aspect, we were not able to improve agreement of the Comp. ND texture predictions with experiment by tuning of parameters without effecting other predictions significantly. We believe that this may be due to a failure to capture the interaction between <c+a> slip and <a> (basal and prism) modes with the simple hardening model used here; since this is the only loading orientation where significant amounts of both <a> and <c+a> slip is required, it is understandable that a failure to capture interactions would have the most significant effect.
3.4.3 Lattice strains

Lattice strains are the elastic strains of families of grains that have a similar orientation; such that they contribute to a measured diffraction peak. How ‘similar’ in orientation the grains must be is determined by a range of factors including incident beam divergence, size of detector, etc.; however, typically it represents grains with a scattering vector ±5° in common. Lattice strains are measured by determining the movement of such a diffraction peak, in an X-ray or neutron diffraction experiment, see e.g. [40] for a review of the technique. Variations in the sharing of the relative fractions of applied load between different lattice orientations can disclose the interaction between the orientations, and hence the operating deformation modes. In the CPFE code, the lattice strains were ‘measured’ by recording the stresses, twinning volume fractions, and Euler angles of each IP at the end of each time step. Euler angles were updated using Eq. 3-16 [41, 42] and, consequently, it was feasible to determine whether or not the IP is capable of contributing to an identified diffraction peak at the end of each iteration.

\[
\begin{align*}
\phi_1 &= -\Omega_{42}^e - \phi_2 \cos \phi \\
\hat{\phi} &= -\Omega_{23}^e \cos \varphi_1 - \Omega_{31}^e \sin \varphi_1 \\
\phi_2 &= -\Omega_{23}^e \frac{\sin \varphi_1}{\sin \phi} + \Omega_{23}^e \frac{\cos \varphi_1}{\sin \phi}
\end{align*}
\] (3-16)

where \( \varphi_1, \phi, \) and \( \varphi_2 \) are Euler angles and \( \Omega^e \) is elastic part of spin tensor defined with respect to the global coordinate. The elastic strain at each IP is then calculated based on the updated orientation and elastic modulus using the current stress state at the IP.

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Fig. 3-7. Comparison between CPFEM results and experiments for tension tests along RD and TD: a) RD/ND; b) RD/RD; c) RD/TD; d) TD/ND; e) TD/RD; f) TD/TD.
Lattice strain evolutions along ND, RD and TD (measured directions) as a function of applied true stress are illustrated in Fig. 3-7. The general trends on lattice strains variations were captured using the current model in all cases; the level of agreement is very similar to that which can be achieved using self-consistent modeling approaches, e.g., Mareau and Daymond [38]. By comparison of lattice strains in tension along RD and TD it can be seen that development of the lattice strains in these two plate directions is very similar. For instance, for tension along RD and measurement along RD (Ten. RD/RD), lattice strains hardly deviate from linearity which is also similar to that seen in Ten. TD/TD. All the strains remain in the positive zone whereas in the Poisson directions strains are in the negative zone initially. The \{0002\} strain remains entirely in the negative zone in Ten. RD/ND and Ten TD/ND while strain in other planes shift to positive zone as a result of strain redistributions.

Grains generally yield sooner in Ten. RD comparing to Ten TD, as seen by deviations from linearity of the lattice strains in the direction measured parallel to the applied load. For instance, \{20\overline{2}1\} strains deviate from linearity at 200 MPa in Ten. RD while they deviated at 300 MPa in Ten. TD. This can be explained by looking at the initial texture (Fig. 3-2); very few plastically hard grains are oriented in RD direction (i.e. grains with \{0002\} orientation in the RD direction) while a moderate number are seen in the TD.

Acceptable results were achieved in terms of yield point prediction for the different lattice strains. For instance, the yield point of the \{2 0 \overline{2} 1\}, \{1 1 \overline{2} 2\}, and \{1 1 \overline{2} 0\} orientations are calculated accurately, although that of \{0 0 0 2\} strain is captured some discrepancy (under predicted) compared to experiment. In Ten RD/ND, two changes in gradient (inflection) are seen in the
former orientations and both are captured by the CPFE model. The first inflection is a move from negative strains towards more positive ones and the second shows a saturation in terms of strain accommodation. Some discussion of the relative contribution of the operation of different slip systems to such inflections can be found in Xu et al. [35] and Mareau and Daymond [38]. It should be noted that, the number of IPs that participate in the strain measurement changes with these inflections, for instance, the number of IPs participate contributing to the \{2 0 2 1\} strain measurement at the beginning of the loading process is 15,547, it reaches a maximum value (17,704) at the beginning of the first inflection and ends up with 15,360. The fluctuations in the values of strain that can be seen in the last stages of the loading are due to the variations in number of the IPs contributing to the calculated strain.
Fig. 3-8. Comparison between CPFEM results and experiments for compression test along TD: a) TD/ND; b) TD/TD; c) TD/RD. Information on eight diffracting planes is separated in two groups of four to avoid clustering.
Lattice strain development for compression along TD with respect to the applied true stress is illustrated in Fig. 3-8. Generally, shifts and yielding in lattice strains are well captured using the CPFE code, with levels of under prediction and over prediction in some lattice strain curves that is comparable to that seen with models reported in the literature.

Because of the anisotropic single crystal elasticity of Zircaloy-2, a different elastic modulus is calculated in different directions using CPFE modeling. The elastic behavior of the material in different directions is well captured revealing that single crystal elastic properties that are used in the CPFEM are appropriate. Different inflections that are observed during loading are a result of activation of different deformation modes. For instance, in Comp TD/TD, three inflections are observed for the \{0 0 0 2\} strain. The first inflection, at -300 MPa, is because of activation of basal slip [35] and is captured by the CPFE model. Between -300 MPa and -370 MPa, the magnitude of this strain increases and then stops due to the second inflection, caused by tensile twinning. At -370 MPa the number of grains oriented in the \{0 0 0 2\} direction increases rapidly since twinning reorients grains into this direction. The reoriented grains are grains with lower strains and hence the contribution of these grains leads to a decrease in magnitude of strain. Table 3-2 shows how the number of IPs that diffract the TD beam for \{0 0 0 2\} direction increases rapidly at -350 MPa. However, it can be seen that the model prediction of this reduced increase in strain is less than that seen experimentally – the ‘S’ shaped nature of the response is not captured. The model predictions of Clausen et al. [21] suggest that this may be due to the fact that newly formed twins are significantly relaxed compared to the parent grain, or at least that this ‘S’ shape is controlled by the relative partitioning of the stress field between the untwinned and twinned
region, factors not yet included in the model reported here, where instead the child grains start with the stress state of their parent.

<table>
<thead>
<tr>
<th>Applied stress (MPa)</th>
<th>(0002) strains (με)</th>
<th>Number of diffracting IP</th>
</tr>
</thead>
<tbody>
<tr>
<td>-107.759</td>
<td>-410.7</td>
<td>3008</td>
</tr>
<tr>
<td>-338.535</td>
<td>-435.80</td>
<td>3537</td>
</tr>
<tr>
<td>-345.603</td>
<td>-4714.3</td>
<td>3988</td>
</tr>
<tr>
<td>-351.369</td>
<td>-503.61</td>
<td>4607</td>
</tr>
<tr>
<td>-356.168</td>
<td>-5299.3</td>
<td>5350</td>
</tr>
<tr>
<td>-360.223</td>
<td>-5531.4</td>
<td>6295</td>
</tr>
<tr>
<td>-363.692</td>
<td>-5708.4</td>
<td>7398</td>
</tr>
<tr>
<td>-377.339</td>
<td>-6272.0</td>
<td>14977</td>
</tr>
<tr>
<td>-383.064</td>
<td>-6427.0</td>
<td>19549</td>
</tr>
<tr>
<td>-389.685</td>
<td>-6553.9</td>
<td>24680</td>
</tr>
</tbody>
</table>

While three inflections are recognizable in \{0 0 0 2\} strain, no such dramatic shift occurs in \{1 0 1 1\} and \{1 0 1 2\} strains and the CPFE model successfully captured their evolution.

In Fig. 3-9, evolution of lattice strains along ND is illustrated as a function of applied load. The trends in the evolution of lattice strains in ND are also well captured with CPFE modeling. In this direction, the texture is dominated by \{0 0 0 2\} grains parallel to the applied load. Unlike the \{0 0 0 2\} strain in Comp. TD/TD, the \{0 0 0 2\} strain in Comp. ND/ND is almost linear with a slight transition in the elastic to plastic zone, as basal and prismatic systems become active [35], and another slight change in the slope because of activation of pyramidal slip (with slightly over
predicted stress in this family of grains). There is insignificant effect of tensile twinning as the
twinning volume fraction is less than 3% at -12% macroscopic strain in Comp ND (resulting from
reorientation of grains with \{0 0 0 2\} plane normal parallel to the TD direction which are
undergoing local tension due to Poisson constraints). Consequently, the variation in the number
of IPs contributing to a diffraction peak is not as strong as that of Comp. TD. Other strain
developments in Comp ND/ND are similar to Comp TD/TD except that because of the low
activity of tensile twinning system, the activity of pyramidal systems causes slightly more clear
change in lattice strain slopes.

In the Poisson directions (Fig. 3-9b), the first and second inflections in the \{0002\} strains are also
related to activation of basal and pyramidal systems, respectively. The differences that are
generally seen between the calculated and measured lattice strains are higher than seen for
measurements parallel to the applied load, as discussed for cubic materials by Oliver et al. [43].
Fig. 3-9. Comparison between CPFEM results and experiments for compression along ND: a) ND/ND; b) ND/TD; c) ND/RD.
3.5 Discussion

3.5.1 Average strain stress curves

The sequence of activation of each slip/twin system varies from loading in one direction to another, but generally the initial yield behavior of Zircaloy-2 is controlled by slip on the prism and basal systems. These activities are controlled first by the CRSS of each system, and secondly by the hardening of the systems. The parameters were implemented in a SC code [38] with the same assumptions for slip and twinning as those given in the modeling section of the current paper for comparative results. As previously stated, the geometry assigned to grains can control the yield behavior; since grains have an ellipsoidal shape in the SC modeling, assigning cube elements to grains causes premature yielding in the CPFE due to higher stress concentration in cubical grains. This was readily tested by comparing ellipsoidal and cubic grains in a homogenous medium with a given mis-orientation with respect to the grain. Results of our CPFE tests confirmed that the peak stress in cubic grains is higher than the ellipsoidal grains, and that the distribution in stress in cubic grains is also larger. Although results of the SC modeling are always stiffer than those of CPFE, SC codes can generate single crystal parameters more efficiently in terms of simulation time. Especially, when the response of the material depends on the direction of loading, e.g., in this case Zircaloy-2, SC models can facilitate the determination of the single crystal parameters as they are an order of magnitude (in some cases two or even higher, depending on the size of the model) faster than CPFE models. Once parameters are identified by SC modeling, just a few adjustments in the CRSSs, and potentially the hardening parameters, could be enough to account for the different stress concentrations present in the CPFE approach.
3.5.2 Lattice strains and texture evolutions

In the previous section it was shown that our first approximation for a stress state in the child grain (equal to that of parent at inception) causes failure to capture the relaxation observed in the \{0002\} grains in Comp. TD/TD. In an alternative second approximation, continuity assumptions (Eq. 3-17) for tractions and elastic displacements across the twin boundaries are enforced [21]:

\[
\begin{align*}
\varepsilon_{11}^{pa,el} &= \varepsilon_{11}^{ch,el}, \\
\varepsilon_{22}^{pa,el} &= \varepsilon_{22}^{ch,el}, \\
\varepsilon_{12}^{pa,el} &= \varepsilon_{12}^{ch,el} \\
\sigma_{33}^{pa} &= \sigma_{33}^{ch}, \\
\sigma_{23}^{pa} &= \sigma_{23}^{ch}, \\
\sigma_{13}^{pa} &= \sigma_{13}^{ch}
\end{align*}
\]

where \(pa\) represents parent grain, \(ch\) represents child grain, \(el\) represents the elastic part of the strain tensor. Eq. 3-17 should be applied in the local coordinate system where axes 1 and 2 are in the twin plane with axes 1 along the shear direction of the twin system, and axis 3 is along the twin plane normal. Knowing the elastic strain tensor, the other six unknowns can be determined. However, since zirconium is not a very elastically anisotropic material, coupled with not localizing the initial twinning plastic strain in the twin, this method yields similar results to those that were achieved using the first approximation i.e., it basically enforces a similar stress state in the parent and child at inception. Using the same assumption for the initial stress state in the newly-created twins, the same results in terms of strain state in grain families were achieved with the SC code (Fig. 3-10b). However, while the SC model makes this calculation Eq. 3-17 at a single grain, the FE code carries out the calculation at an IP, i.e. a location smaller than a grain;
hence, it represents a larger number of interfaces within the grain. Further investigations into determining the initial stress state in the child at inception are clearly required.

Another assumption that affects the local and global response of the material is how load is shared between twin and parent at each IP. In the current model, it is assumed that strain increment is the same for the parent and child and the stress increment is calculated at the end of each step based on the volume average of the parent and child. This assumption basically means that the twin is embedded in the grain and is an upper bound for calculation of the stress. However, the gradual changes in an IP as it convert from ‘parent’ to the ‘child’ suggests the need for a more realistic representation of the evolution of twins, as twins nucleate in the shape of lamina and their volume gradually increases with applied strain. An alternate method is to convert the IP properties from parent to child swiftly at inception. In this case, the results will be significantly mesh sensitive as the representative volume element must be comparable to the twin size. Consequently, this method is useful when twinning in individual grains or interaction between a small number of grains is of concern e.g., when they are compared to high resolution synchrotron X-ray or EBSD results. On the other hand, since many grains are within the scattering volume of a typical neutron diffraction test, it is sensible that the CPFE volume studied will also contain many grains and twins, and hence the scheme of gradually changing properties of the IP that is used here is more efficient.
3.5.3 Direct comparison between SC and CPFE results

The sequence of activation of each slip/twin system varies from loading in one direction to another, but generally the initial yield behavior of Zircaloy-2 is controlled by slip on the prism and basal systems. These activities are controlled first by the CRSS of each system, and secondly by the hardening of the systems. The slip/twinning modeling and the same single crystal parameters as those given in the modeling section of the current paper were implemented in a SC code [38], to provide comparative results a comparison between the predictions of the SC and CPFE models for lattice strains is shown in Fig. 3-10. In all cases grains (families) generally behave more stiffly in the SC due to their shape as discussed in Section 3.5.1, which is also reflected in the predicted average flow curve. Under these assumptions, the results of the CPFE lattice strains are somewhat closer to the experimental results, presumably since more realistic grain–grain interactions are represented in the CPFE, however the difference is small. The
comparable agreement between CPFE and SC codes appears to show that local intragranular stress fluctuations do not significantly affect the average elastic strains that are determined by diffraction peak position, and compared to in this paper. Presumably such intragranular fluctuations do effect the predictions of the distribution of strains about this average. The distribution of strains would affect diffraction peak width, so in principle can be determined, however this is not easy experimentally and is outside the scope of this paper. When comparing texture predictions we see that the SC model tends to overestimate the strength of the peak (maximum and minimum) texture whereas the CPFE results are closer to the experimental results. In Fig. 3-11 results of the SC code and CPFE are compared for predictions of texture after 15% strain in Ten. RD. The better texture prediction is likely explained by the fact that in a SC model each grain starts with a single orientation and just has one option for its final orientation based on the imposed strain path – which means all the necessary rotations will not necessarily be accommodated in a given grain [44]. In contrast in the CPFE model a given initial grain orientation is affected by its neighbours, and hence can have many possible slightly different final orientations, depending on their effects.

Fig. 3-11. A comparison between texture predictions after 15% straining in TEN. RD: a) SC results b) CPFE results.
3.6 Conclusion
A crystal plasticity finite element code has been developed to simulate elastic and plastic
deformation of HCP materials. Slip and twinning are considered the two major deformation
modes in the modeling. It is observed that the current code is suitable for modeling Zircaloy-2,
capturing average strain-stress curves, lattice (internal grain) strains, and the development of
textures very well in comparison to experimental data. A better prediction of texture evolution is
achieved, while trends on lattice strain development are comparably well captured using this
CPFE code in comparison to previously published reports using SC models. Twinning volume
fractions are relatively smaller that those predicted by SC modeling. The model will be used in
the future to consider in detail the effects of grain to grain interactions on twin nucleation and
growth.

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Chapter 4

Internal strain and texture development during twinning; comparing neutron diffraction measurements with crystal plasticity finite element approaches

Different approaches to the modeling of twinning are examined within the framework of a Crystal Plasticity Finite Element (CPFE) code. The model predictions are compared with in situ neutron diffraction experiments previously carried out on zirconium and magnesium alloys. The experiments are used to evaluate different model assumptions regarding the stress state inside newly formed twins at inception, as well as different assumptions to account for the interaction between twin and parent grain during subsequent twin growth. In particular, the relaxation in some grain orientations that is experimentally observed, and is associated with twin-induced stress relief, can be captured by the model under appropriate assumptions.

4.1 Introduction

The ability to discretize a volume of interest within a polycrystalline material into sub-divisions which are amenable to computational solution has resulted in the Crystal Plasticity Finite Element approach becoming a powerful method for capturing deformation at multiple length-scales. Intergranular as well as intragranular deformation effects can be examined, and the evolution of both internal stress and texture described. Texture, the distribution of crystallographic orientations in a polycrystalline material, can be altered by the plastic deformation imposed on a
material during a manufacturing process or imposed strain. Under a static load, slip based plastic deformation normally induces gradual texture evolution as a function of imposed strain. On the other hand twinning causes abrupt rotation in the crystal lattice of a grain, and hence can result in an abrupt change in the texture of the polycrystalline aggregate. Modeling of many aspects of slip based plastic deformation is well developed [1-3], however critical concepts in the modeling of twinning including both initiation and propagation are still poorly understood.

One of the assumptions typically used in modeling of twinning at a polycrystalline level is to consider the plastic relaxation due to twinning in a manner analogous to that of slip, or generally speaking, to consider twinning as a pseudo-slip [4]. In such a case, twinning is a mode of deformation which induces plastic shear on the specific twin plane and in the twin direction. A preliminary assumption in accounting for the swift crystallographic rotation due to twinning was proposed by Van Houtte [5] in which a random grain, chosen based on the “Monte Carlo” approach, is selected and the whole grain is reoriented. This method has subsequently been implemented in many numerical simulations, along with approaches to improve on the same basic assumption. To name a few, Tomé et al. [6] showed that it is necessary to consider a large number of grain orientations to obtain reasonable results using Van Houtte’s assumptions directly; instead, it was proposed to reorient a grain with respect to the most active twinning system, the so-called Predominant Twinning Reorientation (PTR) scheme. Lebensohn and Tomé proposed a volume fraction transfer scheme in which Euler space was divided into cells, where instead of keeping grain volume constant while changing orientation, the volume fraction assigned to each cell evolved [7].

There have been recent successes in the application of the Self Consistent (SC) approach to modeling the “average effects” of twinning, such as internal strains and texture development [8,
Several different assumptions have been suggested in handling the twin-parent grain interaction. Generally, these studies can be divided into two categories: in the first category, the stress state inside the twin at twin inception is investigated. Clausen et al. [10] showed that in order to capture the observed stress state in some newly generated grain orientations, which appeared due to twinning, it is required to consider the effects of back stresses on the relaxation inside both the new “child” twin (where we use “child” to describe the twinned domain) and the original “parent” grain. In the second category, the main consideration is with regards the load sharing or interaction between child and parent. For instance, Proust et al. [11] showed that uncoupling the deformation in the twins and the parents leads to a stiffer material behavior than the coupled condition. Also, in contrast to a PTR scheme, in reality it is likely that more than one twin system could be active in a given parent grain, even if this occurs after the first reorientation due to twinning.

The aforementioned assumptions and others have been used to model deformation in magnesium and zirconium alloys in which an HCP crystal structure, combined with typically having strong textures induced during manufacturing, results in twinning often being a significant or even dominant deformation mode. For instance, the plastic relaxation caused by twinning in AZ31 and AZ31B, was studied by Agnew and his coworkers [12, 13], though without accounting for twinning reorientation. Similar studies were carried out on Zircaloy-2 with and without considering twinning reorientation [14-16]; such studies have shown that accounting for crystallographic twinning reorientation is mandatory not only to capture texture development but also internal strain evolution. Proust et al. [8] have studied the effects of the rotations caused by both twinning and detwinning on texture development during strain path changes in AZ31.
In the present work, a CPFE code is described to model elastic and plastic deformation, accounting for both slip and twinning. Having multiple Integration Points (IPs) within each grain provides the opportunity to capture strain-stress and texture variation within each grain, in contrast to SC models which typically assume a uniform strain state within a grain. Further, accounting for the interaction between each grain and its surrounding neighbours directly, rather than via the homogenous medium approach utilized in the SC approach, allows us to test some of the assumptions already proposed within SC and CPFE models. Here, for twin initiation, we examine three different conditions to determine the stress state within each child. In the first and second conditions equal stress [17] and continuity equations are forced across the twin boundary [18, 19] respectively, whereas in the third condition, the so called Finite Initial Fraction (FIF) [10] is tested to examine the ability to capture the relaxation caused by twinning. In order to provide insight into the mechanics of the average effect of interactions between parent and twin at their interface, for twin propagation, coupling effects between parent and twin (or lack thereof) are considered using two previously published methods [4, 11, 17]. The predictions from these different modelling approaches are compared with experimental neutron diffraction results, previously reported in [10, 20].

4.2 CPFE model
In this section, the modeling framework used to describe polycrystalline deformation in which both slip and twinning can occur is briefly summarized. For detail of the various formulations in CPFE modeling we refer to the review paper by Roters [21]. In the absence of twinning, material flows through the crystal lattice via dislocation motion, whereas the lattice itself, with the material embedded on it, undergoes elastic deformation and rotation [2]. Then the total velocity
gradient (\(L\)) in the current state can be written based on the elastic part (\(F^e\)) and plastic part (\(F^p\)) of the deformation gradient as follows:

\[ L = \hat{F}F^{-1} = F^eF^{-1} + F^e\hat{F}^pF^{-1}F^e^{-1} \]  \hspace{1cm} (4-1)

where \(L\) can be expressed as

\[ L = D + \Omega = \text{sym}(L) + \text{asym}(L) \]  \hspace{1cm} (4-2)

and \(D\) and \(\Omega\) are symmetric and asymmetric parts of the velocity gradient and are the symmetric rate of stretching and spin tensors, respectively. \(D\) and \(\Omega\) can also be decomposed into elastic parts (\(D^e, \Omega^e\)) and plastic parts (\(D^p, \Omega^p\)). Let us assume that slip based plastic deformation can occur in the both parent and child, then

\[ \varepsilon^p_{\text{Pa}} = \sum_{\alpha=1}^{N^\text{Pa}} p^\alpha \gamma^\alpha; \varepsilon^p_{\text{ch}} = \sum_{\delta=1}^{N^\text{ch}} p^\delta \gamma^\delta; \varepsilon_{\text{tw}} = \sum_{\beta=1}^{N^\text{tw}} p^\beta \gamma_0; \]  \hspace{1cm} (4-3)

where \(p^\alpha\) is the symmetric part of the Schmid factor (\(S^\alpha\)) of system \(\alpha\), \(\gamma\) is the shear on the slip or twinning system, \(\gamma_0\) is the characteristic twin shear, and \(N\) represents the number of slip system available in parent (\(\text{Pa}\)) and child (\(\text{ch}\)). \(N^\text{tw}\) is the total number of twin systems that can be potentially active in the parent. The total inelastic strain, consequently, is comprised of three different terms: the plastic slip in parent, the plastic slip in the child, and the volume fraction of twins. Eq. 4-4 elaborates the contribution of each term to the total inelastic strain.

\[ \varepsilon^\text{in}_T = \left[ 1 - \sum_{\beta=1}^{N^\text{tw}} f^\beta \right] \varepsilon^p_{\text{Pa}} + \sum_{\delta=1}^{N^\text{ch}} f^\delta p^\delta \gamma^\delta + \sum_{\beta=1}^{N^\text{tw}} f^\beta p^\beta \gamma_0 \]  \hspace{1cm} (4-4)

where \(f^\beta\) is the twin volume fraction associated with shear on the twin system \(\beta\). The plastic part of the velocity gradient can now be extracted by taking the derivative of Eq. 4-4 with respect to time:
It is worth noting that the velocity gradient defined here is the complete formulation, although the
effect of twin volume fraction rate on the accumulated plastic shear on slip systems in the parent
and child, the last two terms in the right hand side of the Eq. 4-5, has been historically neglected
[4, 22-24].

In our current model, a rate dependent formulation is implemented by which all slip and twinning
shear rates can be calculated following Asaro and Needleman [3]:

\[ \dot{\gamma}^\alpha = \dot{\gamma}_0 \left( \frac{\tau^\alpha}{g^\alpha} \right)^n \text{sign} \left( \frac{\tau^\alpha}{g^\alpha} \right) \]  

(4-6)

In the above formulation, the rate dependency can be controlled by \( n \); \( \dot{\gamma}_0 \) is a reference shear
strain rate. \( \tau^\alpha \) and \( g^\alpha \) are resolved shear stress on the slip or twinning system \( \alpha \) and strength of
this system, respectively.

The strain rate of the twinning systems is related to twinning volume fraction with the following
equation [4]

\[ \dot{f}^\beta = \frac{\dot{\gamma}^\beta}{\dot{\gamma}_0}, \quad f^\beta \geq 0, \sum_{\beta} f^\beta \leq 1, \text{if } \tau^\beta > 0 \]  

(4-7)

\[ \dot{f}^\beta = 0 \text{ if } \tau^\beta \leq 0 \]

The restrictions that are imposed on Eq. 4-7 indicate that twinning volume fraction cannot be
negative, the sum of the twinned volume cannot exceed the parent grain volume itself and, in this
formulation, the twinned regions are not allowed to detwin. \( \tau^\alpha \) is a function of imposed stress and Schmid factor [2]:

\[
\tau^\alpha = P^\alpha \Psi
\]

where \( \Psi \) is the Kirchoff stress and the Jaumann rate of this stress is related to the elastic part of the rate of deformation and elastic tensor as:

\[
\dot{\Psi}^e = \mathcal{L} : \bD^e \quad \text{where} \quad \dot{\Psi}^e = \dot{\Psi} - \Omega^e \Psi + \Psi \Omega^e
\]

The strength of each slip and twinning system is assumed to follow an extended Voce hardening:

\[
g^\alpha = g_0^\alpha + (g_1^\alpha + \theta_1^\alpha \Gamma) \left( 1 - \exp \left( - \frac{\theta_0^\alpha \Gamma}{g_1^\alpha} \right) \right)
\]

where \( g^\alpha \) is the Critical Resolved Shear Stress (CRSS), \( g_0^\alpha \) is initial CRSS, \( \Gamma \) is accumulated shear on all slip/twin systems, \( \theta_0^\alpha \) is initial hardening rate, and \( g_1^\alpha \) and \( \theta_1^\alpha \) determine asymptotic characteristics of hardening. The rate of evolution of CRSS, \( \dot{g}^\alpha \), on each slip or twinning system \( \alpha \) is related to the rate of strain as:

\[
\dot{g}^\alpha = \sum_{\beta} h_{\alpha \beta} \dot{\gamma}^\beta
\]

where \( h_{\alpha \beta} \) is self hardening and \( h_{\alpha \beta} \) is latent hardening and both are functions of total accumulated shear strain on all slip and twinning systems. The hardening law described here is chosen primarily for ease of use, and for comparison with other models where it has been used extensively. More complicated hardening laws could be readily included in the future, most obviously including dislocation density terms. We have implemented all of the above assumptions in a UMAT code, where at the beginning of each time step, for each IP, the FE solver passes strain and time increments to the code. The code then solves for the total stress increment and Jacobian matrix (the variation of stress increment with respect to the variation of strain increment).
4.3 Twin models

4.3.1 Twin inception

In a CPFE simulation, depending on the size of the representative volume element, a given element and/or integration point (IP) could represent a family of grains, a grain, or a small part of a grain, so, while one of the IPs of an element is ‘twinned’, other IPs of the same elements are not necessarily twinned, see Fig. 4-1b. The inception of a twin at an IP, in the study reported here, is totally controlled by the stress state inside the given IP. In the presence of shear stress on a twin system, the associated twin volume fraction is calculated using Eq. 4-6:8; i.e., twinning occurs independently of the twin volume fraction of any surrounding IPs. For creation of a child in an IP, a parameter ($\xi$) is introduced representing the minimum twin volume fraction required at that IP before crystallographic reorientation occurs. That is, whenever the twin volume fraction on the system $\beta$ reaches the value $\xi$, the systems inside the parent at that IP are reoriented to the new orientation using the twin plane normal of system $\beta$ and a simple reflection equation. This newly created twin then occupies $\xi$ volume percent at that IP initially, and its volume fraction then evolves with the shear on the twin system $\beta$. In this concept, the twin volume fraction then increases gradually until twin/twins take the total volume of the IP. Two different schemes are followed here for the generation of twins at each IP. In the first scheme, only one twin is generated at an IP, with the orientation decided to be that of the (initially) most active twin system. This scheme is also known as Predominant Twin Reorientation (PTR) [10]. Although since there is a non-homogenous distribution of stresses inside a grain, due to interaction with neighboring grains and grain boundary geometry, the predominant twin system can potentially be different in one location of a grain to another, the general physical interpretation of PTR is that one has parallel twins inside a grain where their volume fractions increase until the grain is fully
consumed. In the second scheme, up to six twins are allowed to be created at each IP, and the volume fraction of each increases independently to accommodate the imposed shear strain. This scheme we will call the Multiple Twin (MT) Scheme. Hence, in contrast to PTR, in the MT scheme one might expect a more complicated change in the texture with twinning for example.

Fig. 4-1. The input model used for simulations: (a) FE input: grains with same orientation have similar color (b) schematic showing example of how integration points might map on a grain

The stress state inside the twin is identified here using three different proposed approaches. For the first development of the model, twin and parent grain were assumed to have equal stresses (ES) at twin inception, as previously described [17]. In the second method, continuity equations (CE) for tractions and displacements across the twin boundary are enforced, as previously used in a SC approach [10]; see also [18, 19]. Assuming axis 1 is along the shear direction and axis 3 is along the normal to the twin plane then continuity equations (CE) lead to:

\[
\begin{align*}
\varepsilon_{11}^{\text{Pae}}, \varepsilon_{22}^{\text{Pae}}, \varepsilon_{12}^{\text{Pae}} &= \varepsilon_{11}^{\text{ch}}, \varepsilon_{22}^{\text{ch}}, \varepsilon_{12}^{\text{ch}} \\
\sigma_{33}^{\text{Pae}}, \sigma_{23}^{\text{Pae}}, \sigma_{13}^{\text{Pae}} &= \sigma_{33}^{\text{ch}}, \sigma_{23}^{\text{ch}}, \sigma_{13}^{\text{ch}}
\end{align*}
\] (4-12)
All other unknowns are determined using the elastic modulus of child and parent. The ES and CE approaches imply different equilibrium conditions that are likely not satisfied immediately at twin inception, based on experimental results [25]. However, during twin growth and evolution, parent and twin could potentially return to such equilibrium conditions.

A third method, the “Finite Initial Fraction (FIF)” approach [10] is also used to examine to what extent the code is able to capture relaxation due to twinning. In this assumption the plastic shear on the twin system induces back stresses on both parent and child due to constraint of the surrounding crystals. This back stresses can be determined as:

\[ \sigma^0 = \mathcal{L} \varepsilon^0, \varepsilon^0 = -S \xi / \gamma^0 \]  

(4-13)

where \( S \) is the Schmid tensor. This back stress arises because in the absence of surrounding grains, a change in shape in the parent-child grain might be created right at the inception; however, the constraints imposed by neighboring grains prevent or limit this phenomenon [25]. Generally, twin formation starts with accumulation of enough dislocations to form a stable embryo, this is also called nucleation; once a twin nucleates, it propagates across the parent grain and then widens. Nucleation in the FIF assumption is slightly different to what is used so far in our CPFE terminologies; that is, FIF is when the twin volume fraction reaches a value that can cause notable effect. If the IP is a significant portion of the grain, the FIF is somewhere between nucleation and propagation; if the grain is descretized using lots of IPs, it will be closer to nucleation.

### 4.3.2 Twin growth

Once twinning occurs, the response of the parent grain and material in general is substantially affected by the load sharing between twins and grains. Hence the way that deformation of twins
and parent are coupled could effectively change both the internal and average stress state in a grain. In the current implementation, an IP has a volume fraction of both ‘twin(s)’ and ‘parent’ (in contrast to SC models where a grain is either a twin or parent), hence an assumption as how to handle the allocation of the stress and strain increment associated with the IP between the twin and parent is a requirement of the modeling approach; the twin and parent can never be totally uncoupled. We report here two different conditions that have been used: In the first approach, which we term the “uncoupled” condition, the total strain increment in parent and child at each time step is assumed to be the same. The stress and rotation increments for parent and child are then determined separately. The total stress increment and also the Jacobian matrix for the IP are then determined based on the volume fraction average of the twins and parent:

\[ \sigma_{\text{new}} = \sigma_{\text{old}} + \Delta\sigma \]

\[ \Delta\sigma = \left[ 1 - \sum_{\beta=1}^{N^{\text{tw}}} f_\beta \right] \Delta\sigma_{\text{Pa}}^{\text{Pa}} + \sum_{\delta=1}^{N^{\text{ch}}} f_\delta \Delta\sigma_{\delta,\text{ch}}^{\delta,\text{ch}} + \sum_{\delta=1}^{N^{\text{ch}}} \Delta f_\delta (\sigma_{\delta,\text{ch}} - \sigma_{\text{Pa}}^{\text{Pa}}) \]  

(4-14)

Since in this method the twin and parent at each IP are “uncoupled” in terms of stress interaction, the twin-grain coupling terms in Eq. 4-5. vanish, i.e., the right hand side of this equation reduces to a simple plastic slip in the twins and just the first and the third terms remain in the parent side. Here, just the PTR scheme has been investigated with the “uncoupled” case (i.e., \(N^{\text{ch}} = 1\)). The physical interpretation of an “uncoupled” assumption is that the stress interaction between parent and twin at the twin boundary is not as strong as in the coupled case (see below). However, interaction between twinned IP and surrounding IPs (which may or may not have twinned) due to the compatibility and force equilibrium equations still exist and indirectly account for twin/parent interaction.
In the second or “coupled” approach, the same elastic strain increment is assumed for both parent and child, as proposed by Kalidindi [4]. In such a case, all of the equations to determine plastic deformation inside both parent and twin(s), must be solved simultaneously. So, a strong interaction between twins and parent grain exists and none of the terms in Eq. 4-5 can be neglected. To obtain a sense of the effects of these different coupling terms, four different cases have been studied. In Case I, the rate effects are basically ignored, i.e. the last two terms in the right hand side of Eq. 4-5 are neglected. In Case II, the Twin Volume Fraction Rate Effects (TVFREs) on child are considered but that on a parent is neglected, i.e. the fourth term in Eq. 4-5 is neglected. In Case III, the TVFREs on the child is neglected but that on parent is not neglected. In Case IV, none of the coupling terms are neglected. In this coupled approach, not only are the elastic increment of parent and twin(s) equal, but solving Eqs. 4-1:5 results in equal elastic rotation increments for parents and twin(s). The physical conclusion of this assumption is that small twins ‘follow’ the rotation of the parent grain, while once their volume fraction have decreased sufficiently, the parent grain will ‘follow’ the twin(s). Note that though the elastic strain increment is identical in parent and twin(s), the crystallographic elastic anisotropy means that the stress increment is not identical. In this approach we have examined both PTR and MT schemes.

It is worth repeating that at each IP, there is a parent grain, and one or more twins. In contrast to SC modeling [11], in this CPFE code the twin and parent material at a given IP can never be totally uncoupled, as they must share the total strain increment (or part of it) associated with that IP – this is a constraint of the FE approach. We have described here then two different approaches for assigning this shared strain increment between the twin and parent.
A third approach that could be used, would be to divide the total strain increment such that continuity equations (Eq. 4-12), the stress-strain relationship, and Eqs. 4-14:15 are satisfied at each time increment.

\[
1 - \sum_{\beta=1}^{N_{tw}} f^{\beta} \Delta \epsilon_{i}^{Pa} + \sum_{\delta=1}^{N_{ch}} f^{\delta} \Delta \epsilon_{i}^{\delta, ch} - \Delta \epsilon_{i} = err, \quad i = 1:6
\]  

(4-15)

where err is the error, which is minimized. This method represents the most physically realistic interaction between twin and parent that we considered, as instead of making assumptions as to assignment of the total strain increment (as in the coupled and uncoupled cases), an additional iterative loop is made to evaluate the contribution of both twin and parent to the total stress and strain increment. If more than one twin is created at an IP, finding a solution to Eq. 4-15 will become a computationally tedious process. In order to simplify these equations, it was assumed in initial testing of this third method that there is just one twin at each IP and that it could be treated as being fully elastic. Even in this case, finding an answer that would satisfy all of the aforementioned equations turned out to be extremely time consuming within the CPFE framework. Hence, based on the available computational resources, it did not make sense to pursue this method, and we do not report it further here, though in the future it is undoubtedly an avenue that should be pursued.

4.4 Simulation conditions

The detailed description of the input file of the simulations can be found elsewhere [17], but in brief, the measured texture (by neutron diffraction) was used as the input to the FE code, assigning a Number of Elements (NE) of each crystallographic orientation within the model in proportion to the volume fraction of that orientation. A cube with 36x36x36 first order elements
(C3D8; brick elements, each with eight IPs and nodes [26]) were used and elements of each orientation were clustered in the form of cubes with eight elements (2×2×2) to permit some stress variation inside each grain. Periodic boundary conditions were applied at the surfaces, i.e. effectively representing an infinite aggregate, and uniaxial loads were applied at specified nodes with a nominal macroscopic strain rate of 5.5E-5 s⁻¹. Tables 1 and 2 show single crystal properties used in the simulations.

**Table 4-1. Single crystal properties of Zircaloy-2**

<table>
<thead>
<tr>
<th>n</th>
<th>y₀</th>
<th>g₀</th>
<th>g₁</th>
<th>β₀</th>
<th>β₁</th>
<th>h⁺⁺</th>
<th>h⁻⁻</th>
<th>h⁺⁻</th>
<th>h⁻⁺</th>
<th>t=Pri</th>
<th>t=Bas</th>
<th>t=Pyr</th>
<th>t=TTW</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pri</td>
<td>20</td>
<td>3.5×10⁴</td>
<td>0.12</td>
<td>0.33</td>
<td>0.01</td>
<td>0</td>
<td>5</td>
<td>5</td>
<td>5</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>Bas</td>
<td>20</td>
<td>3.5×10⁴</td>
<td>0.168</td>
<td>0.22</td>
<td>0.05</td>
<td>0</td>
<td>5</td>
<td>1</td>
<td>5</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>Pyr</td>
<td>20</td>
<td>1.0×10⁴</td>
<td>0.331</td>
<td>0.27</td>
<td>0.62</td>
<td>0.28</td>
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<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>TTW</td>
<td>20</td>
<td>1.0×10⁴</td>
<td>0.25</td>
<td>0.2</td>
<td>0.05</td>
<td>0</td>
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<td>5</td>
<td>5</td>
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<td>1</td>
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<td></td>
</tr>
</tbody>
</table>

All slip and twinning systems (basal, prismatic, and tensile twinning) used for simulations are considered the same for both Zircaloy-2 and AZ31 except that pyramidal slip systems {1 0 T 1} are allowed to be active in Zircaloy-2 [16] whereas second order pyramidal {1 1 2 2} are used for AZ31 [27]. The single crystal elastic constants that were used for Zircaloy-2 are those determined by Fisher and Renken [28]: C₁₁=143.5 GPa, C₃₃=164.9 GPa, C₁₂=72.5 GPa, C₁₃=65.4 GPa, and C₄₄=32.1 GPa, and for AZ31 are those determined by Simmons and Wang [29]: C₁₁=59.75 GPa, C₃₃=61.7 GPa, C₁₂=23.24 GPa, C₁₃=21.7 GPa, and C₄₄=16.39 GPa. The plastic properties are those previously used in SC models [15], with some changes as described in [17].
Table 4-2. Single crystal properties of AZ31 [30]

<table>
<thead>
<tr>
<th></th>
<th>( n )</th>
<th>( \dot{\gamma}_0 )</th>
<th>( g_0 )</th>
<th>( g_1 )</th>
<th>( \theta_0 )</th>
<th>( \theta_1 )</th>
<th>( h^{zz} )</th>
<th>( h^{tt} )</th>
<th>( h^{xz} )</th>
<th>( h^{xt} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pri</td>
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<td>0.01</td>
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<td>0.08</td>
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<td>Bas</td>
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<td>0.001</td>
<td>0.012</td>
<td>0.01</td>
<td>0.24</td>
<td>0.0</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Pyr</td>
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</tr>
</tbody>
</table>

4.5 Results and discussion

4.5.1 Coupling effects

The experimental flow curve for tension along the Normal Direction (ND) of a piece of warm-rolled slab of Zircaloy-2, with most of basal planes oriented in ND direction and prone to twin in tension along ND [20], are compared with numerical results in Fig 4-2a. The sensitivity of the model predictions to the assumptions described in Section 4.3 as to load sharing between twin and parent grain can be seen. Figure 4-2a compares different assumptions as to TVFRE. In the absence of the TVFRE on child and parent (Case 1), “coupling” the twin and parent causes a harder response. Interestingly, in contrast to the negligible effects of TVFREs in the parent grains (compare Case 2 and Case 4), the flow curve is significantly affected by the twin rate term (see Case 3). As the twin rate term is a result of accumulated slip shear in the twin multiplied by the twin volume fraction, it’s interesting to see the impact of this term even at the very beginning of the plastic deformation. “Coupling” with rate effects results in softer results (compare Coupled Case 4 with Uncoupled) which is in agreement with the results of SC modeling reported by Proust at al. [11].
Fig. 4-2. Comparison between measured and calculated average flow curves: (a) results of modeling Zircaloy-2 for tension along ND: coupling and uncoupling of twin-parent interactions and twin volume fraction rate effects on the both twin and parent: case I: all TVFREs are ignored; case II: with TVFREs on child; case III: with TVFREs on Parent; case IV: with TVFREs on parent and child; (b) average flow curve of AZ31 for compression along axial direction (see Section 4.5.2 for model assumptions).

4.5.2 Twin growth

In the magnesium modeling, a “rod texture” which is typically generated during extrusion is used as the input texture to the FE code. Since in this rod texture basal plane normals are perpendicular to and are distributed symmetrically about the rod axis, compression in the rod axial direction cause tensile strains in the Poisson direction and hence a significant amount of tensile twinning. In Fig. 4-2b, the general flow curve measured for compression along the rod axis is compared with CPFE results. In this simulation, a “coupled” PTR scheme is used where twins are assumed to behave elastically in order to capture the rapid stress increase in the average flow curve. At twin inception we would expect a strong Hall-Petch effect in the twins, since twins are small in size hence having elastic twins is likely reasonable at low TVFs. At low TVFs, slip dislocations are hard to move in twins as the mean free path of dislocations is small; only slip planes near to
parallel with the twin plane would effectively be active in the twins [11]. Thus, while the assumption of elastic twins will not be valid once they grow in size, it is used to represent the strong restrictions on plasticity associated with twin formation.

The early yield that is observed in the numerical results is related to using plasticity constants that are generated by optimizing SC model predictions (Table 4-2) without adjusting the CRSS of deformation systems, as discussed in [17].

The validity of the PTR scheme for twin growth is examined by inspecting the internal strains, the strains in a family of grains that satisfy the Bragg conditions for diffracting an incident beam in a particular orientation [31], and texture development of AZ31. The results for axial and Poisson direction strains are compared with the calculated strains in Fig. 4-3 a-b, using both the PTR and MT schemes. In the PTR scheme at the inception, shear on all twin systems, with the exception of the predominant one, are deactivated by assigning a very high value to their current strength. This assumption is required since with increase in twin volume fraction (TVF) at an IP, the orientation of the IP changes from the parent orientation into the twin orientation; if other twin systems were to remain active, the predominant twin system in the parent will not necessarily remain the predominant one as twin pseudo-slip is accommodated on other twin systems. This is a quite different case from what is assumed in the SC modeling presented in [10] where relaxation due to pseudo-slip on other twin systems do still exist even after twin inception. General trends in lattice strain development are captured using the PTR scheme; however, the inflection observed at -120 MPa in {0002} planes in Transverse Direction (TD) is not captured. On the other hand, although the MT scheme causes no significant changes compared to the PTR scheme in the average flow curve or the lattice strain evolution in the axial direction, the inflection of {0002} planes in TD is somewhat better captured using the MT scheme. Although
the large relaxation at the yield point is not captured by the MT or PTR schemes, the inflection towards compressive stresses in the \{0002\} family is eventually captured by the MT method (with some under prediction in terms of magnitude of the inflection). The expense of capturing the \{0002\} strain inflection in the MT scheme is a significant increase in the simulation time as the mathematical equations are required to be solved for up to five additional twin systems at each IP. Interestingly, however, the texture evolution that is observed by using a PTR scheme is in fact substantially closer to what is measured experimentally (Fig. 4-4).

![Fig. 4-3. Comparison between PTR and MT schemes for internal strain development in AZ31: (a) axial (b) transverse direction](image)

Fig. 4-4a-c show the measured initial and final texture of AZ31 and calculated final texture of AZ31 using the PTR scheme. The model qualitatively and quantitatively captured the main features of the pole figures, i.e., the positions of the maximum and minimum concentrations of the texture components and changes associated with twinning. In contrast to the lattice strains evolution, for texture prediction significantly better results were achieved using a PTR scheme than in the MT scheme (MTS results are not shown due to space constraints). The main difference is that although in the MT scheme the model was able to capture reorientation of basal
normals from radial direction into axial direction, the intensity of these basal normals was too low compared to what is measured experimentally and achieved numerically with the PTR scheme. This is basically related to the evolution of volume fraction of each of the twins created through the simulation (Fig 4-4d for PTR scheme). Considering both simulation time and the results achieved for lattice strains and texture development, the PTR scheme can be considered a better at modeling average behavior of AZ31 than the MTS.

Fig 4-4. (a) initial texture of AZ31; (b) measured final texture of AZ31 after 10% of straining [10]; (c) results of CPFE for final texture of AZ31 after 10% of straining; (d) comparison between numerical and experimental [10] results of TVF evolution in AZ31.
4.5.3 Twinning relaxation

The capability of three different methods, described in section 3.1, in determining stress state inside twins is investigated in this section. In Fig. 4-5a the measured lattice strains of AZ31 in parent grains and twins are compared with numerical results. Twinning causes normals to the basal planes that were previously perpendicular to the rod axis to become parallel with this axis. Hence, the \{1 0 \bar{1} 0\} grains reorient to become the \{0 0 0 2\} grains that appear at around -120 MPa. The measured data shows that while parent grains are in compression, the new grains appear in tension. As shown in Fig. 4-5a, since the elastic constants of Mg are nearly isotropic, application of either the ES or CE approaches lead to approximately the same results. These two approaches basically enforce the same stress state inside parent and twin grains at the twin inception. On the other hand, the FIF method can generate twins with tensile stresses relative to the parent. There is a negligible difference between the results of this approach and the other two approaches once lattice strain inside the new twins reach around -2000µε. It is worth noting that, in the simulation with FIF assumption, \(\xi\) for twin inception is set at 3%; assigning a higher value to \(\xi\) will cause more tensile stress states inside the new born twins but also causes an instability in the CPFE simulation due to the very rapid change in both the Jacobian matrix and the stress state at the IP. One could fine tune the value of \(\xi\) to obtain a value that exactly captures the exact value of initial twin stresses measured experimentally; however we must consider if such small changes in this value would be physically meaningful.

The FIF method, along with the two other methods, is also applied to model uniaxial compression along Transverse Direction (TD) of Zircaloy-2. In Fig. 4-4b the lattice strains in \{0 0 0 2\} grains with Bragg condition in either ND or TD are compared with those of the CPFE predictions. Xu et al [20] showed that the second inflection observed around -360 MPa in \{0 0 0 2\} TD grains is due
to the reorientation of \{0 0 0 \} ND grains into \{0 0 0 \} TD grains by twinning. The response of the \{0 0 0 \} lattice reflection in the TD direction is due to the strains in the original population of \{0 0 0 \} TD grains combined with the strain of the newly formed \{0 0 0 \} TD grains which are caused by twins. \{0 0 0 \} ND parent grains, are in tension just prior to twin inception since compression along TD results in the Poisson direction being in tension. Similar to the Mg case, application of ES and CE approaches causes almost the same stress state inside parent and new born twins and hence these two methods again result in similar \{0 0 0 \} TD strains. Since in both ES and CE approaches the twins are in tension at twin inception, the average \{0 0 0 \} TD response goes into compression more slowly, however, the significant relaxation that is observed experimentally was not captured using these two approaches. On the other hand, this relaxation is captured by FIF assumption for high value of $\xi$. The results shows that for $\xi = 2\%$ there is negligible difference between the three approaches; however for $\xi = 15\%$, the FIF approach is capable of replicating features of the relaxation due to twinning (although not the magnitude). This is interesting as the value of $\xi$ in the model is directly related to the density of twinning-related dislocations in the actual material. That is, since $\xi$ itself is a critical twin volume fraction, which is proportional to the shear that take place on twin system (Eq. 4-6, 4-7, 4-10), a large value of $\xi$ basically means that a larger dislocation accumulation is required for twin inception [32]. However, this value of $\xi$ seems unrealistically large, compared to experimental (microscopy) observations of twin sizes. With the application of the SE and CE approaches, a sufficient relaxation might be captured if the twin volume fraction was able to increase very rapidly once the twin has initiated, i.e. that once the twin nucleated it was capable of easy propagation [18, 32]. The authors of this paper are now applying this code to grain scale
Fig. 4-5. Comparison between ES, CE and FIF assumptions for twin inception: lattice strains in the parent and twin of (a) AZ31 and (b) Zircaloy-2

4.6 Conclusion

Various methods for twin-parent interaction have been examined using CPFE modeling, and compared to neutron diffraction results. Examining the complete form of velocity gradient that is introduced in this paper showed that the effect of twin volume fraction rates on shear in child can cause huge relaxation even right after inception. Also, comparing multiple experimental data sets, and different approaches, it was observed that the PTR scheme gives acceptable results for both texture and internal lattice strain development. For twin inception, it was observed that the FIF approach is able to explain the relaxation due to twinning once the parameter for twin inception is assigned appropriately, but that an unrealistically large value of initial twin size may be required to obtain such results. Considering the full range of experimental data types considered (macroscopic flow curve, internal lattice strain and texture evolution) the PTR scheme with FIF
assumption for twin inception and use of an uncoupled twin/parent interaction resulted in the best agreement between model and experiment.

Reference List


Chapter 5
Multi-scale modeling and experimental study of twin inception and propagation in hexagonal close-packed materials using a crystal plasticity finite element approach; Part I: average behavior

A Crystal Plasticity Finite Element (CPFE) code is used to study the effect of grain boundary geometry and texture on twin inception and propagation. Three dimensional grains with random shapes are generated using Voronoi tessellation and used for simulations. The results are compared with previously published Electron Backscattered Diffraction (EBSD) studies carried out on zirconium and magnesium. It is shown here that the majority of phenomenae observed experimentally regarding the average (statistical) behavior of twins can be captured by considering the grain boundary geometry. It is observed that twins are prone to initiate at grain boundaries and specifically at the conjunction of more than two grains. The various stress conditions and concentrations at grain boundaries also result in selection of different twin variants.

5.1 Introduction
Plastic deformation in polycrystalline materials can generally be explained by movement of dislocations in the slip plane in a slip direction where under static loading, plastic slip is accompanied by gradual changes in the crystallographic orientation of grains [1-4]. Due to lack of easy-slip systems, on the other hand, materials with Hexagonal Close-Packed (HCP) crystals
often accommodate imposed deformation by a rapid change in the crystallographic orientation which is known as twinning [5-7]. The whole twinning process can be divided into four stages. In the first stage, which will be called nucleation, twinning related dislocations accumulate where twins are embryos that may or may not lead to a successful twin. In the second stage, typically called inception, dislocations related to twinning reach a critical value that can trigger a twin; in the third stage, called propagation, twins form with a needle shape typically crossing the grain, and in the fourth stage, called propagation, the propagated twin thickens. Texture, the distribution of crystallographic orientation of grains with respect to an external coordinate, of an HCP material can change drastically during plastic deformation due to twinning which can alter mechanical behavior of the material. Hence, in order to have a better understanding of deformation mechanisms in HCP materials it is necessary to study parameters that can influence twinning.

Deformation twinning has been studied at different length scales by several experimental and numerical procedures. At a macroscopic length scale, the average behavior of families of twins has been experimentally studied using in-situ neutron diffraction tests [8, 9]. Some fundamental questions about mechanisms involved in texture devolvement [10, 11], interaction between twins and parent grains or other twins [12], twinning and detwinning [13], as well as the stress state inside twins at inception [14] have been investigated. The effects of local parameters on twins, e.g. grain boundary geometry or stress fluctuations within a given grain, are some of the major missing parameters in such experiments. Two major numerical approaches, i.e., Self Consistent (SC) and Crystal Plasticity Finite Element (CPFE), have been implemented to rationalize behavior of materials under these experiments [15, 16]. In the SC approach, a grain has an ellipsoidal shape with homogenous stress and is embedded in a homogenous medium that
represents the average response of all of the other grains [17]. Hence, in conventional SC modeling the effect of grain boundary and stress heterogeneity inside each grain are simply neglected. Nevertheless, a short simulation-time, in comparison to CPFE models, has empowered SC models to provide a significant contribution in explaining physics behind twinning induced by plastic deformation [18-20]. On the other hand, although grain boundaries are not discernable in a neutron diffraction experiment, in terms of modeling, different grain shapes, e.g. cube or more realistic can be used, and many Integration Points (IPs) can be assigned to each grain in a CPFE simulation hence capturing stress and rotation variation inside each grain [21-24].

At a microscopic length scale, statistical study of twins has been experimentally carried out via Electron BackScattered Diffraction as well as micro x-ray diffraction [25-27]. Effects of a wide variety of parameters such as mis-orientation between two neighboring grains and grain diameter or volume on nucleation of twins or twin variant selection have been studied. In terms of modeling, the assumption of having homogenous stress distribution within each grain or ellipsoidal shaped-grain, where stress concentration due to grain boundary geometry are basically ignored, in SC models, results in missing local effects on twin inception and consequently difficulty in interpreting experimental data. Recently, by introducing new parameters which are chosen with the aid of atomistic models, modification has been applied to the current existing SC models to take in to account the probability of having some susceptible / probable twinning sites in a grain boundary. For instance, Beyerlein and Tomé [28] introduced new parameters to virtually create susceptible sites for twinning in their SC model. Also, virtual fluctuations were induced on the Resolved Shear Stress (RSS) of each twin variant to generate deviations from the average RSS calculated from the homogenous stress of the grain; reflecting in reality both the variation in RSS within the parent grain and the potential for variation in RSS required for twin
inception due to grain boundary type. With these considerations, it was shown that grains with both high and low tendency to twin can twin, where the probability of having twins increases with grain tendency to twin based on Schmid factor. More recently, the modified code was connected to an atomistic model [29] to calculate a statistical distribution of grain boundary defects. Effects of these statistical defects in grain boundaries as well as local stresses on twin inception are studied in Beyerlein et al. [30]. At a lower length scale, effects of various parameters on twin formation have been studied within an atomistic modeling framework. To name some key observations from this area, Serra and Bacon [31] showed that plastic slip is not transferred from one crystal to the other with a residual dislocation left at the interface; instead, the matrix dislocation decomposes into interfacial defects. Hence matrix slip dislocations can become a new source of twinning dislocations; these then produce twin growth when the appropriate stress is applied to the crystal. Studies of nucleation mechanisms of deformation twins within an atomistic simulation framework showed that, in HCP metals, a stable twin nucleus consists of multiple atomic layers [32, 33]. Also, a molecular dynamic study by Wang et al. [29] showed that low angle tilt boundaries contain a uniform array of large misfit grain boundary dislocations that when exposed to a local stress concentration, the grain boundary dislocations dissociate into small number of twin partial dislocations which then coalesce into a single twin nucleus. In comparison with the range of work using SC models and atomistic simulations, little attention has been paid to the statistical study of twins using CPFE approaches. In the current study, grains with random shape are mapped into a FE solver to study the effects of texture variation, grain boundary geometry, and stress fluctuation within grains on twin inception and propagation. The CPFE results are compared against previously published experimental EBSD data on zirconium [25]. The question that is tried to tackle here is to what extent
conventional crystal plasticity FE models can rationalize the statistically observed data – given that such models do not include atomistic information about grain boundary character, but only the impact of grain shape and stress concentration.

5.2 CPFE description

5.2.1 General mathematical formulation

In this section, the general formulation and assumptions of the code is explained; details of the code are described in Abdolvand, Daymond et. al. [34]. For a general solid mechanics problem, fifteen equations are required to be solved simultaneously: three force equilibrium, six compatibility equations, and six equations of state, i.e., stress-strain relationships. At the beginning of each time increment, the ABAQUS [35] FE solver sends the total strain, rotation, and time increment to the User MATerial (UMAT) subroutine where the corresponding stress increment, the six equations of state, and Jacobian matrix (the variation of stress increment with respect to the variation of strain increment) must be calculated. The nine remaining equations relating to equilibrium and compatibility are determined by the FE solver. Twin(s), which we will refer to as ‘child(ren)’ of parent grains, can potentially nucleate inside a given grain during plastic deformation. In the presence of both plastic slip and twinning, the total inelastic strain comprises of three terms as follows [36]:

\[
\varepsilon_{\text{in}} = \left[ 1 - \sum_{\beta=1}^{N_{\text{tw}}} f_\beta \right] \sum_{\alpha=1}^{N_{\text{Pa}}} p_\alpha \gamma_\alpha + \sum_{\delta=1}^{N_{\text{ch}}} f_\delta p_\delta \gamma_\delta + \sum_{\beta=1}^{N_{\text{tw}}} f_\beta p_\beta \gamma_0
\]  

(5-1)

where the first term in the right hand side of Eq. 5-1 represent plastic slip inside the parent grain, the second term represent plastic slip inside twins, and the last term represents the strain
accommodated by the volume fraction of twins present. \( f^\beta \) is the twin volume fraction associated with shear on the twin system \( \beta \), \( P^\alpha \) is the symmetric part of the Schmid tensor \( (S^\alpha) \) of a system \( \alpha \), \( \gamma \) is the shear on the slip or twinning system, \( \gamma_0 \) is the characteristic twin shear, and \( N \) represents the number of slip system available in parent (Pa) and child (ch). \( N^{tw} \) is the total number of twin variants (six in this case) that can be potentially active in the parent. In the model reported here, secondary twinning i.e., twins within twins are not allowed.

The Schmid tensor is a function of normal to the slip/twin system \( (n^\alpha) \) and slip/twin direction (\( d^\alpha \)):

\[
S^\alpha = d^\alpha \otimes n^\alpha
\]  
(5-2)

The plastic part of the velocity gradient can be written as [37]:

\[
L^p = \left[ 1 - \sum_{\beta=1}^{N^{tw}} f^\beta \right] \sum_{\alpha=1}^{N^{Pa}} S^\alpha \dot{\gamma}^\alpha + \sum_{\delta=1}^{N^{ch}} f^\delta S^\delta \dot{\gamma}^\delta + \sum_{\beta=1}^{N^{tw}} \dot{f}^\beta S^\beta \gamma_0
\]  
(5-3)

The shear rates on each twin/slip system in Eq. 5-3 are calculated using a rate-dependent formulation proposed by Asaro and Needleman [38]:

\[
\dot{\gamma}^\alpha = \dot{\gamma}_0 \left| \frac{\tau^\alpha}{g^\alpha} \right|^n \text{sign} \left( \frac{\tau^\alpha}{g^\alpha} \right)
\]  
(5-4)

where \( \dot{\gamma}_0 \) is a reference shear strain rate and \( n \) controls the rate dependency. \( \tau^\alpha \) and \( g^\alpha \) are the resolved shear stress on the slip or twinning system \( \alpha \) and strength of this system, respectively.

The twin volume fraction rate in Eq. 5-1 and 5-3 correlates with shear rate on each twin system in the parent grain as [37]:

\[
\dot{f}^\beta = \frac{\dot{\gamma}^\beta}{\gamma_0}, \ f^\beta \geq 0, \ \sum_{\beta} f^\beta \leq 1, \text{if } \tau^\beta > 0
\]  
(5-5)

\[
\dot{f}^\beta = 0 \text{ if } \tau^\beta \leq 0
\]
The imposed restrictions in Eq. 5-5 indicate that twin volume fraction cannot be negative, the sum of the twinned volume cannot exceed the parent grain volume itself and the twinned regions are not allowed to detwin. \( \tau^\alpha \) is a function of imposed stress and Schmidth tensor [4]:

\[
\tau^\alpha = P^\alpha; \Psi
\]  

(5-6)

where \( \Psi \) is the Kirchhoff stress and the Jaumann rate of this stress is related to the elastic part of the rate of deformation and elastic tensor as:

\[
\ddot{\Psi}^e = L^e D^e \text{ where } \ddot{\Psi}^e = \dot{\Psi}_e - \Omega^e \dot{\Psi} + \Psi \Omega^e
\]  

(5-7)

where \( D^e \) and \( \Omega^e \) are the symmetric and anti-symmetric part of the elastic part of the velocity gradient. The strength of each slip and twinning system is assumed to follow an extended Voce hardening:

\[
g^\alpha = g^\alpha_0 + (g^\alpha_1 + \theta^\alpha_1 \Gamma) \left( 1 - \exp \left( -\frac{\theta^\alpha_0 \Gamma}{g^\alpha_0} \right) \right)
\]  

(5-8)

where \( g^\alpha \) is the Critical Resolved Shear Stress (CRSS), \( g^\alpha_0 \) is initial CRSS, \( \Gamma \) is accumulated shear on all slip/twin systems, \( \theta^\alpha_0 \) is initial hardening rate, and \( g^\alpha_1 \) and \( \theta^\alpha_1 \) determine asymptotic characteristics of hardening. The rate of evolution of CRSS, \( \dot{g}^\alpha \), on each slip or twinning system \( \alpha \) is related to the rate of strain as:

\[
\dot{g}^\alpha = \sum_{\beta} h_{\alpha\beta} q_{\alpha\beta} \dot{\gamma}^\beta
\]  

(5-9)

where \( h_{\beta\beta} \) is self hardening and \( h_{\alpha\beta} q_{\alpha\beta} \) is latent hardening; \( h_{\alpha\beta} \) and \( h_{\beta\beta} \) can be calculated using Eq. 5-8 and 5-9 (see Eq. 34 in Appendix A), and \( q_{\alpha\alpha} \), and \( q_{\alpha\beta} \) are the constants given in Table 5-1.

All of the above assumptions are implemented in the UMAT code where for each Integration Point (IP), both slip and twinning (as a pseudo-slip) are considered to be potentially active.
following Eq. 5-4 and 5-5. Time integration of Eq. 5-3 results in the plastic strain and rotation increment, and given the total strain and rotation increment by FE solver, the elastic strain and rotation increment can be calculated. Following the methodology described in Abdolvand and Daymond [36], one twin is allowed to be created at each IP whose orientation is calculated by reflecting the parent orientation using the normal of the predominant twin system of the IP. The creation of this predominant twin variant is as follows; initially all twin variants are allowed to operate (based on Eq. 5-4 and 5-5), this can be considered the nucleation step when low levels of shear strain can accumulate on each twin system. When the nominal twin volume fraction at an IP reaches a critical value (ξ), a twin is ‘created’ at that IP, with crystallographic reorientation and transfer of volume fraction from parent to the twin [36]. The reorientation step is termed the inception step here to distinguish it from nucleation. Other twin variants are then deactivated at that IP. Twin growth and propagation is also allowed using Eq. 5-5.

5.2.2 The model input
In order to generate random grain geometries, the Voronoi tessellation [39] is used where 3D space is divided by space filling polyhedrons. For this purpose, random points are generated as each polyhedron’s seed point where any point inside each polyhedron is closer to this seed point than any other ones. As we aim to solely study the effect of texture and grain boundary geometries, in the current study, grain boundaries are assumed to be coherent interfaces with no vacancies or defects; however one can study the effects of imperfections with the current model, but in that case very fine meshes must be used and simulation time will be increased drastically. Depending on the number of grains, the generated microstructures were assigned to cubic arrays of elements of appropriate size. A sample input file with 1000 grains is shown in Fig. 5-1.
As cubic elements facilitate finding each element’s neighbors (for programming purposes) as well as applying desired boundary conditions, first order cubic elements with eight IPs per element (C3D8) are used to discretize the grains. Material properties of a Zircaloy-2 plate, given in Table 5-1, with HCP crystal structure are used here to be able to compare the CPFE results with both experiments on pure zirconium [25] and the second part of this work [40]. Plastic deformation in Zircaloy-2 is mostly controlled by prism \(<11\overline{2}0\>\), basal \(<1\overline{1}\overline{2}0\>\), and pyramidal \(<11\overline{2}\overline{3}\>\) slip as well as tensile twinning \(<10\overline{1}1\>\) [10, 41]. The elastic properties of the single crystal is assumed to be identical to those of pure Zirconium determined by Fischer and Renken [42]: $C_{11}$=143.5 GPa, $C_{33}$=164.9 GPa, $C_{12}$=72.5 GPa, $C_{13}$=65.4 GPa, and $C_{44}$=32.1 GPa.

At the beginning of the simulations, orientation variation inside each grain is neglected and one unique orientation is assigned to all of the elements of a grain; however, with loading, due to local variations in local environment, IPs of a particular grain can experience different rotations leading to an orientation gradient within the grain. In order to study the effects of texture, two different strategies are followed. In the first strategy, the top 200 and 1000 strongest orientations
of the Zircloy-2 plate, as measured by neutron diffraction [10], are assigned to cube arrays of elements with $36^3$ (S36 series) and $58^3$ (S58 series) elements, respectively. Then a static load ($\dot{\varepsilon} = 5.5 \times 10^{-5} \, \text{s}^{-1}$) is applied along the Normal Direction (ND) of the plate. The distribution of grains in the S58 series is shown in Fig. 5-1. Textures of the mentioned cases are also illustrated in Fig. 5-2. In the second strategy, the effects of texture variations are studied by changing loading direction from ND to the Transverse Direction (TD) and also sense of loading. In order to study the effects of neighboring grains, while keeping texture and grain shape unchanged, the orientations used for generating S58TD model were assigned to different grains in S58TDN. A random texture was also generated for comparison with other cases. Each model is named as follows:

- Simulation with $36^3$ elements and tensile loading along ND: S36ND
- Simulation with $36^3$ elements and tensile loading along TD: S36TD
- Simulation with $58^3$ elements and tensile loading along ND: S58ND
- Simulation with $58^3$ elements and tensile loading along TD: S58TD
- Simulation with $58^3$ elements and compression loading along TD: S58TDC
- Simulation with $58^3$ elements and tensile loading along TD (grains neighbours are altered): S58TDN
- Simulation with $58^3$ elements with a random texture: S58RND

Hence, the same input model is used for S58ND, S58TD and S58TDC and just loading direction or sign are changed. Grain geometries and the texture of the model in S58TDN are not changed compared to S58TD, yet each grain will have different orientation and different neighbors.
S58RND has the same input model as S58TD in terms of grain geometry, but with a random texture.

### Table 5-1. Single crystal properties of Zircaloy-2 [34]

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<th></th>
<th>n</th>
<th>$\dot{\gamma}_0$</th>
<th>$g_0$</th>
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<th>$\theta_0$</th>
<th>$\theta_1$</th>
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<th>$q^{\text{td}}$</th>
<th>$q^{\text{pr}}$</th>
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<tbody>
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<td></td>
<td>s$^{-1}$</td>
<td>GPa</td>
<td>GPa</td>
<td>GPa</td>
<td>(self)</td>
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<td>t=Basal</td>
<td>t=Pyramidal</td>
<td>t=Tensile twin</td>
<td></td>
</tr>
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<td>Tensile twin</td>
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<td>$1.0\times10^{-8}$</td>
<td>0.25</td>
<td>0.2</td>
<td>0.05</td>
<td>0</td>
<td>1</td>
<td>5</td>
<td>5</td>
<td>1</td>
</tr>
</tbody>
</table>

On average, each grain will have $\sim$1866 IPs in S36 series and $\sim$1560 IPs in S58 series; it has been shown that 350 IPs per grain will result in reasonable estimation of inter- and intra-granular stress heterogeneities [43, 44]. As the average grain size of grains in Zircaloy-2 slab is 13 $\mu$m, each IP will correspond to $\sim$851 nm in S36 series and $\sim$903 nm in S58 series. In terms of element size, each element side represents $\sim$1.7 $\mu$m in the S36 series and $\sim$1.8 $\mu$m in S58 series.

In the two texture files used here, most of the normals to the basal planes are oriented toward the ND direction which results in higher tendency to twin for tension along ND or compression along a perpendicular direction. In case (a) in Fig. 5-2, the crystals’ c-axis are oriented more toward TD than RD whereas in the case (b) it is more axi-symmetric about ND which is closer to the experimental case study in Capolungo et al. [25]. The texture of the pure zirconium used for that experimental study is shown in Fig. 5-2c. For the experimental study In Plane Compression (IPC) was applied to the experimental sample to cause tensile stress in the Poisson direction and activate twinning. Hence, in terms of twin variant selection, it is expected that the S58TDC would be the closest to the experimental results reported by Capolungo as the generated texture for the
model is close enough to the experiment and loading direction is the same. The calculated average flow curve of each case is shown in Fig. 5-2d.

Fig. 5-2. Input texture assigned to (a) 200 grains: S36 series and (b) 1000 grains: S58 series; (c) texture of the pure zirconium used in the experimental study by Capolungo et al. [25]: 1 and 2 are in-plane directions and normal to this plane is ND (d) average flow curves of the seven different cases considered in this study.

Periodic boundary conditions, similar to that described in Abdolvand, Daymond et al. [34], are applied to the free surfaces of the models by which each free surface is virtually in touch with its corresponding opposite surface, e.g., ABCD in Fig. 5-1 is in touch with EFGH, and deformation across these surfaces is continuous. The physical interpretation of such conditions is to simulate
an infinite lattice with a unit cell of the cube illustrated in Fig. 5-1. External load is applied at points G (for ND series) or E (for TD series) to enforce deformation up to 10% true strain.

### 5.2.3 Post-processing

The tendency of each slip or twin system to accommodate plastic shear can be explained by the system’s Schmid factor. The value of the Schmid factor can be calculated using Eq. 5-10. [28].

\[
SF^\alpha = \frac{p^\alpha \cdot \sigma}{\|\sigma\|}
\]  

(5-10)

where \(SF^\alpha\) represents the Schmid Factor of slip/twin system \(\alpha\), and \(\|\sigma\|\) is the norm of the stress tensor. Depending on where one uses local stresses or the far-field applied stress, two different values can be assigned to \(SF^\alpha\). Due to the stress and orientation gradient inside each grain, the \(SF^\alpha\) of each IP within a grain will be different from the others; in this context, we use Local Schmid Factor (LSF) to refer to the \(SF^\alpha\) that corresponds to using the local stresses at each IP \((\sigma^{IP})\) in Eq. 5-10. On the other hand, Geometrical Schmid Factor (GSF) refers to the \(SF^\alpha\) that corresponds to using the average (far-field applied) stresses in Eq. 5-10., e.g. for the ND calculations \(\sigma^{ND} = \frac{1}{N} \sum \sigma^{IP,ND}\) where \(N\) is the total number of IPs. These terminologies are used inside a post-processor to calculate LSF and GSF at each time step. In addition neighbours of an element \((E_i)\) are noted in the post-processor as the elements having a common face with \(E_i\). Although one can consider common nodes or lines for neighbor selection, face neighbours exert a greater constraint on the deformation of the neighbor than node or line [45]. It is shown for dodecahedron elements that the effect of face neighbors on deformation is higher [45]; so face neighbours are the only neighbors considered here.
As indicated in Section 5.2.1, plastic shear due to twinning is initially modeled as pseudo-slip (this is the nucleation stage). In the current study, twin ‘formation’ is introduced as the reorientation event, i.e. inception, not the plastic relaxation that exists before reorientation (see Eq. 5-4. and 5-5.), i.e., once the TVF reaches $\xi$, there is a crystallographic reorientation and part of the IP is ‘twin’. Following this terminology, in the post processor a Twin Inception Site (TIS) is introduced as an IP of an element $E_1$ in grain $G_1$ that just twinned with respect to the twin variant $v_i$, while none of the surrounding IPs in the same element and also neighboring elements inside $G_1$ twinned regarding to $v_i$. Hence, if because of stress heterogeneity inside an element two or more variants of the twin system are active and cause twins, two or more inception sites can exist inside even one element. The physical interpretation of such an assumption is that some of the elements can represent multiple-junctions, where two or more grain boundaries meet, and due to the large stress gradients inside the element, different variants can be active and cause twin formation. The frequency of these types of elements occurring depends on the generated microstructure as well as how finely a grain is discretized. Further, each TIS is assumed to be a unique twin, although different IPs twinned with the same twin variant within a grain may meet at some point during deformation and make a single twin.

The statistical study of twins can be performed within two different frameworks: In the first one, for the sake of having more twins for statistical study, many grains can be mapped into the FE solver to increase the number of potential sites for twin inception. In this method, twins with real shape can be studied, i.e. considering inception and propagation simultaneously for twin identification, yet it is computationally very expensive as many grains need to be mapped to the FE solver. This methodology will be used in the second part of the current study [40] for a study on local behaviour.
In the second framework, instead of using many grains, a few can be used, but with the application of PBC. In this case features of each grain, e.g. grain boundaries, mis-orientation between two grains, etc, are repeated infinitely. Also, with the current terminologies we use here for twins, each grain will have many twins (or inception sites) which results in a good representation number of twins at lower computational cost. This methodology will be used in the current report and it has been shown [34, 36] that this second methodology represents average statistical behavior of twins, as typically seen in an in-situ neutron diffraction experiment, fairly well. Hence, what we call a twin from now on is the *inception site* not the propagated twin at the end of the deformation test; propagation is allowed (but not forced after inception) in the model.

Here a summary of all of the assumptions are given; twin inception is allowed once the twin volume fraction of a given twin system at an IP reaches a critical value. This value represents the critical dislocation density required for twin inception. Twin orientation is a function of the predominant twin variant as a better agreement with experiments can be achieved using the PTR scheme [34, 36]. Also, each TIS is assumed to be a ‘twin’ in this part of the study.

### 5.3 Results

The majority of twins in zirconium at room temperature are caused by the \( \{1 \, 0 \, \bar{1} \, 2\}\{1 \, 0 \, \bar{1} \, 1\} \) tensile twinning system [7]. This system has six variants and the SF of each can be calculated using Eq. 5-10. For the sake of comparison with experimental results, in all of the figures shown in the results section, the applied stress is used for the SF calculation, i.e. the geometrical Schmid factors are used. Also, when making comparisons between the six variants, the variant with the highest GSF will be called the first variant, i.e. GSF\(_1\) and the one with the lowest GSF will be
GSF. In what follows, the initial orientations of grains are used for GSF calculation unless otherwise stated.

5.3.1 Grain distributions
The initial distribution of (potential parent) grains with respect to the highest available twin GSF for four model cases is shown in Fig. 5-3. As shown, in S58ND and S58TDC most of the grains have a high tendency for twinning with only a few grains having low twin SF; on the other hand, while a more continuous distribution of grains in GSF1 space is presented, most of the grains in the S36TD and S58TD models have a very low tendency for twinning with only a few of them well-aligned for twinning. The average GSF1 in each model and number of grains having GSF1 higher than the average value are indicated in Table 5-2.

Table 5-2. The average GSF1 in each model and number of grains having GSF1 higher than the average value

<table>
<thead>
<tr>
<th>model</th>
<th>average GSF1</th>
<th>number of grains with GSF1 higher than the average value</th>
</tr>
</thead>
<tbody>
<tr>
<td>S58ND</td>
<td>0.315</td>
<td>644</td>
</tr>
<tr>
<td>S58TD</td>
<td>0.066</td>
<td>360</td>
</tr>
<tr>
<td>S58TDC</td>
<td>0.261</td>
<td>656</td>
</tr>
<tr>
<td>S58RND</td>
<td>0.138</td>
<td>437</td>
</tr>
<tr>
<td>S36ND</td>
<td>0.346</td>
<td>100</td>
</tr>
<tr>
<td>S36TD</td>
<td>0.077</td>
<td>81</td>
</tr>
</tbody>
</table>

As the CRSS for activating twinning in Zr crystals is higher than that of basal and prism slip (see Table. 5-1), grains oriented for twinning can be considered as “hard grains”. As a consequence, the probability of a soft grain being surrounded by hard grains is high in the ND series whereas the reverse trend is expected in the S36TD and S58TD models.
5.3.2 Twinned-grains distribution

The distribution of the fraction of twinned grains with respect to $G_{SF_1}$ after 5% and 10% straining is shown in Fig. 5-4. For calculating twin fractions, the number of twinned grains (grains having at least one inception site in the CPFE simulations) is divided by the total number of the grains having a given value of the $G_{SF_1}$. As expected, the fraction of twinned grains increases as the $G_{SF_1}$ increases. A comparison with experimental results is shown in Fig. 5-4a.
and 4c (the model directions with more tendency for twinning). The trend in the CPFE results is very similar to the experimentally observed one especially for S58TDC case (Fig. 5-4a). Two points should be mentioned here: first, in the CPFE results all of the grains with GSF\textsubscript{1} higher than 0.38 have twinned in all cases (hence all of the grains in S36ND are twinned) whereas experimental observation showed that not all of the grains with GSF\textsubscript{1} higher than 0.4 are twinned (~10\% not twinned). Different factors could be responsible for missing the 10\% in the experiment; for instance, twins in the grains with high GSF\textsubscript{1} may form under the surface or their size might be too small to be discernable at the resolution used for the EBSD measurement (scanning step size for the experimental study was 0.2 \(\mu m\)). Second, in agreement with the experimental observation, some of the grains with low GSF\textsubscript{1} are twinned in the CPFE reflecting the effects of local stresses and grain-grain interactions on twin nucleation.
Fig 5-4. Comparison between Experiment (Exp) [25] and simulation results: fraction of twinned grains at different loading stage for (a) S58TDC, (b) S58TD, (c) S58ND, and (d) S36TD.

5.3.3 Twin variant selection

The contribution of each twin variant to the total number of twins, as a function of twin variant is shown in Fig. 5-5. Twin variants are ordered from the maximum (GSF₁) to the minimum (GSF₆). A similar trend to the experimental data is captured, especially in the S58TDC simulation (Fig. 5-5a), the texture and loading sense closest to the experimental study. Most of twins form based on
the predominant twin variant (GSF), but not all of them. The frequency of twins decreases as the variant SF decreases. This is interesting as it reflect the effect of local stresses on twin inception. As described in section 2.1 a Predominant Twin Reorientation (PTR) scheme is used in the current modeling where once twin volume fraction reaches a critical value, crystallographic reorientation occurs based on the predominant variant, i.e. the most active variant up to that time step. Two possibilities arise here for rationalizing the results. First, the twin variant SFs are calculated based on the applied stress which is a uni-axial load. As the value of these variants are calculated at the beginning of the simulation, i.e. at the first time step when there is no rotation variation within each grain, grain rotation can cause re-ordering of the variants. Hence, rotation variation within a grain is one possible reason for reordering twin variants; given the small rotations associated with plastic slip, (e.g. 3° rotation after 7% straining of a Zircaloy-2 single crystal with initial Euler angle of (0,50,0) and loading along the sample’s z-axis) to these low strains this seems likely to have a relatively minor contribution. The second possibility and likely larger effect is the variation in local stresses. In the discussion, as well as in [40], we show that there is a large fluctuation in the twin SF within a grain if LSF is used for the calculation instead of GSF. Thus there is not a unique predominant twin system everywhere inside a grain, and depending on the orientation of the neighboring grains and shape of the grain boundaries, a significant variation can exist in the twin SF. Hence all of the twin variants are active in the S58TD case whereas just three of them are active in the S36TD series.
Fig. 5-5. Number fraction of each twin variant ordered from the highest geometrical Schmid factor to the lowest for (a) S58TDC, (b) S58TD, (c) S58ND, (d) S36ND, (e) S36TD, and S58RND.
5.3.4 Twin variant distribution

The geometrical Schmid factor of each individual twin variant is normalized by GSF$_1$ and is plotted as a function of GSF$_1$ in Fig. 5-6a:6e. Different symbols and colors are used for each twin variant. A similar trend to the experimental observation (Fig. 5-6a) is captured in all of the CPFE simulations. The results of S58TDC (Fig. 5-6b) are very close to those of the experiment. All of the twin variants are active in the grains with higher GSF$_1$ and in most of the cases just the top three strongest twin variants are active at lower GSF$_1$. The frequency of each variant is also plotted as a function of twin SF normalized by GSF$_1$ in Fig. 5-6f:6j.
Fig. 5-6. Distribution of the active twin variant Schmid factor normalized by the GSF$_1$ as a function of GSF$_1$ in (a) experiment, (b) S58TDC, (c) S58TD, (d) S58RND, and (e) S58ND. Frequency of each active variant as a function of the GSF$_1$ for (f) experiment, (g) S58TDC, (h) S58TD, (i) S58RND, and (j) S58ND.
In order to explain why at higher GSF\textsubscript{1} most of the twin variants are active a closer look at the variation of SFs with crystal orientation is required. The variation of twin Schmid factor as a function of the mis-orientation between normal to the basal plane and loading axis is shown in Fig. 5-7a and 5-7c; tension along z-axis for the ND series in the CPFE simulations, and compression along y-axis for IPC in the experiment and S58TDC in the simulation, respectively. When the mis-orientation is less than 20 degrees for tension along z-axis, all of the twin variants more or less have equal SFs. Hence, near equal probability exists between all of the variants to create a twin. That is why in the ND series, as well as the S58TD case, at higher GSF\textsubscript{1} twins resulting from all six variants are observed. When rotating the crystal about the x-axis, two of the twin variants will have a negative SF (and hence should not be able to generate twins as twinning cannot happen with a negative SF [46]). Nevertheless, four of the twin variants have almost equal positive SFs resulting in the creation of the twins at lower GSF\textsubscript{1} as it is shown in Fig. 5-6e and 5-6j.

Similar reasons can be used to explain the results from the experiment. When comparing Fig 5-6a with Fig 5-6b it can be seen that most of the features observed in experiment are captured. This is significant as we have just created a random microstructure (grain boundaries and shapes), which is definitely not the same as the observed in the experiment. There is another feature in Fig 5-6a and 6b which is intriguing, which is the existence and population of the sixth and fifth variants at higher values of GSF\textsubscript{1} (>0.4). While the S58TDC simulation confirms the existence of the fifth variant at the higher GSF\textsubscript{1}, in contrast to the experiment, the population of this variant and the existence of the sixth variant are not those observed in experiment. Crystal imperfections, point defects and atomistic boundary effects, which are neglected in CPFE simulations, are the most
probable reasons for this discrepancy as stress states close to these areas could be totally different from the rest of the grain.

In Fig 5-6c and 5-6d results for S58TD and S58RND are shown. It appears from these two figures that in textured materials when the loading direction does not really favor twinning, twin inception follows the trends observed in materials with a random texture, although the population of twins in the random texture is a little higher than the textured one.

Fig. 5-7. Variation of twin Schmid factor variants with rotating an HCP crystal about x-axis for (a) tension along z-axis and (c) compression along y-axes; θ is the mis-orientation between normal to the basal plane and z-axis, where x- and z- directions are defined relative to the sample as shown in (b).

5.3.5 Grain boundary mis-orientation effects

The distribution of the grain boundary mis-orientations in the S58 and S36 series are shown in Fig. 5-8a. For the sake of consistency with the experimental data, the total mis-orientation at the grain boundaries is calculated as follows [28]:

\[
\theta = \min \left[ \cos^{-1} \frac{\text{trace}(R_A R_B^T) - 1}{2} \right]
\]  

(5-11)

where \( R_A \) and \( R_B \) are the rotation matrix of grains A and B converting the crystal axis to the sample axis. As HCP crystals are transversely isotropic, \( \theta \) greater than 90 degrees can be replaced
by $180 - \theta$. The distribution of grain boundary mis-orientations in the microstructure generated for S58 series is closer to the experiment than the S36 series. In order to investigate the average effects of neighboring grains on twin inception, the fraction of twinned grain boundaries as a function of $\theta$ for ND and TD series are shown in Fig. 5-8b and 8c, respectively. The experimental observation shows a slight correlation between mis-orientation and twinning with fewer twins observed at higher mis-orientations. The CPFE results for ND series show a slight increase in the fraction of twinned boundaries up to 10 degrees mis-orientation, then from 10 to 45 degrees almost no change is observed. In both S36ND and S58ND simulations, the fraction of twinned boundaries decreases once mis-orientation become greater than 50 degrees. The trend captured in S58TD is very similar to ND series, however, in the S36TD simulation, the number of twinned boundaries increases constantly as the mis-orientation increases. The difference between the last two simulations indicates the complex effect of texture and grain boundary geometry, and neighboring grains on twin inception.
5.3.6 Size effects

The distribution of grain size in the S58 and S36 series are shown in Fig. 5-9a. and 5-9b. A more homogenous distribution of grain sizes was observed in the experiment (in the experiment the EBSD step size was 0.2 microns; no grains smaller than 3 micron diameter are reported; also, the grain size distribution in CPFE are not similar to that of experiment, in the next chapter a real size...
distribution is used to allow a more direct comparison. It worth noting here that grains in the CPFE models have equiaxed shapes as a result of using Voronoi tessellation for creating microstructures. This is in agreement with the equiaxed grains used for the experimental study [25]. In both experiment and model, grains with at least one twin are categorized as a twinned grain. Experimental data show a slight increase in the number of twinned grains as the size of the grain increases. Likewise, the same trend is observed in S58ND and S36TD models, although in the S58TD model the trend is weaker.

As no size effect, e.g. Hall-Petch effect, is included in the current constitutive equations of each IP, the neighbors, grain boundary geometry and mis-orientation between grains are responsible for all the CPFE results. That is, regardless of grain size, a grain with high GSF\textsubscript{1} will twin as shown in Fig. 5-4. The probability of having a twin in a soft grain increases with grain size as bigger grains within the given population have larger grain boundaries and hence more neighbours than average sized grains. As the number of neighbours increases, the probability of facing onto a hard grain increases and due to the stress incompatibility at the grain boundary, twins will likely be induced in the bigger grain. Also, with more grain boundary, the probability of having triple junctions at the boundary increases; it is shown in the next section (Section 5.3.7) that triple junctions and elements with more non-identical neighbours are more susceptible to twin initiation.
Fig. 5-9. Distribution of grains diameter in (a) experiment and S58 series and (b) S36 series. Fraction of twinned grains as a function of grain size in (c) experiment and S58 series and (d) S36TD.

5.3.7 Grain boundary geometry

The influence of grain boundary geometry on twin nucleation is studied by categorizing elements of each model based on the number of non-identical grains they face onto. Non-identical neighbours of the element $E_1$ is identified as the number of elements having a common face with $E_1$ and belonging to different grains. For instance, if the number of non-identical neighbours of the element $E_1$ in the grain $G_1$ is 2, it means there are two elements from two different grains...
having contact with $E_1$. As each cubic element has six faces, the other four faces of $E_1$ in this 
example have contact with the elements inside $G_1$. Hence, in this example $E_1$ represent a triple 
junction. In Fig. 5-10a it is shown that the frequency of finding a TIS is the highest at a triple 
junction or interface of two grains, but beyond that the TIS frequency decreases with the number 
of non-identical neighbours. If the number of TISs of a certain element category is normalized 
with the total number of available elements within that category, the trend shown in Fig. 5-10b is 
achieved. Fig. 5-10b thus shows the effects of stress incompatibility at grain boundaries where 
with more non-identical elements, stress concentration increases and is more likely to cause twin 
inception. It is worth noting that having more than three grains contributing to a boundary in our 
simulations is a result of discretizing grain domains with cubic elements. Remembering that twin 
inception is allowed anywhere in a grain based on the stress state, having more than 95% of the 
TISs at the grain boundaries reflects the important role of grain boundary as a source of stress 
concentration for twin inception. It should be noted that experimental evidence suggests that 
twins can only nucleate at grain boundaries, due to the required dislocation arrangements for twin 
nucleation [29]. It is thus interesting that even though we do not force twin nucleation to occur at 
a grain boundary, the model rarely predicts that it will occur away from one.
5.4 Discussion

Different CPFE simulations have been performed to study the effects of texture and grain geometry variation on twin inception. A deterministic method [28] has been used for generating twins by which once twin volume fraction reaches a critical value a twin is generated using reflection about normal to the predominant twin system. The CPFE results are compared against 2D experimental studies by EBSD. Many of the experimental observations for pure zirconium [25] have also been observed for magnesium [26], another HCP material with high twin activity, confirming that the results represent some of the inherent properties of twin formation. Similar trends have been observed in the CPFE results reported here and compared against the experimental results.

In Fig. 5-4., it was shown that grains with a high GSF, will eventually twin in CPFE simulations regardless of the grain size or grain boundary geometry. The slightly different textures and lack of information about sub-surface twins in 2D EBSD experiments could be responsible for the 10%
discrepancy between CPFE and experiment at high GSF\textsubscript{1}. Also, in this study we are just using a stress criteria for twin inception, i.e., the stress state at an IP is the only factor controlling inception; this 10\% discrepancy could also originate from neglecting other factors such as twin surface energy, the elastic energy associated with the twin formation process, or the characteristics of dislocations required for twin nucleation. A three dimensional experimental study and atomistic calculations would be needed to investigate these hypotheses. It was also shown, in agreement with experimental results, that twins can form in grains with low GSF\textsubscript{1}. Local stress concentrations result from grain boundary geometry, as shown in Fig. 5-10., or hard-to-soft grain contact are two reasons, in our model, for inducing a twin in a soft grain. The effects of the local stresses on some selected results are shown in Fig. 5-11. Local stresses at the initial loading stage (at the beginning of each simulation, i.e., the first simulation step) are used to calculate each grain LSF where the average stress of each grain is used for the LSF calculations; the distribution of grains and the fraction of twinned grains against LSF\textsubscript{1} is shown in Fig. 5-11a and 11b, respectively. The ratio between LSF\textsubscript{1} to GSF\textsubscript{1} at the initial loading stage, i.e., in the elastic zone, for the 5000 IPs that will twin during the simulation in S58TD series is shown in Fig. 5-11c. On average, the LSF\textsubscript{1} are 16\% higher than GSF\textsubscript{1} for the twinned IPs in S58TD. Although wide fluctuations are observed in the ratio, the trend shown in Fig. 5-11a and 5-11b does not show a substantial change in the trends shown by using GSF\textsubscript{1}. On the other hand, if SF is calculated based on the local stresses at the reorientation stage, where the effect of plastic flow on stress fluctuations is larger, a bigger difference is revealed between LSF\textsubscript{1} and GSF\textsubscript{1}. In Fig. 5-11d the ratio of LSF\textsubscript{1} to GSF\textsubscript{1} by using local and applied stresses at the inception stage is shown. On average, LSF\textsubscript{1} are 35\% higher than GSF\textsubscript{1} for twinned IPs in S58TD. Comparison between Fig. 5-11c and 5-11d shows that load sharing between two grains and the geometry of the grain
boundary, which has a direct influence on stress incompatibility at the boundary, have far more significant influence during plastic deformation than elastic deformation. That is, a grain that starts with a very low twin LSF, may eventually twin as a result of load sharing or grain-boundary geometry during plastic deformation.

Fig. 5-11: (a) distribution of grains as a function of the highest local twin Schmid factor for S58TD; (b) fraction of twinned grains as a function of the highest local twin Schmid factor for S58TD; ratio of the highest local Schmid factor to the highest geometrical Schmid factor for 5000 twinned integration points at (c) initial loading stage and (d) twin inception stage.
In terms of neighbor effects on twin variant selection, we note that the S58TDN geometry is made where texture and grain shapes are not altered, comparing to S58TD, yet the orientations are assigned to different grains. Hence each grain has different neighbors. The propensity and distribution of each twin variant are shown in Fig 5-12a and 5-12b. In comparison with Fig. 5-5b and Fig. 5-6c, it is clear that the position of grains, as well as neighbours of a grain, does not really influence variant selection on a statistical basis; the major parameter, in this regard, is instead the texture of the material. Further, in comparison to the experiment, random shapes are assigned to grain shapes, yet the results are impressively close (Fig. 5-6a and 5-6b). One of the implications of these results is the inherent properties of twins when they are studied statistically. That is, regardless of the actual position (or shape) of each individual grain in the aggregate, similar trends for effects of various parameters on twin-variant selection will be achieved on a statistical basis. This reason rationalizes why in the recent statistical study of twins [30] within a self-consistent framework, where virtual grain boundaries are generated and no neighboring effects are included, close agreement can be obtained with experimental data. However, in the next part of this study we will show that when considering an individual grain, twin nucleation sites and twin propagation direction in the grain are strongly influenced by the local conditions [40].
Fig. 5.12. CPFE results for S58TDN: (a) number fraction of each twin variant, (b) Distribution of the active twin variant Schmid factor normalized by the GSF as a function of GSF - color code is given in Fig. 5-6, (c) fraction of twinned grain as a function of grain diameter, and (d) fraction of the twinned grain boundaries as a function of grain boundaries misorientation.

In terms of grain size, in Fig. 5-12c it is shown that distribution of the twinned grains is slightly affected by alternating neighboring grains (compare to Fig. 5-9c) reflecting the minor role of grain position in triggering twinning. In Fig 5-12d, on the other hand, it is shown that distribution of twinned grain boundaries is affected by changing grain position in the aggregate.
In order to understand the effects of misorientation at the grain boundary on twin inception two further models were generated. In the first model, a Zircaloy-2 single crystal is subjected to a uni-axial loading along z–direction (parallel to the basal plane normal). The orientation of the crystal is changed by rotating it about x-axis as shown in Fig. 5-7b, the load is then applied in the z-direction (load direction does not change). The variation of elastic and plastic response of the single crystal with respect to the misorientation between normal to the basal plane and loading direction is shown in Fig. 5-13a. As a result of decreasing twin activity, the single crystal become plastically harder up to 20 degrees misorientation (see Fig. 5-7a.), however, more misorientation activates basal and prism systems causing a softer response. Elastically, the crystal becomes softer with increasing misorientation up to 56˚, after which it becomes slightly harder.

In the second model, two single crystals of Zircaloy-2 are simulated to study the effects of grain boundary misorientation on twin inception. The first single crystal has constant orientation (0, 0, 0 in Euler space) with normal to the basal plane parallel to the loading direction, which is always in z-direction. The second crystal, on the other hand, is chosen with various rotation about x-axis (orientation: 0, \(\theta\), 0 ). The second crystal is placed to the side of the first crystal (normals to the common prism planes are parallel for the two crystals) and PBCs are applied to the model. The stress and strain state along the loading direction in the first crystal as a function of misorientation between the two crystals at twin inception is shown in Fig. 5-13b. In spite of the fact that the first single crystal has a constant orientation, variation of orientation in the neighboring crystal results in complicated variation of stress as well as strain state inside the first crystal. Comparison between Fig. 5-13a and 13b shows that, for the second case study, crystal orientation has a strong influence on the twin inception in the neighboring grain.
A complicated combination of mis-match between elastic and plastic responses of neighboring crystals (e.g. Fig. 5-13b.), absolute orientation of each crystal with respect to the loading direction (e.g. Fig. 5-13a), grain boundary geometry, and number of different grains contributing to form a boundary (e.g. Fig. 5-10b.) influence compatibility equations and deformation of elements at grain boundaries. Hence, although the trends observed on mis-orientation effects on twin inception (Fig. 5-8b and 5-8c) can to some extent be explained by single crystal observations, there is not a unique way to explain exactly how twin inception is affected by grain misorientation for all of the case studies provided here. Nonetheless, comparison of Fig. 5-8b and 8c reveals the strong effects of initial texture on twin inception where two completely different trends are seen for misorientation effects on twin inception.

The general comparison between CPFE and experimental results shows that most of the trends observed experimentally can be explained by the orientation and geometry of grains. These two
parameters affect stress fluctuations within a grain and cause activation of different twin variants within a grain. No doubt, at the expense of higher computational cost, one could get an even closer description of twin inception by considering effects of local defects.

5.5 Conclusion

Various FE simulations in a conventional crystal plasticity framework have been performed to examine the effects of grain boundary geometry, misorientation, and texture on twin nucleation. We showed local stress concentration and stress variation within a grain causes activation of different twin variants in the grain. In agreement with experimental results, CPFE simulations showed that not all of the twins will result from the highest GSF, although the frequency of twins formed by this variant is the highest. CPFE simulations shows as a result of stress incompatibility at the grain boundary, grains with low tendency to twin can still twin and the probability of inducing a twin in those grains increases as the size of the grain increases. It is also shown the frequency of finding twins at triple junctions and interfaces of two grains is the highest, yet, as a result of stress incompatibility, the probability of twin nucleation at a boundary increases with the number of grains contributing in the boundary.

The study of twin Schmid factors shows that use of local stresses instead of applied stresses can cause significant changes in the SF evaluation, especially due to load sharing between soft and hard grains; the changes in SF are more tangible during plastic deformation. Also, we have showed that when twins are studied statistically, the propensity and population of twin variants are not affected by grain neighbours, assuming that the correct texture is used.

Without increasing complexity in the conventional crystal plasticity frameworks we showed that stress heterogeneity within grains resulted from load sharing with neighboring grains and that the
geometry of grain boundaries are two major parameters controlling twin inception. For the sake of lower computational cost, existence of random defects in crystal structure is neglected in this study, yet some differences between model and experimental observations would likely be explained by considering them.

Reference List


Chapter 6

Multi-scale modeling and experimental study of twin inception and propagation in hexagonal close-packed materials using a crystal plasticity finite element approach; Part II: local behavior

*In-situ* tensile tests are performed on Zircaloy-2 samples with various grain sizes to study twin inception and propagation. Orientation maps of some areas at the surface are measured before and after deformation, using the Electron BackScattered Diffraction (EBSD) technique. Strain fields of the same areas are determined using the digital image correlation technique and are compared with results from Crystal Plasticity Finite Element (CPFE) simulations. Different assumptions are made within the CPFE code to simulate twin propagation. It is observed that the predictions of different models does not really change from one model to another when statistical information on the twins is compared, yet local predictions for each grain, i.e. twin direction, twin variant selection, and twin inception site, do change. Also, it is shown that the twin Schmid factor can vary drastically within grains, and that for those grains with a low tendency for twinning this variation may make them susceptible to twinning.

6.1 Introduction

Characterization of the mechanical response of materials under varied loading conditions can provide insight into the operating micro-deformation mechanisms. Various experimental and numerical methods have been implemented to answer critical questions about deformation
mechanisms with the goal of e.g., improvement of in-service life-time of materials. While in-situ deformation studies, such as neutron or synchrotron diffraction are very powerful, and can provide extensive data as to the operating micro-mechanisms [1] they can be difficult or expensive to perform. Hence laboratory based techniques, such as digital image correlation (DIC), are also an important characterization tool. DIC is a versatile technique that has been used to understand deformation at various length scales from micro to macro. The basic concept behind image correlation is to find features in the images taken from interested area at different loading stage and try to find one-to-one correspondence between positions of these features [2-6]. Once the relations between images are resolved, strains can be extracted and deformation evolution can be studied. As the images are usually captured from the surface, strains at the surface can be measured and bulk information, in contrast to penetrating diffraction methods, is not monitored. Crystal plasticity in the finite element framework has been used in parallel with image correlation techniques to answer experimentally-irresolvable questions. Study of materials at this scale usually consist of mapping of grain shapes into a finite element solver and investigating the effects of grain-grain interaction on the average and local behavior of materials [7-11].

Because of their low absorption cross sections towards neutrons, zirconium and its alloys have been extensively used in nuclear reactors. Alpha-zirconium has Hexagonal Close-Packed (HCP) crystal structure with high tendency to twin under tensile loading along the c-axis of the crystal. It is known that twins form readily at the stress concentrations of crack tips in zirconium alloys [12]. Hence, a precise understanding of the interaction of local neighbourhood on twinning has potentially significant practical interest as well as providing insight into the physical mechanism
of twinning. In this paper, we report a study of twin formation, including both inception and propagation, in Zircaloy-2 samples.

Deformation twinning at the grain scale in a CPFE framework has been studied to some extent. Texture evolution as well as deformation and activity of twin variants of each grain were studied by Prakash et al. [13] and Choi et al. [14]. To reduce numerical instability, an implicit-dynamic formulation was implemented by Barton et al. [15] to model twin formation in a 125 grain polycrystal. A good picture of twin formation is presented in Barton et al.’s work, but the lack of CPFE results being compared with experiment, leaves questions as to the assumptions made.

Formation of twins in single crystal zinc has been studied by Forest and Parisot [16] where twin nucleation was virtually controlled by introducing a geometrical defect and twin growth was the result of the motion of the localization front on one or both sides of the twin, in the spirit of Maugin [17]. In the current study, local twin formation in Zircaloy-2 polycrystal samples is studied experimentally as well as numerically. Grain orientations and geometries at the surface of the samples are measured for different samples before and after uniaxial straining. In-situ tensile tests are carried out in an SEM chamber where grains’ strains are measured by the digital image correlation technique. Grain maps are imported into the ABAQUS FE solver to study inception and propagation of twins using different assumptions within a crystal plasticity formulation. The CPFE results are compared against experimental results both locally and statistically.

### 6.2 Experimental procedure

Set one of dog bone samples (S1) with 14mm gauge length, 3 mm width, and 2 mm thickness were prepared from a previously well characterised Zircaloy-2 slab. The nominal composition of Zircaloy-2 is 1.2-1.7 wt% Sn, 0.07-0.2 wt% Fe, 0.05-0.15 wt% Cr, 0.03-0.08 wt% Ni, 1400 wt
ppm Oxygen [18-20]. The initial texture of the slab is shown in Fig. 6-1a. Due to having a relatively small grain size (~13 μm) and an inability to readily resolve grain boundaries in S1, cubes from the original slab were cold-rolled to 10% (compression along previous rolling direction with 10% thickness reduction) and then heat treated at 720 °C for 48 hours. The heat treatment was conducted in an Argon gas environment to prevent oxide layer formation. The heat treatment resulted in a material with equiaxed grains and an average grain size of 50 μm from which a second set of dog-bone samples (S2) were prepared, with the same dimensions as S1. One side of each sample was mechanically polished down to 1200 grid and then with 6, 3, and 1 micron diamond paste. Subsequent attack polishing of the samples was performed with a solution of 5% H₂O₂, 5% HNO₃, 5% HF, and 85% H₂O for 15 seconds several times until it resulted in a shiny surface with no visible scratches. A micro-indent was then placed on each sample’s surface to define the sample coordinate system for pre- and post-loading EBSD as well as image analysis on the same area. Samples were finally electro-polished for 60 seconds at 25 volts in a -30 °C solution of 10% perchloric acid and 90% methanol. To prevent formation of oxide layers on the polished-surface, samples were then quickly moved into the SEM vacuum chamber. The quality of indexing process at each point can be characterized by a parameter called Mean Angular Deviation (MAD) that reflects how close the indexed pattern is to the standard values available in the internal library of the indexing program. In our EBSD measurement, points with MAD < 0.7 are considered as un-indexed point. Also, for identification of grain boundaries, more that 5˚ misorientation was not allowed within each grain; hence, the maximum deviation at each point inside a grain, from the average calculated orientation of the grain cannot exceed 5°.

Orientation maps of some selected areas in S2 samples were measured before applying load; three different areas with a total 775 grains were investigated in this set. The initial texture of the S2 set
achieved from these areas is shown in Fig. 6-1b. Similar to S1 set, the normal to basal planes are mostly oriented toward Normal Direction (ND). Hence, tensile load was applied along the ND to activate twinning; the tensile stage was placed in a JEOL-840 SEM chamber where images from the selected areas were captured at different loading steps. The loading process was under load control during elastic deformation and strain control ($\dot{\varepsilon} = 5.5E - 5$ s$^{-1}$) during plastic deformation. The average flow curves of the S1 and S2 series are shown in Fig. 6-1c. Orientation maps of the selected areas were measured again after 3% straining. Fig. 6-1d shows the post deformation texture of the S2 set.

Due to difficulties in achieving good post-deformation EBSD patterns on the small grain size material, we did not carry out pre-deformation EBSD and image analysis on the S1 set. Instead, post deformation orientation maps of two different areas were measured from an annealed S1 sample. As the recrystallization temperature of Zircaloy-2 is 450 °C [21], S1 samples were annealed at 300 °C for an hour; this recovered sufficient dislocation density that EBSD mapping could be achieved, while it should not remove twins [21]. In order to create a ‘starting’ microstructure for modeling, the twins were identified by orientation relationship and shape, then removed from the grain map; these modified approximate starting maps were used for the starting point of the CPFES simulations. In total 1016 parent grains were investigated in the S1 set.
Fig. 6-1: (a) pre deformation texture of S1 set; (b) pre deformation texture of S2 set; (c) comparison between calculated and measured average flow curve of S1 and S2 sets; (d) post deformation texture of S2 set

6.3 CPFE simulation

6.3.1 Input models

The pre-deformation orientation maps of grains, either directly determined (S2) or extrapolated (S1) were used to generate input files for the FE solver. For this purpose, the average orientation of each grain was calculated [22, 23] and used as the initial input orientation of each grain. Hence, orientation variations within grains before deformation are neglected. Grain maps were subsequently imported into the FE solver and meshed with C3D8 cubic elements with 8 Integration Points (IP) per element. As in a typical 2D orientation map measurement information
from grains beneath the surface are not available, the grain map of each input model was extruded in the third direction; this will give us the opportunity to introduce different boundary conditions in the third dimension (see below). A sample input file is shown in Fig. 6-2. On average 339 and 137 elements are assigned to each grain in the S2 and S1 sets (2712 and 1096 IP per grain), respectively. Hence, each IP at the surface of the model (neglecting the IPs existing thorough the thickness of the model) represent ~1.3 μm and ~690 nm of the sample in S2 and S1, respectively, which are less than half of the step size used for the EBSD scans. Grain boundaries are assumed to be coherent and the existence of other defects, e.g. point defects or variation in alloying-elements such as Sn, Fe, Cr, Ni, and Oxygen in Zircaloy-2 [24], is neglected. The single crystal material properties are extracted based on the average alloy response to uniaxial loads imposed in different directions relative to the texture [25]. Equations are introduced at the models’ free surfaces to simulate plane strain and plane stress conditions, to study the upper and lower bound responses of the model, as well as periodic conditions, which represents between the two. Given that polished samples are deformed in situ and studied, we might expect that plane stress conditions would be closest to the experiment; however this neglects the fact that twin initiation may occur subsurface. The applied equations are such that for plane strain \( \langle \varepsilon_{zz} \rangle = \langle \varepsilon_{xx} \rangle = \langle \varepsilon_{xy} \rangle = 0 \), and for plane stress \( \langle \sigma_{zz} \rangle = \langle \sigma_{xx} \rangle = \langle \sigma_{xy} \rangle = 0 \), where \( A_i \) represent average value of \( A \) in the \( i \) direction of the model. Applied equations for periodic boundary conditions are presented in Abdolvand et al. [25]. All of the simulations comprised of two steps; in the first step, the model is cooled down from a higher temperature to account for thermal residual stresses produced during manufacturing process of S1 set [26] or our heat treatment on S2 set. In the second step, models are loaded uni-axially in the ND with the same strain rate we used for the experiments. Due to crystal anisotropy of Zircaloy-2, initial thermal stresses have an effect on
material response especially when results for loading along transverse direction are compared
with those of loading along normal direction; however, not including initial thermal effects won’t
change qualitative results.

a.  
b.  
c.  
d.  

Fig. 6-2. Sample EBSD maps and FE input files: (a) An EBSD map of one of the S1 sample
with no twins. (b) A pre deformed EBSD map of one of the S2 samples; (c) A sample FE
input file from the EBSD map shown in Fig. 6-2b; (d) XY view of the same model. Colors
are assigned randomly to each grain.
Single crystal material properties reported in Abdolvand et al. [25] and first part of this report [27] are used for samples in the S1 set. For samples in the S2 set they were modified, to respect the changes observed in average flow curve, hence reflecting the recrystallization and grain growth which has occurred, as well as the different texture (Fig. 6-1). Estimated single crystal material properties of samples in the S2 set are presented in Table 6-1; \( g_0 \) and \( \theta_0 \) have decreased slightly (7.5 % and 12 %, respectively) compared to S1, while other parameters have been left the same. There is no explicit Hall-Petch formulation included in the model so the change in parameters incorporates both the change in grain size, and any changes in initial dislocation density that have occurred due to the heat treatment.

<table>
<thead>
<tr>
<th>N</th>
<th>( Y_0 ) ( s^{-1} )</th>
<th>( g_0 ) GPa</th>
<th>( g_1 ) GPa</th>
<th>( \theta_0 ) GPa</th>
<th>( \theta_1 ) GPa</th>
<th>( q_{s}^{t} ) (self)</th>
<th>( q_{t}^{t} ) t=Prism</th>
<th>( q_{t}^{t} ) t=Basal</th>
<th>( q_{t}^{t} ) t=Pyramidal</th>
<th>( q_{t}^{t} ) t=Tensile twin</th>
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<td>0</td>
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<tr>
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<td>3.5×10^{-4}</td>
<td>0.156</td>
<td>0.222</td>
<td>0.044</td>
<td>0</td>
<td>5</td>
<td>1</td>
<td>5</td>
<td>1</td>
</tr>
<tr>
<td>Pyramidal</td>
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<td>1.0×10^{-4}</td>
<td>0.307</td>
<td>0.272</td>
<td>0.551</td>
<td>0.28</td>
<td>1</td>
<td>1</td>
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<td>1</td>
</tr>
<tr>
<td>Tensile twin</td>
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<td>0.232</td>
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</tbody>
</table>

6.3.2 Twinning assumptions

The mathematical equations used for simulations are the same as those presented in the previous part of this report [27] (Section 5.2.1). The key features and modifications imposed for twin inception and propagation are explained in this section. Later in section 6-4.1 we will show that these modifications are mandatory if twins with right geometry wanted to be modeled. In contrast to our previous approaches in modeling average behavior of twins [25, 28], here, attention is paid on the formation of the shape and propagation direction of twins. A twin
inception site could be anywhere in a grain, however, in the previous part of this report, grain boundaries are shown to be more susceptible places. As before, the decision on twin inception is made based on a deterministic approach, where once the total twin volume fraction reaches a critical value ($\xi$), twin formation, i.e. twin reorientation, is permitted toward the predominant twin variant, and other twin variants are deactivated (in terms of accommodating further shear strain) at that IP. Once $\xi$ is reached in an IP (which could be anywhere in a grain), a subroutine is called to generate a Subset of Elements (SOE) that can potentially represent a twin. For this purpose, first the predominant twin variant, i.e. the most active one, of the twinned IP is identified; the twin normal of this variant ($n_{tw}$) and the position of the element that the twinned IP belongs to are used to generate the shape of the twin plane (red lines in Fig. 6-3). To identify which elements in the grain belong to the SOE, we start from the inception site and find elements in the XY plane (Fig. 6-3.) and then extrapolate them in both positive and negative Z direction. Once a twin inception site is identified, the neighboring elements, elements with a common face, of the inception site in the XY plane are checked to determine which one (out of four) is the closest to the twin plane. The closest element, let us call it $E_1$, will fall into the twin zone ($T_1$ in Fig. 6-3) and is added to the SOE. The same trend is applied to the neighbours of $E_1$ to find the next candidate for assigning to a SOE. The process of finding the next element continues until the last element hits a grain boundary or another already existing twin. Fig. 6-3b shows a sample simulation for a single crystal of Zircaloy-2. It is worth noting that, being an element in SOE does not necessarily mean that reorientation will happen in that element; the $\xi$ must also be reached for these elements so that the reorientation event can take place. This assumption means that twin propagation is solely controlled by the stress state at each IP. Also, to be consistent with reality,
elements in SOE are only allowed to reorient with respect to the identified predominant variant of the inception IP.

Fig. 6-3. (a) A schematic of how twin incept and propagate in the CPFE code; (b) Results for a single crystal Zircaloy-2: blue circles are untwinned elements and green circles are twinned elements.

Different assumptions were tested for the grain behavior after SOE formation. The results we present here are just for three of many different approaches that have tested in the CPFE code to describe twin propagation. In the first approximation (will be called M1), all of the IPs that do not fall into the SOE are prohibited from accommodating twin relaxation, i.e. twin relaxation (pseudo-slip) just happens in the IPs that belong to SOE and nowhere else in the grain. This assumption allocates all of the twin relaxation into the twin and hence forces twin propagation; it relatively increases stresses in both the untwinned part of SOE and the rest of the grain. It is also commonly believed that twin propagation requires less driving force than twin formation [29-31]. Twin propagation in the IPs of the SOE can also be facilitated once reorientation takes place by assigning either a higher value to $\gamma_0$ or decreasing the critical resolved shear stresses required for further twinning to occur [32]. The results we present here are for increasing twinning $\gamma_0$ by a
factor of 10 for propagation in the grain. In this concept, an increased shear strain rate is applied to the twin tip so that the propagation stage happens faster. In order to simulate twin broadening, i.e. growth in the thickness direction, one could write the energy equations to find the optimum value for the thickness [33]; the energy terms can also reveal when a second twin must be created in the parent grain [34]. However, here for simplicity we simply introduce an empirical parameter that reflects the saturation of the IPs in the SOE, i.e. whether the IPs in the SOE have been fully or partially transferred to twins, and growth will be allowed to happen. The saturation parameter could be set to any value; for instance, if the saturation parameter is set to 50% it means that once 50% of the IPs in the SOE are fully or partially twinned, the next twin is permitted to be formed in the grain. This new twin will be wherever a new inception site is favoured, potentially next to the first twin (i.e., effectively a thickening of the original twin), or at a distance, i.e. a second twin. It is also worth noticing that, broadening or propagation in the lateral direction can also originate in a sense from twin volume transfer from matrix at each integration point, i.e., at the twin inception, small portion of each IP twins, and with more loading and shear stress acting on that IP, twin volume fraction increases or effectively the twin broadens.

The second approach (M2) is similar to the M1, with the exception that twin relaxation is not prohibited in the grain, i.e. pseudo slip is allowed to continue everywhere in the grain even after twin inception. All other assumptions are the same for M2 as M1. The last approach (M3) is the one that is presented in the previous part of this report [27] were twin propagation is not controlled in this manner, i.e. twin reorientation can happen anywhere in the grain that the RSS allows. The value $\dot{\gamma}_0$ of is not increased in the M3 approach once twinning occurs at an IP.
6.4 Results

6.4.1 Twin inception and propagation

Results of the simulations for the two cases shown in Fig. 6-2a and 6-2b are shown in Fig. 6-4 and 6-5, respectively. The M1 scheme is used for both cases with the implementation of plane stress boundary conditions (see section 6-4.3). Random colors are assigned to each grain in Fig 6-4a and 6-4b; however, black dots in Fig. 6-4b represent the reoriented (twinned) elements. The size of these black dots is proportional to the number of reoriented IPs in each element. In order to compare CPFE results with the EBSD map, each grain is given a color code in Fig. 6-4c; green grains are not twinned in both experiment and simulation, blue grains are twinned in both experiment and model, red grains are twinned in the experiment but not in the simulation, purple grains are twinned in simulation but not experiment, and twin formation was not discernable (in the experiment) in white grains. To be consistent with our EBSD map resolution, twins smaller than 500 nm in the CPFE simulations are not included in the post-processing analysis. The tendency of each grain to accommodate deformation by twinning under a tensile load is related to the misorientation between normal to the basal plane of the grain and loading direction; the smaller the misorientation, the higher the tendency [27]. Based on the initial orientation of each grain, in Fig. 6-4d, a color is assigned to each grain to represent the aforementioned misorientation. Alternatively, each color in Fig. 6-4d is proportional to the value of the highest geometrical Schmid factor of each grain (GSF in terminology [27]). An example stress distribution calculated for grains after 0.2% strain is also shown in Fig. 6-4e. A similar set of figures is made for an S2 case sample, presented in Fig. 6-5, with the exception that the post deformation EBSD map of the sample is presented in Fig. 6-5a (the sample is not annealed hence indexing of this sample is worse than S1).
Fig. 6.4. (a) Twin map of the grains (an S1 sample) shown in Fig. 6-2b after 3% straining; (b) CPFE result for the same model, black dots are reoriented elements; (c) comparison between CPFE result and experiment: green area: not twinned in FE and not twinned in experiment; blue area: both FE and experiment twinned; red area: not twinned in FE and twinned in experiment; purple area: twinned in FE and not twinned in experiment; white area: not discernible; (d) distribution of the misorientation between normal to the basal plane and loading direction before loading: colors are proportional to the cosine of the
Comparison between Fig. 6-4a and 6-4b shows that, on average, many features related to twin inception and propagation are captured in the simulations. A glance over these figures shows that twins normally intercept at grain boundary, and typically at the junction of more than two grains. From the model predictions we determine that the inception always occurs at the boundary. This is clear in both Fig. 6-4b and 6-5b and is compatible with our previous Voronoi simulations [27]. Interestingly, even in soft grains, i.e., grains with lower twin Schmid factor in Fig 6-4d and 6-5d, twins can occur due to the stress concentration and incompatibility at the triple junctions; however they do not grow in size or propagate across the grain. The stress concentration at triple junctions is also responsible for the existence of many black dots in the model predictions of Fig 6-4b and 6-5b. There are many explanations for the existence of the twins that incept but do not propagate. To mention a few, recalling that in our model both twin inception and propagation are solely controlled by stress state at each IP, in the grains with a low tendency for twinning, there can be enough local stress for inception (nucleation) but not enough stress or driving force to cause propagation. In grains with higher Schmid factors, twin propagation may require more straining (more than the maximum 3% that we applied here) or it may be that the load sharing with soft neighboring grains on the opposite side of the grain to the inception point suppress twin propagation across the grain. It is also worth mentioning that, the incompatibility and stress concentration at the triple junction are highly affected by the number and order of the elements used for simulation [35-37]. A better stress gradient will be captured by using a higher number of elements especially at the grain boundary; however, this becomes computationally expensive, and prohibitive when trying to generate statistical information about twinning.
In order to demonstrate how the twins form in CPFE simulations, some twins are selected as case studies. Region 1 in Fig. 6-4b and 6-5b are the twins that represent model agreement with experiment for both inception site (assuming that inception occurred at the grain boundary in the experiment) and propagation direction (Fig. 6-4a and 6-5a). The inception site is the grain boundary where the twinned grain intersects with some other soft or hard grains. The stress distribution in the twinned grains is high enough to cause propagation (see Fig. 6-4e and 6-5e). The limit that is imposed in this model for generation of a second twin is 50% saturation, which is not reached at the macroscopic strains applied.

Region 2 represents the twins that form in the same grains as observed experimentally, but the model inception and/or direction is not what is observed. Existence of different triple junctions within a grain leads to having multiple susceptible sites for twinning in the grain; the one with higher stress concentration or incompatibility is the one that triggers a twin in the model. In terms of twin propagation direction, which also represents the twin variant selection in this concept, grains that are almost perfectly aligned for twinning are shown to have more than two twin variants that are very nearly equally active [27] and the probability of picking one of them is almost the same. Consequently, the propagation direction is highly influenced by the stress state inside the grain. We need to emphasize here that the stress state inside each grain is significantly affected by the sub-surface grains [38-40], and that those missing grains are likely one of the strongest reasons for not capturing the correct stress distribution, i.e. twin variant selection, inside a grain.

The Region 3 in Fig. 6-4b represents some of the cases that are observed in both experiment and in our simulations where a twin has incepted in one grain and propagated into another
neighboring grain. In the CPFE simulations, the excessive shear at the twin tip, resulted from prohibiting elements out of the SOE from accommodating pseudo slip, and making propagation easier for twins by changing power law parameters, coupled by the presence of a low angle grain boundary is responsible for propagation of a twin across more than a grain. This phenomenon has been observed in grains with small misorientation in experiments [41-43] as well as in the current CPFE simulations.

The Region 3 in Fig. 6-5b reveals the propagation of a twin once a SOE is generated. In Fig 6-5e it is seen that the twin in Region 3 forms at the intersection of three grain boundaries where a high stress concentration exists. For the same reason, some elements also reorient at the far side of the grain, but after 3% applied strain these two ends of the twin do not meet. What we can conclude for the propagation trend observed in this grain as well as some other grains, that higher stresses are mandatory to form a twin, but not enough to capture the fast propagation that is observed in experiments. The pseudo slip scheme that has been used for modeling twinning basically considers twinning as a gradual plastic deformation, however, at least at the inception stage, twin formation is a dynamic process and that need to be taken into account. Other schemes, e.g. shock wave equations in modeling phase transition fronts, could be more appropriate to simulate the inception and initial nucleation stage [16, 17].

Region 4 in Fig. 6-4b and 5b represents grains with low twin Schmid factor, that still have twin(s) formed in them. It has been observed that some soft grains can occasionally twin in experiment; in the finite element simulations however, grain boundary geometry and the presence of hard neighbor grains did not trigger a twin in those grains. This emphasizes the role of sub-surface
grains and crystal imperfections that are distributed randomly in the crystal structure in twin nucleation.

On the other hand, in Region 5 (Fig. 6-4b and 6-5b) although the grain is well aligned for twinning, no twin is observed in the experiment. The first probable explanation for this observation is the formation of twins under the EBSD surface which did not leave any evidence on the surface. Another alternative is the size (thickness) of the twins which could be substantially smaller than the resolution we used to create our EBSD maps. 3D experiments could represent a better insight on these two potential contributions.

The agreement between Fig. 6-4a and 4b and also between Fig. 6-5a and 6-5b in terms of parent grains that twinned and or did not twin (Fig. 6-4c and 6-5c) is higher than 78 percent.
Fig. 6.5. (a) Twin map of the grains (an S2 sample) shown in Fig. 6-2a: the post deformation EBSD map; (b) CPFE result for the same model, black dots are reoriented elements; (c) comparison between CPFE result and experiment: green area: not twinned in FE and not twinned in experiment; blue area: both FE and experiment twinned; red area: not twinned in FE and twinned in experiment; purple area: twinned in FE and not twinned in experiment; white area: not discernible; (d) misorientation between normal to the basal...
planes and loading direction; (e) a sample stress distribution among the gains.

A sample result of simulations using M2 scheme is shown in Fig. 6-6a. In comparison to the results for the same input model where the M1 scheme was applied (Fig. 6-4b), statistically, the average twin inception/propagation characteristics are unchanged. For instance, twins form at grain boundaries where higher stress concentration exists and propagation direction in some cases coincides with what is observed experimentally. In agreement with what is observed for the M1 case, more than 78 percent agreement exists between the CPFE simulation and experimental result in terms of determining if a grain twins or does not. In terms of local behavior, however, the twin propagation and inception sites are changed for some grains, which reflects the effect of the assumption we made in terms of prohibiting/encouraging twin relaxation in the elements that are outside/inside of the SOE, respectively. In our current approach, the twin propagation direction is decided by the predominant twin variant at inception; therefore, at the early stage of plastic deformation. On the other hand with the M2 scheme, twins form approximately at the same sites observed when using the M1 scheme and also have the same propagation directions. However, since elements outside the SOE zone in M2 scheme are allowed to accommodate pseudo-slip, with more plastic deformation the observed twin inception sites, as well as propagation directions, no longer necessarily coincide with what is observed using the M1 scheme. That is, the permitted pseudo-slip alters the potential stress concentration sites in neighboring grains and consequently changes twin inception sites and propagation directions.

A sample application of M3 scheme in modeling one of the samples in S1 set is shown in Fig. 6-6b. In this scheme, twin can incept anywhere in a grain and no restriction is placed on the propagation or inception of the next twin. Hence, reorientation initially takes place at IPs with
higher stress concentration (region one in Fig. 6-6b; similar locations to M1 and M2), and with more straining other parts of a grain will experience it. In contrast to the other two mentioned schemes, different twins can form as a result of having different predominant twin variants even inside a particular grain. This is a reflection of the fact that different grain neighbours cause various stress conditions at the grain boundary and hence causes activation of different twin variants. In comparison to our EBSD experiments, this method could not explain local behavior or propagation of twins, yet we showed that it is a reasonable approach to model the average behavior of polycrystals when compared against experiments carrying information about average grain family response, e.g. neutron or x-ray synchrotron diffraction experiment where the representative volume element is big enough that each element in CPFE effectively represents many grains [25, 28].

Fig 6-6. Application of (a) M2 approach and (b) M3 approach in modeling samples in S1 set. Black dots are reoriented elements.
6.4.2 Average behavior

All of the investigated grains (~1800 grains) are used to present a statistical comparison between results of the CPFE simulations and experiments. In Fig. 6-7a, the propensity of grains with respect to the highest Geometrical twin Schmid Factor (GSF₁ as defined in [27]) is shown. Samples in both the S1 and S2 sets are relatively textured and loaded favourably for twinning, hence many grains have a high GSF₁. Nevertheless, grains with lower GSF₁ also exist in the body of samples, especially in the S2 set due to the heat treatment process applied. The fraction of twinned grains as a function of GSF₁ is plotted in Fig. 6-7b. All in all, 295 grains are twinned in the experiments with a total 392 twins. The M1 scheme is used here to compare CPFE results with those of our experiments. The general trend observed in experiments is also observed in the CPFE simulations (with over prediction occurring at higher GSF₁). Twins can form in grains with both higher GSF₁ and lower one, and the propensity for twinning increases with higher GSF₁. The contribution of each twin variant to the total number of twins is presented in Fig. 6-7c. Local stress concentrations caused by grain boundary geometry, neighboring grains, having certain boundaries (also called atomistic boundary) that can help twin initiation [44, 45], and local crystal imperfections are the main reasons for activating other twin variants in experiment. The CPFE simulations demonstrate that even neglecting the contribution of crystal imperfections and also the sub-surface layer, a good statistical approximation of twin variant selection can be provided; this reflects the dominant effect of grain boundary geometry and grain orientation.
Fig. 6-7. (a) Propensity of grains with respect to the highest geometrical twin Schmid factor; comparison between experiment and simulation results: (b) fraction of twinned grains against highest geometrical twin Schmid factor and (c) number fraction of each twin variant ordered from the highest geometrical twin Schmid factor to the lowest.

The distribution of Grain Boundaries Misorientations (GBM) and fraction of twinned boundaries as a function of GBM are shown in Fig. 6-8a and 8b, respectively. At lower misorientations, the discrepancy between CPFE results and experiment is higher; however, the discrepancy decreases at higher misorientations. Having a smaller number of grain boundaries with lower
misorientations could explain the discrepancy, as a small variation in the number of twinned grain boundaries can result in big variation in the fractional value at lower GBM.

The distribution of grain diameters and fraction of twinned grains as a function of grain diameter are shown in Fig. 6-8c and 6-8d, respectively. As more than half of the grains have ~13 µm of grain size (grains in S1 set) a higher grain frequency exists at diameter less than 10 µm (Fig. 6-8c). The experimental results shows than grains with higher grain size normally have higher tendency to twin (Fig. 6-7d); a similar trend is also observed in the CPFE simulation and better agreement is achieved at higher grain diameters. However as mentioned before, in the current version of the CPFE code, grain size effects are not explicitly included and the increased propensity for twinning in larger grains arises due to the larger surface area. Effects associated with dislocation–grain interaction are not captured, and are likely associated with the discrepancies that exist when size effects are studied. Hence the model undepredicts twinning at large grain size, and overpredicts at small grain size compared to the experimental data.
Fig. 6-8. (a) distribution of grain boundaries misorientations; (b) fraction of the twinned grain boundaries as a function of grain boundaries misorientation: CPFE vs. experiment; (c) distribution of grains diameter; (d) fraction of twinned grains as a function of grain size: CPFE vs. experiment.

6.4.3 Image analysis

Images were captured during the in-microscope deformation of samples to measure strain, using the image correlation technique. A sample image of an undeformed microstructure is shown in Fig. 6-9a; This is the same area we studied in Fig. 6-5. The image correlation process was carried out using Istra 4D software (see appendix B for more detail). Images are needed to be subdivided
into smaller pieces, called facets; the software tries to find one-to-one correspondence between
facets of an image with those of the previous image. Hence, each facet must be big enough to
contain reasonable number of features for correlation purposes; at the same time, the facet size
must not be too big since that causes a reduction in spatial resolution.

In order to measure strain in individual grains, one may map a regular pattern on the sample
surface [46, 47], however, these induced patterns usually produce irregularity on the surface and
cause resolution reduction in EBSD patterns of deformed samples. Hence, as each individual
grain didn’t have enough features for the correlation process, a family of grains was used for
generation of the surface in-plane strain map. Two investigated areas, Poly 1 and Poly 2, are
shown in Fig. 6-9a. Measured strains are compared with CPFE results with different boundary
conditions in Fig 6-9b to 6-9f. Errors shown in Fig 6-9 are those related to the correlation process
where based on covariance matrix, during correlation process, and by using error propagation
method the uncertainties in the measured data is calculated. They thus are measures solely of the
error within the data analysis, and will hence be the minimum possible error on the measurement.
A sense of the size of the true error bar can be obtained from the scatter in the data when it should
be changing smoothly, e.g. low stress region in Fig 6-9b.

The whole deformation process can be divided into elastic and plastic deformation, where once
measured strains are plotted against applied stress better insight into the former can be achieved
(Fig. 6-9b and 6-9d to 6-9f) while the plot of measured strain against applied strain reveals more
information about the latter (Fig. 6-9c). Simulations with different boundary conditions resulted
in equal prediction in the elastic zone, however, the yield point and plastic prediction are
significantly affected by the boundary condition. The plane strain normally causes the hardest
response due to the triaxality of the stress state whereas planes stress causes the softest response. The periodic boundary condition is somewhere between these two extremes. As the traction force normal to the free surface is zero, the measured state in samples is closer to the plane stress condition, (hence why the plane stress results were presented in section 6-4.1 and 6-4.2). Further, the comparison between CPFE and measured strains shows that the single crystal parameters we produced for explaining deformation in the big grain size samples are also reasonably good when describing the response of a grain ensemble.
Fig. 6-9. (a) Pre deformation configuration of the sample shown in Fig. 6-2b with Poly1 and Poly 2 as two investigated areas; comparison between measure strain and CPFE results for (b) normal to the loading direction in Poly 2: measured strain vs. applied stress, (c) normal to the loading direction in Poly 2: measured strain vs. applied strain, (d) along the loading direction in Poly 2: measured strain vs. applied stress, (e) normal to the loading direction in Poly 1: measured strain vs. applied stress, (f) along the loading direction in Poly 2: measured strain vs. applied stress.

6.5 Discussion

First we would like to summarize our CPFE observations and discussions. A CPFE code has been used to study twin inception and propagation in different measured microstructures of Zircaloy-2 samples. In the current approach, the stress state at each IP is the only parameter controlling twin inception and propagation; it is shown that twins tend to initiate at grain boundaries in both “soft” and “hard” grains due to stress concentration originating from mismatch between elastic and plastic properties of two different neighboring grains whereas in soft grains they don’t propagate far into the grain. It is observed that some twin inception sites and propagation directions are captured very well by the model, whereas some other cases are not. Different factors could be responsible for the discrepancy seen in the CPFE compared to experimental results. To name a few, first of all, the existence of various crystal defects inside each grain, e.g. distribution of
alloying elements for this alloy, and specially at the grain boundary is neglected, where these defect sites can act as the potential twin inception sites due to their contribution to stress concentration. Secondly, it has been shown that sub-surface grains can have tremendous effects on stress distribution inside each grain at the surface [38-40] where these effects are basically neglected in the current approach. A three dimensional grain map, such as the one presented in Aydiner et al. [48] or Abdolvand et al. [49], is required to confirm more precisely the trends observed in this report. Third, to facilitate element numbering for twin propagation purposes, i.e. communicating between different elements, as well as applying desired boundary conditions, first order element are used where the ultimate number of them is totally controlled by the capabilities of the machine used for simulation. Using higher order elements and/or more elements per grain can surely improve the results.

In the current model, the criteria for creating the second twin inside a grain is simply based on the saturation of the elements inside the SOE in terms of twin accommodation. It was observed that not more than one twin formed inside each grain during 3% straining, based on the parameters used, whereas our experimental results revealed existence of more than one twin in some grains. Obviously, there is a plenty of room available for completing this part of the research by implementing other purposed methods such as energy methods presented in Fischer et al. [33] or Zhang et al.[34] and [50]. Similar trends can be used for twin thickening.

In terms of statistical study of twin formation, i.e. Fig. 6-7 and 6-8, general trends observed in our experiments are captured using the CPFE. In the previous part of this study [27], twin inception sites were used to represent twins in CPFE; here, attention was paid to both inception and propagation where more or less similar trends were captured. It is observed in Fig. 6-7b and 6-7c
that twins can form in grains with both high and low GSF. To shed light on this particular observation, the stress variations found inside grains are reported here. In Fig. 6-10a the distribution of Von Mises stresses as a function of misorientation between the normal to the basal plane and the loading direction (θ) is shown. Von Mises stresses are extracted from our CPFE simulation at a step just before macroscopic yielding where twins had not yet formed. The misorientation (θ) is calculated based on the initial orientation of IPs in each grain. As expected, at higher θ grains are softer since prism and basal systems are active compared to the grains with smaller θ where twinning, with a higher CRSS is more active. What is more interesting is the distribution of stresses; at higher θ, there are many IPs that act as if they were low θ IPs. These IPs belong to soft grains (with basal and prism as two main deformation mechanism); however, due to neighboring effects where the soft grain is facing a “hard” grain, they experience high stresses. In order to have closer look at these IPs we introduce a Concentration Factor (CF) as:

$$CF = \frac{A_{ip}^{n}}{\langle A_{ip}^{n} \rangle}$$  

where $A_{ip}^{n}$ is the value of the parameter A at the IP that belongs to the grain n and $\langle A_{ip}^{n} \rangle$ is the average value of the A in all of the IPs in the same grain. Von Mises stress concentration variation inside each grain as a function of θ is shown in Fig. 6-10b. The distribution of Von Mises stress CF shows that stresses in hard grains do not vary as much as they do in soft grains, where more than 60% higher stresses (compared to the grain average value) are observed in some cases. A similar study can be conducted on Schmid factors using the local stresses. In Fig. 6-10c. the variation of maximum Local twin Schmid Factor (LSF) as a function of θ is presented. In comparison to the Von Mises stresses, a similar trend is observed; however, because of carrying information from both orientation and local stress state, one can argue that the LSF represents a
better insight into the effect of local environment on twin inception. For instance, at $\theta \sim 80$ there are many IPs for which the twin activity in them, or $(LSF_1)$, is as high as (or even higher than) that in IPs of “hard” grains, although these IPs belong to “soft” grains, i.e. the grains have a low $GSF_1$. These IPs are the places where twin inception occur in CPFE simulations for low $GSF_1$ grains. These points also likely represent the nucleation sites in soft grains where twins would incept, with an initial overshoot in size at nucleation [51], but due to the low resolved shear stress that acts on them, the twin does not thicken or propagate. $LSF_1$ Concentration Factors of IPs are shown in Fig. 6-10d. As the average $LSF_1$ in soft grain is very close to zero, at the higher $\theta$ the concentration factor can reach very large values (60 in this case). We therefore emphasize the first 50 degrees misorientations with the rest of the scale shown in the figure inset.
Fig. 6-10. (a) Von Mises stresses as a function of the misorientation between normal to the basal planes and loading direction (θ); (b) stress concentration factor as a function of θ; (c) maximum Local twin Schmid Factor (LSF₁) as a function of θ; (d) LSF₁ concentration factor as a function of θ.

The statistical study of twins revealed that stress concentrations resulting from grain boundary geometry, orientation of grains and that of neighboring grains can cause twin formation in both
“soft” and “hard” grains. The statistical trends showed in Fig. 6-7 and 6-8 apparently are not really a function of which scheme is used for twin propagation (M1, M2 or so on), yet the local behavior, e.g. twin inception sites and propagation directions, are truly a function of the local behavior and applied scheme.

6.6 Conclusion
Various different approaches are tested in a CPFE framework to investigate the ability of CPFE to explain twin formation in an HCP material. Two dimensional measured grain maps are implemented as the input files for FE simulations. It is assumed that twin inception and propagation are exclusively controlled by stress state at each IP and the predominant twin variant is responsible for twin formation. CPFE simulations revealed that twins tend to form at grain boundaries especially at the intersection of more than two grains, due to the existence of higher stress concentration at those locations. It is observed that while some of the twins in CPFE form with respect to the same variant observed in experiment, some other don’t follow the same trend. Many reasons could be responsible for the discrepancies such as effects of sub-surface grains or neglecting the role of lattice imperfections. In terms of average behavior, most of the experimentally observed phenomena are captured in CPFE simulations. It is shown that twin forms in both “soft” and “hard” grains and with respect to different twin variants. Enormous fluctuation in local stresses and consequently in the highest local Schmid factors are shown to be one of the strongest reason for formation of twins in soft grains.
Reference List


Chapter 7
Conclusions and future work

7.1 Conclusions

Crystal plasticity constitutive equations have been implemented in a UMAT subroutine and used to study various aspects of deformation by slip and twinning in HCP crystals, with an emphasis on studying deformation in Zircaloy-2. The ability of the code to model material deformation has been tested at different length scales by comparing results with those of in-situ neutron diffraction measurements of texture as well as lattice strain evolution. At a lower length scale, twin inception and propagation in each grain have been investigated and the results are compared against 2D EBSD measurements, both carried out by the author and from the literature. Following are the general conclusions of this study:

1) Chapter 3: Cubic-shape grains were assigned to pre-deformation measured orientations of Zircaloy-2. Grains were randomly dispersed in the body of the model and periodic boundary conditions applied at the free surfaces such that the ‘cube’ can be considered as a unit cell of an infinite array of grains. It is shown that the rate dependent equations can adequately describe both macroscopic and microscopic deformation of Zircloy-2 under six different loading conditions, relative to the parent texture. Many inflections observed in the lattice strain measurement are captured and explained by the CPFE code. It is shown that relaxation due to twin inception is responsible for some of the inflections observed in lattice strains. As a result of stress and rotation heterogeneity within each grain good texture predictions are achieved by CPFE especially when results are compared with self consistent models. In terms of internal strain evolution, both CPFE
and the self consistent model used in this dissertation show equal power in describing experimental observations.

2) Chapter 4: Various assumptions in modeling twinning were tested to study the pros and cons of each over the others. Results were compared against neutron diffraction experiments on both Zircaloy-2 as well as the Mg alloy AZ31B. It is shown that, in the developed CPFE code, the predominant twin reorientation scheme provides better agreement with experiment than having multiple twins at each integration point in terms of texture evolution prediction. Three different scenarios were followed for estimating the stress state inside twins at inception; it is shown that between equal stress conditions (twin and parent have equal stress at inception), continuity equations (continuity equations are satisfied at the twin boundary), and the FIF assumption (considering back stresses resulted from constraint applied by neighboring integration points) the third can explain significant relaxation observed at the twin inception. It is also observed that decoupling the twin from parent grain once the twin is formed, in terms of load sharing, works the best in our current approach to modeling twinning.

3) Chapter 5: Grains with random shape were generated using Voronoi tessellation and mapped into the FE solver to statistically study twin formation in HCP materials. CPFE results were compared against EBSD measurements from the literature; it was shown that by considering initial texture and grain boundary effects most of the trends observed experimentally can be captured in the CPFE simulations. It is shown that twins can form in grains with both high and low twin Schmid factor, where the probability of having a
twin is higher in grains with higher Schmid factors. Also, neighboring grains are one of the potential reasons for generating stress concentration and forming twin in “soft” grains, i.e. grains with a low twin Schmid factor. Local and global stresses are used for calculating the twin Schmid factor, termed LSF and GSF, respectively. Due to stress variations within each grain, twins can form not necessarily just based on the predominant variant (if GSF terminology is used) where depending on the loading direction and initial texture, all six twin variants can contribute to twin formation. CPFE simulations show that due to stress concentrations, twins tend to incept at the conjunction of more than two grains, where the probability of having a twin at conjunctions increases with the number of grains contributing to the conjunction. While some of the statistical parameters, e.g. twin variant selection or fraction of twinned grain, are not affected by the position and neighbours of grains, some others, e.g. fraction of twinned grain boundary or fraction of twinned grains, are affected by those parameters. GSF have been used in the literature to characterize twin variants; it is shown here that as a result of variation in local stresses there is a significant difference between GSF and LSF, especially in the plastic zone, which makes GSF an unreliable variable in explaining grain tendency for twinning. Finally, it is shown if twins are studied statistically, i.e. local behavior is not of primary interest, with initial texture and creating random grain shapes most of the phenomena regarding twin variant selection can be explained with CPFE simulations.

4) Chapter 6: Orientation maps of samples made of Zircaloy-2 were measured before and after deformation. In-situ tensile tests, inside an SEM chamber, were performed on each sample in the plate-normal direction to monitor twin formation within each grain. Pre-
deformation orientation maps of grains were mapped into the finite element solver and local twin formation studied. In addition, the previously described approach to modeling twinning was modified in order to consider local twin geometry. Results from CPFE simulations are compared against post deformation EBSD maps. It is observed that, due to stress concentration twins tend to form at grain boundaries, especially at the conjunction of more than two grains. In comparison to the experimental results, some twins formed in CPFE have similar form and direction to the measured ones and some do not. The major potential reason for discrepancies between calculations and measurements is the effects of sub-surface grain that are neglected in the 2D geometry simulations. Neglecting the existence of crystal imperfections and other elements in the structure of each grain are other reasons for discrepancies. Different approaches in modeling twin formation were tested in the CPFE code; it is observed that CPFE-experiment statistical comparisons do not really change from one approach to another, yet local twin formation does change as a result of changing stress states inside each grain. As twin inception and propagation in the current study are controlled solely by the stress state at the twin tip, it is shown that higher stresses are required for twin propagation, but that is not enough - the rapid twin formation at the inception stage could not be captured. Strains in families of grains were measured using the image correlation technique and compared against CPFE results. Between different applied boundary conditions, plane stress was shown to have the closest approximation of strain distribution, as expected since stress in the direction normal to the free surface is zero in the experiment. Stress concentration analysis within each grain revealed high fluctuations in stresses from one side of a grain to another. Also, the twin Schmid factor analysis revealed that Schmid factors in “soft”
grains can be as high as those in “hard” grains as a result of neighboring effects and grain boundary geometry; that is one of the reasons why twins can readily form in “soft” grains.

Discretizing each grain with many integration points and having the force equilibrium and compatibility equations satisfied for each integration point empowers the finite element scheme in capturing inter- and intra-granular stress heterogeneities and hence provides improved insight to the material behavior in the existence of deformation by twinning than non-local schemes. In this dissertation, it is shown that average and statistical behavior of twins can be properly simulated by the methodologies implemented in developing the UMAT code, however, lots of work is needed in studying the local behavior of twins. The final aim of this study is to apply the developed code for investigating deformation at the crack tip of materials, with an emphasis on nuclear materials; having known the pros and cons of the code, it may now be used to studying deformation of grains at various stress concentrations.

7.2 Future work
The long term goal of this research is to develop a CPFE code to be used for crack modeling. In the current research, different approaches are used to understand powers and weaknesses of the developed code under different loading conditions; besides, different aspects of deformation in HCP polycrystals are studied, yet some further studies are required to confirm some of the reported phenomena in the current work:

1) Some parameters for modeling deformation twinning in the current research are calibrated by comparing results of the CPFE code with those of different experiments on polycrystalline Zircaloy-2. Better insight into the twin inception and propagation can be
achieved by modeling single crystals and comparing the results with experiments. The experimental set-up could comprise of several *in-situ* synchrotron X-ray diffraction experiments where notched single crystal zirconium are loaded at different angles with respect to the normal to the basal planes while twin inception, stress state inside twin and parent grain, and twin propagation direction can be monitored simultaneously. This test can confirm many controversial aspects of twin formation; for instance, is twin formation a random process or is it a deterministic one, i.e. is there a certain load/dislocation density that must be reached to produce a twin or not? What is the stress state inside the twin at the inception if there is no constraint by neighboring grains and how does twin propagate in the absence of these constraints? How much twin relaxation can be recorded at the twin inception and how does the stress tensor vary with distance from the twin plane? How does the twin thicken and when does the next twin incept? These are some fundamental questions that are still not answered clearly and can be modeled/investigated using the current CPFE code.

2) The statistical study of twins in the current research is based on 2D EBSD measurements where in many cases, uncertainty in the result and discussion rises because of missing information from grains under the surface; 3D synchrotron X-ray diffraction technique can be used to study the same parameters in 3D and confirm the trends in 3D. Also, the stress state inside twin at inception and during propagation can be measured with this technique and used in parallel with the CPFE code to understand the mechanism of twin inception.
3) Modeling deformation of HCP polycrystals shows that the current code is well capable of predicting deformation when the representative volume element contains information from many grains, i.e. when compared against neutron diffraction experiments and families of grains are studied at the same time; it is expected that the current code is able to model deformation at the crack tip in the aforementioned length scale; however, if the interaction of crack and each individual grain is desired in a polycrystal, more studies are required to understand twin propagation and the interaction between crack tip with each individual twin.

4) The developed code uses crystal plasticity constitutive equations in the finite element framework where plastic deformation is a result of slip and twinning. The code is a general code and can be used to study different deformation mechanisms at different length scale. To name a few, interaction between grains, grain boundary mechanics, texture evolution, effects of crystal imperfections on various parameters such as inception of twins.
Appendix A
Formulation of the crystal plasticity constitutive model

In this section, equations used for modeling plastic deformation in the developed UMAT are explained. At the beginning of each time step, total strain and rotation increment as well as time increment are calculated by ABAQUS FE solver [1] and are passed to the UMAT subroutine. The aim of the UMAT is to calculate the total stress increment and Jacobian matrix (variation of the stress increment with respect to the variation of strain increment) and pass them back to the FE solver at the end of each time step; Also, state dependent variables, e.g., current resolved shear stress, current strength, total accumulated shear, and current orientation of slip/twin direction and normal to the slip/twin planes of all of the slip/twin systems must be updated inside the UMAT.

In order to explain the equations, we first start with the simpler case where the material flows because of pure slip and then modify equations to include twinning. It worth mentioning that there must be a stage where at each Integration Point (IP) material flows only by slip as twinning reorientation and creation of the new crystal (child grain) happens once twinning shear (pseudo-slip) reaches a critical value.

Let us introduce following agreements:

Lowercase alphabets with arrows represent vectors, uppercase alphabets represent second order tensors (except for Jacobian, see Eq. 10), and script letters represent fourth order tensors. Also, we will follow summation convention as follows:

\[ \vec{v} = v_i \text{ where } i = 1:3 \]

\[ if \vec{v} = P \vec{v} \text{ then } \dot{v}_i = P_{ij} v_j \]  \hspace{1cm} (1)
1. Deformation by pure slip

The UMAT code is developed based on the mathematical equations developed for rate dependent equations by Hill [2], Hill and Rice [3], Asaro [4], and Asaro and Needleman [5]. We follow the same trend introduced by Huang [6] in developing slip based plastic deformation within a UMAT subroutine. The total deformation can be decomposed into the elastic part, which causes lattice reorientation and stretching, and the plastic part which causes movement of dislocation in slip plane in slip direction. It is assumed that plastic slip does not produce any lattice reorientation. Hence, total deformation gradient \( F \) can be decomposed to:

\[
F_{ij} = \frac{\partial \mathbf{x}_i}{\partial x_j} 
\]

(2)

\[
F = F^e F^p
\]

where \( \mathbf{x}_i \) is the displacement field in the current configuration, \( x_j \) is the displacement field in the initial configuration, and \( F^e \) and \( F^p \) are the elastic and plastic parts of the deformation gradient, respectively. The velocity gradient \( (L) \) can now be achieved by taking derivative of Eq. (2) with respect to time:

\[
L = \dot{F} F^{-1} = \dot{F}^e F^{e-1} + F^e (\dot{F}^p F^{p-1}) F^{e-1} 
\]

(3)

\[
L = L^e + L^p \quad \text{where} \quad L^e = F^e F^{e-1}, \quad \text{and} \quad L^p = F^e (\dot{L}^p) F^{e-1}, \quad \text{also} \quad \dot{L}^p = F^p F^{p-1}
\]

Following Asaro [4], the rate of elastic and plastic stretching \( (D) \) and spin \( (\Omega) \) tensors are correlated to the velocity gradient as:
\[ D^e + \Omega^e = L^e = T^e F^{e-1} \]
\[ D^p + \Omega^p = L^p \]
\[ D = D^e + D^p, \text{and } \Omega = \Omega^e + \Omega^p \]

It is shown by Hill [2], Rice [7], and Rice and Hill [3] that \( D^p, \) and \( \Omega^p \) can be extracted from shear on slip systems:

\[ L^p = D^p + \Omega^p = \sum_{\alpha=1}^{N^s} (\overline{m}^{\alpha} \otimes \overline{n}^{\alpha}) \hat{\gamma}^\alpha \]  \[ (5) \]

where \( N^s \) is the total number of slip systems than can be active, \( \hat{\gamma}^\alpha \) is the shear rate on the slip system \( \alpha, \overline{m}^{\alpha}, \) and \( \overline{n}^{\alpha} \) are the normal to the slip plane and shear direction of the system \( \alpha \) in the current configuration (please note that \( L^P \) is Eq. 3 is push forward of \( \overline{I}^p \) which means plastic rates are calculated on the current configuration). \( D^p, \) and \( \Omega^p \) are also introduced as the symmetric and skew symmetric part of \( L^p \) by which:

\[ D^p = \text{sym} (L^p) = \sum_{\alpha=1}^{N^s} P^{\alpha} \hat{\gamma}^\alpha, \text{and } \Omega^p = \text{skew}(L^p) = \sum_{\alpha=1}^{N^s} W^{\alpha} \hat{\gamma}^\alpha \]  \[ (6) \]

where

\[ P^{\alpha} = \frac{1}{2} (\overline{m}^{\alpha} \otimes \overline{n}^{\alpha} + \overline{n}^{\alpha} \otimes \overline{m}^{\alpha}), \text{and } W^{\alpha} = \frac{1}{2} (\overline{m}^{\alpha} \otimes \overline{n}^{\alpha} - \overline{n}^{\alpha} \otimes \overline{m}^{\alpha}) \]  \[ (7) \]

The Jaumann rate of Kirchoff stress (\( \Psi \)) is related to the rate of elastic stretching tensor as [4]:

\[ \overline{\Psi}^i = \mathcal{L} : D^e \]  \[ (8) \]

where \( \mathcal{L} \) is the fourth order elastic modulus of the crystal, and \( \overline{\Psi}^i \) is the corotational rate of the Kirchoff stress on the axis that rotates with crystal lattice:

\[ \overline{\Psi}^i = \Psi - \Omega^e \Psi + \Psi \Omega^e \]  \[ (9) \]
As in the UMAT, stresses are the Cauchy corotational stresses [1], the Kirchoff stress should be converted to the Cauchy stress using the following Equation:

$$\Psi = J \sigma, \text{where } J = \text{Det } (F)$$  \hspace{1cm} (10)

where $J$ is the Jacobian (it’s different from the ABAQUS Jacobian matrix, this is a scalar value).

Before we extract the rest of the equations, we need to mention two equations that will be used in future; first, the derivative of the Jacobian with respect to time is related to velocity gradient or the stretching tensor as follows [8]:

$$\frac{dj}{dt} = \dot{J} = J \times (D : I) = J \times \text{tr}(D) = J \times (D^e : I) = J \times D^e_{ij} : \delta_{ij}$$ \hspace{1cm} (11)

where $I$ is the second order identity tensor, and $\delta_{ij}$ is the Kronocker delta symbol and is:

$$I = \delta_{ij} = \begin{cases} 1 & \text{when } i = j \\ 0 & \text{when } i \neq j \end{cases}$$ \hspace{1cm} (12)

Now we can use Eq. 12 to derive a very important relationship between $J$ and volume change:

$$\frac{dj}{dt} = J \times D_{ij} : \delta_{ij} \xrightarrow{yields} \ln(J) = \Delta \epsilon_{kk}$$ \hspace{1cm} (13)

where $\Delta \epsilon$ is the strain increment. If we assume that volume change is small, following Eq. 14, $J$ can be replaced by 1:

$$\ln(J) = J - 1 - \frac{1}{2} (J - 1)^2 + \cdots \approx J - 1 \hspace{1cm} (14)$$

$$J = 1 + \Delta \epsilon_{kk} \approx 1$$

The corotational Cauchy stress on lattice and material coordinates are:

$$\tilde{\sigma}^t = \dot{\sigma} - 2\sigma + 2\sigma \Omega^e \text{ on lattice coordinate}$$

$$\sigma = \dot{\sigma} - 2\sigma + 2\sigma \Omega \text{ on the material coordinate}$$ \hspace{1cm} (15)

Using Eq. 9-15, Eq. 8 can be rewritten based on Cauchy stresses as:

$$\tilde{\sigma}^t + (I : D^e) \sigma = L : D^e$$ \hspace{1cm} (16)
Having known that:

\[
\Delta \varepsilon^e = \int_t^{t+\Delta t} D^e \, dt, \quad \text{and} \quad \Delta \varepsilon^p = \int_t^{t+\Delta t} D^p \, dt = \sum_{\alpha=1}^{N^p} P^{i \alpha} \Delta \gamma^\alpha
\] (17)

\[\Delta \sigma = \bar{\sigma} \times \Delta t \quad \text{and} \quad \Delta \varepsilon^e = \Delta \varepsilon - \Delta \varepsilon^p\]

The total stress increment can be extracted from Eq. 15-17 and Eq. 6-7 as:

\[
\Delta \sigma_{ij} = L_{ijkl} \Delta \varepsilon_{kl} - \sigma_{ij} \Delta \varepsilon_{kk} - \sum_{\alpha=1}^{N^p} \left[ L_{ijkl} (P^{i \alpha}_{kl} + W^{i \alpha}_{ik} \sigma_{jk} + W^{i \alpha}_{jk} \sigma_{ik}) \Delta \gamma^\alpha \right]
\] (18)

Hence, once \(\Delta \gamma^\alpha\) is determined, stress increment can be calculated. Now we step by step draw equations required for updating state variables base on the \(\Delta \gamma^\alpha\). First we start with slip direction where following relationship exists between slip direction in the current configuration \((m')\) and that of initial configuration \((m)\) [4]:

\[
m' = F^e m
\] (19)

Taking derivative of Eq. 19 with respect to time yields:

\[
\dot{m}' = F^e \dot{m} = F^e F^e^{-1} \dot{m}' \xrightarrow{\text{Eq. (4)}} \dot{m}' = (D^e + \Omega^e) m'
\] (20)

By taking integration of Eq. 20 over time and using Eq. 6 and 17 slip direction increment can be evaluated as:

\[
\Delta m_i'^{\alpha} = \left[ \Delta \varepsilon_{ij} + \Omega_{ij} \Delta t - \sum_{\beta=1}^{N^p} \left( P_{ij}^{\alpha \beta} + W_{ij}^{\alpha \beta} \right) \Delta \gamma^\beta \right] m_j'^{\alpha}
\] (21)

Similar equations can be extracted for normal to the slip plane [4]:

\[
\tilde{n}' = \tilde{n} F^e^{-1}
\] (22)

And the rate form is:

\[
\dot{\tilde{n}}' = \tilde{n} \dot{F}^e = \tilde{n} F^e \dot{F}^e^{-1}
\] (23)

Also:
\[
\frac{d}{dt} \left( f^e f^{-1} = I \right) \Rightarrow f^e f^{-1} + f^e \dot{f} f^{-1} = 0 \Rightarrow f^e f^{-1} = -f^e \dot{f} f^{-1} \quad (24)
\]

now Eq. 23 can be rewritten as:
\[
\dot{n'} = \vec{n'} f^e \dot{f} f^{-1} = -\vec{n'} f^e \dot{f} f^{-1} \quad (25)
\]

By taking integration of Eq. 25 over time and using Eq. 6 and 17, the slip direction increment can be evaluated as:
\[
\Delta n'_i^\alpha = -n'_j^\alpha \left[ \Delta \varepsilon_{ji} + \Omega_{ji} \Delta t - \sum_{\beta=1}^{N_s} \left( p_{ji}^{\beta} + W_{ji}^{\beta} \right) \Delta y^\beta \right] \quad (26)
\]

Now we will develop the incremental format of resolved shear stress. Generally, resolved shear stress on each slip system can be written as [4]:
\[
\tau^\alpha = \tau'^\alpha, \quad \Psi = \tau'^\alpha : J \sigma \quad (27)
\]

taking derivative of Eq. 27 with respect to time and using Eq. 15, 20, 25 yields:
\[
\dot{\tau}^\alpha = \vec{n'} \left[ \vec{\sigma}^\alpha + \sigma (D^e: J) - D^e \sigma + \sigma \dot{D}^e \right] \vec{n'} \quad (28)
\]

having known that the transpose of \( D^e \) and \( \Omega^e \) are \( D^e \) and \( -\Omega^e \), respectively, Eq. 28 can be rewritten as:
\[
\dot{\tau}^\alpha = \left[ L_{ijkl} : p_{ijkl}^{\alpha} + W_{ijkl}^{\alpha} \sigma_{jk} + W_{ijkl}^{\alpha} \sigma_{ik} \right] : D_i^e = A_{ij}^\alpha : D_i^e \quad (29)
\]

and in incremental format:
\[
\Delta \tau^\alpha = A_{ij}^\alpha : \left[ \Delta \varepsilon_{ij} - \sum_{\beta=1}^{N_s} p_{ij}^{\beta} \Delta y^\beta \right] \quad (30)
\]

In rate dependent materials, shear rate on each slip/twin system correlates with resolved shear stress on that system and current strength of the system \( (g^\alpha) \) as follows [5]:
\[
\dot{\gamma}^\alpha = \gamma_0 \left[ \frac{\tau^\alpha}{g^\alpha} \right]^n \text{sign} \left( \frac{\tau^\alpha}{g^\alpha} \right) \quad (31)
\]
where $\dot{\gamma}_0$ and $n$ are the power law constants. With plastic deformation, strength of each system evolves following these equations:

$$\dot{g}^\alpha = \sum_{\beta=1}^{N^s} h_{\alpha\beta} \dot{\gamma}^\beta \quad \text{or} \quad \Delta g^\alpha = \sum_{\beta=1}^{N^s} h_{\alpha\beta} |\Delta \gamma^\beta|$$  \hspace{1cm} (32)

Different equations can be used (and are included in the UMAT) for evolving strength of each slip/twin systems, here we present Voce hardening [9] as an example:

$$g^\alpha = g_0^\alpha + (g_1^\alpha + \theta_1^\alpha \Gamma) \left(1 - \exp \left(-\frac{\theta_0^\alpha \Gamma}{g_1^\alpha}\right)\right)$$ \hspace{1cm} (33)

$$\Gamma = \sum_{\alpha=1}^{N^s} \int_0^t |\dot{\gamma}^\alpha| \, dt$$

where $g_0^\alpha$ is initial Critical Resolved Shear Stress (CRSS), $\Gamma$ is accumulated shear on all slip/twin systems, $\theta_0^\alpha$ is initial hardening rate, and $g_1^\alpha$ and $\theta_1^\alpha$ determine asymptotic characteristic of hardening. Combining Eq. 33 and 32 yields:

$$\frac{d g^\alpha}{dt} = \frac{dg^\alpha}{d\Gamma} \cdot \frac{d\Gamma}{dt} \quad \text{yields}$$

$$h_{\alpha\beta} = \left(1 - \exp \left(-\frac{\theta_0^\alpha \Gamma}{g_1^\alpha}\right)\right) \theta_1^\alpha + (g_1^\alpha + \theta_1^\alpha \Gamma) \left(\frac{\theta_0^\alpha}{g_1^\alpha} \exp \left(-\frac{\theta_0^\alpha \Gamma}{g_1^\alpha}\right)\right) q_{\alpha\beta}$$ \hspace{1cm} (34)

where $q_{\alpha\beta}$ is a constant and represent interaction between slip/twin system $\alpha$ and $\beta$.

So far all of the state variables are written based on the $\Delta \gamma^\alpha$. We used the same numerical scheme implemented by Huang [6] in a UMAT in the spirit of Pierce et al. [10] for calculating $\Delta \gamma^\alpha$:

$$\Delta \gamma^\alpha = \gamma^\alpha_{t+\Delta t} - \gamma^\alpha_t$$

$$\Delta \gamma^\alpha = \Delta t [(1 - \theta) \dot{\gamma}^\alpha_t + \theta \dot{\gamma}^\alpha_{t+\Delta t}]$$ \hspace{1cm} (35)
where $\theta$ is a parameter between 0 and 1. For solving these nonlinear equations we use a Newton-Raphson iteration scheme where the initial guess to the $\Delta \gamma^\alpha$ is given by Taylor expansion of $\dot{\gamma}_{t+\Delta t}^\alpha$ (Eq. 36) and solving Eq. 37.

$$\dot{\gamma}_{t+\Delta t}^\alpha = \dot{\gamma}_t^\alpha + \frac{\partial \dot{\gamma}^\alpha}{\partial \tau^\alpha} \Delta \tau^\alpha + \frac{\partial \dot{\gamma}^\alpha}{\partial g^\alpha} \Delta g^\alpha$$  \hspace{1cm} (36)

Now by substituting Eq. 30, 32, and 36 in Eq. 35, the initial guess for $\Delta \gamma^\alpha$ can be given by:

$$\sum_{\beta=1}^{N^2} \left\{ \delta_{\alpha \beta} \theta \Delta t \frac{\partial \dot{\gamma}^\alpha}{\partial \tau^\alpha} A_{ij}^\alpha ; P_{ij}^\beta - \theta \Delta t \frac{\partial \dot{\gamma}^\alpha}{\partial g^\alpha} h_{\alpha \beta} \text{sign}(\dot{\gamma}^\beta) \right\} \Delta \gamma^\beta$$

$$= \dot{\gamma}_t^\alpha \Delta t + \theta \Delta t \frac{\partial \dot{\gamma}^\alpha}{\partial \tau^\alpha} A_{ij}^\alpha ; \Delta \epsilon_{ij}$$ \hspace{1cm} (37)

For Newton-Raphson iterations, we rewrite Eq. 35 as:

$$R^\alpha = \Delta \gamma^\alpha - \Delta t [(1 - \theta) \dot{\gamma}_t^\alpha + \theta \dot{\gamma}_{t+\Delta t}^\alpha]$$

$$\dot{\gamma}_{t+\Delta t}^\alpha = \dot{\gamma}_t^\alpha \left| \frac{\tau^\alpha + \Delta \tau^\alpha}{g^\alpha + \Delta g^\alpha} \right|^n \text{sign} \left( \frac{\tau^\alpha + \Delta \tau^\alpha}{g^\alpha + \Delta g^\alpha} \right)$$ \hspace{1cm} (38)

And we try to set $R^\alpha$ equal to zero by following equation:

$$\Delta \gamma_{\tau+1}^\alpha = \Delta \gamma_t^\alpha + u_t^\alpha \text{ where } K_{\tau}^\alpha u_t^\beta = -R_{\tau}^\alpha$$

$$K_{\tau}^{\alpha \beta} = - \frac{\partial R_{\tau}^\alpha}{\partial \Delta \gamma_{\tau}^\beta}$$ \hspace{1cm} (39)

where $\tau$ represents the $r^{th}$ iteration. By substituting Eq. 38 in Eq. 39 and working out derivatives, following equation need to be solved during each iteration to determine $u_t^\alpha$:

$$\sum_{\beta=1}^{N^2} \left\{ \delta_{\alpha \beta} + \theta \Delta t \frac{\partial \dot{\gamma}^\alpha}{\partial \tau^\alpha} A_{ij}^\alpha ; P_{ij}^\beta - \theta \Delta t \frac{\partial \dot{\gamma}^\alpha}{\partial g^\alpha} \left[ h_{\alpha \beta} \text{sign}(\dot{\gamma}^\beta) + \sum_{\theta=1}^{N^2} \frac{\partial h_{\alpha \theta}}{\partial \Delta \gamma_{\tau}^\beta} \left| \Delta \gamma_{\tau}^\theta \right| \right] \right\} u_{\tau}^\beta$$

$$= -\Delta \gamma_{\tau+1}^\alpha + \Delta t [(1 - \theta) \dot{\gamma}_{\tau+1}^\alpha + \theta \dot{\gamma}_{\tau}^\alpha]$$
2. Deformation by slip and twinning

Different versions of UMAT are developed for modeling slip and twinning and each are discussed in detail through chapters 3 to 6. Here we introduce the general mathematical formulation for adding twinning to the presented equations. As discussed in chapter 3 and 4, there are various methods for introducing velocity gradient. Here, we introduce three different methods for modeling twinning. In the first method (will be referred as M1), the plastic part of the velocity gradient for twin and parent grain are written as:

\[
I_{pa}^P = \left(1 - \sum_{\beta=1}^{N_{\text{tw}}} f^\beta \right) \sum_{\alpha=1}^{N_{\text{tw}}} P^\alpha \dot{\gamma}^\alpha + \sum_{\beta=1}^{N_{\text{tw}}} P^\beta \gamma_{0}^{\text{tw}} \dot{f}^\beta
\]

\[
I_{ch}^P = \sum_{\alpha=1}^{N_{\text{tw}}} P^\alpha \dot{\gamma}^\alpha
\]  

(41)

where \(N_{\text{tw}}\) is the total number of twin system that can be active in the parent grain, \(\gamma_{0}^{\text{tw}}\) is the characteristic twin shear, and \(f^\beta\) is the volume fraction of the twin resulted from \(\beta^{th}\) twin system. The strain rate of the twinning systems is related to twinning volume fraction with the following equation [11]:

\[
\dot{f}^\beta = \frac{\dot{\gamma}^\beta}{\gamma_{0}^{\text{tw}}} , \quad f^\beta \geq 0, \quad \sum_{\beta=1}^{N_{\text{tw}}} f^\beta \leq 1, \text{if } \tau^\beta > 0
\]

(42)

\[
\dot{f}^\beta = 0.0 \text{ if } \tau^\beta \leq 0
\]

The restrictions that are imposed on Eq. (42) indicate that twinning volume fraction cannot be negative, the sum of the twinned volume cannot exceed the grain volume itself, and the twinned regions are not allowed to untwin. In the M1 Method twins are generated at each integration points where twin and parent will have equal total strain and rotation increment, but different
stresses. Following Eq. 1-40 these equations are solved separately for twin and parent (considering the modification implemented in Eq. 41) and once stresses for twin and parent are calculated, the total stress increment can be evaluated using Eq. 43:

$$\sigma^{new} = \sigma^{old} + \Delta \sigma$$

$$\Delta \sigma = \left(1 - \sum_{\beta=1}^{N_{tw}} f^\beta\right) \Delta \sigma^{parent} + \sum_{\beta=1}^{N_{tw}} f^\beta \Delta \sigma^{\beta,child} + \sum_{\beta=1}^{N_{tw}} \Delta f^\beta \left(\sigma^{\beta,child} - \sigma^{parent}\right)$$  \hspace{1cm} (43)

Please note that in this method parent and twin will have different elastic and plastic rate of stretching and spin as different plastic gradient are assumed for each.

In the second version (M2) we will use Kalidindi’s approach [11] in modeling twinning where the twin is embedded in the parent grain and both experience the same elastic deformation gradient (or equal elastic velocity gradient):

$$L_{pa}^e = \left(1 - \sum_{\beta=1}^{N_{tw}} f^\beta\right) \sum_{\alpha=1}^{N_s} P^{\alpha,\alpha} + \sum_{\beta=1}^{N_{tw}} f^\beta \sum_{\delta=1}^{N_{s-tw}} P^{\delta,\delta} + \sum_{\beta=1}^{N_{tw}} f^\beta P^{\beta,\beta} y_{0}\,^{tw}$$  \hspace{1cm} (44)

where $$N_{s-tw}$$ is the number of slip systems that can be active in each twin. All of the equation can now be again written with respect to the shear strain increment and elastic and plastic part of the strain increment can be evaluated. In the M2 method, the stress in each twin and in the parent can be calculated as [11]:

$$\sigma_{pa} + (I:D^e) \sigma_{pa} = L_{pa}:D^e$$

$$\sigma_{ch} + (I:D^e) \sigma_{ch} = L_{ch}:D^e$$  \hspace{1cm} (45)

$$L_{ch}$$ is the elastic modulus of the twin which can be calculated having known the orientation of the twin. In order to bring each vector in the parent domain to the twin domain at the inception, the following rotation matrix can be used [12]:
\[ R_{tw} = 2\vec{n}_{tw} \otimes \vec{n}_{tw} - I \]  
\hspace{1cm} (46)

where \( \vec{n}_{tw} \) is the normal to the twin plane at the inception. Total stress increment in the M2 method can also be evaluated using Eq. 43.

In the third approach (M3) we modify plastic part of velocity gradient in order to introduce total inelastic strain as follows:

\[ \varepsilon_{\text{total}}^p = \left( 1 - \sum_{\beta=1}^{N_{tw}} f^\beta \right) \sum_{\alpha=1}^{N_s} p^\alpha y^\alpha + \sum_{\beta=1}^{N_{tw}} f^\beta \sum_{\delta=1}^{N_{s-tw}} p^{\beta \delta} y^{\delta} + \sum_{\beta=1}^{N_{tw}} p^{\beta \delta} f^\beta y_{0}^{tw} \]  
\hspace{1cm} (47)

hence the total plastic velocity gradient will be:

\[ I_{pa}^p = \left( 1 - \sum_{\beta=1}^{N_{tw}} f^\beta \right) \sum_{\alpha=1}^{N_s} p^\alpha \dot{y}^\alpha + \sum_{\beta=1}^{N_{tw}} f^\beta \sum_{\delta=1}^{N_{s-tw}} p^{\beta \delta} \dot{y}^{\delta} + \sum_{\beta=1}^{N_{tw}} f^\beta p^{\beta \delta} y_{0}^{tw} \]  
\hspace{1cm} (48)

Now we can again write the rest of the equations based on the shear strain increment and determine the shear strain increment on each slip/twin system by solving modified version of Eq. 37 and 40. Equations 43 and 45 can consequently be used to calculated total stress increment and stress increment in each twin and parent.

Reference List


Appendix B

Image analysis

In this section, a brief description of the principal of image correlation technique is presented. Digital Image Correlation (DIC) is a versatile technique that has been used to understand deformation at various length scales from micro to macro. The basic concept behind image correlation is to find features in the images taken from interested area at different loading stages and try to find one-to-one correspondence between positions of these features [1-5]. Once the position of each feature is determined, the strain field can be extracted. In order to explain the methodology that DIC is constructed based on, let’s start with the image given in Fig. B-1 and deform it to Fig B-2 [2]. The first step is to subdivide the images into discrete rectangular subsets known as facet, which can then be located and compared from one image to the next. Each facet must have enough features for correlation; hence, facet size must be chosen to be big enough so that each facet contains a reasonable number of features, but it shouldn’t be too big as bigger facets will reduce the spatial resolution. A feature in this context is a region of high contrast that clearly stands out from the ‘background’, i.e. the dark spots in Fig. B-1 and B-2.
Fig. B-1 and B-2: Discretization of the field of deformation field to subregions; B-1: before deformation and B-2: after deformation [2].

Different strategies are employed to carry out the comparison of facets. A number of image correlation algorithms have been developed to cross-correlate grayscale pixel intensity variations from the facets, employing a number of mathematical and computational strategies; these include simple least squares approaches, Fourier transforms or Bayesian probability methods. Some series of displacements and rotations is typically applied to a facet from the undeformed image so
that it correlates with the deformed image. Typically, the quality of the fit between facets as a result of these transformations is given by a correlation coefficient, which is iterated until it is minimized below some threshold error value. If the correlation coefficient cannot be minimized below the prescribed value, then the correlation will fail for that facet [6].

The determination of the uncertainty for every data, in the DIC method used in this study, is based on the co-variance matrix which is calculated during the correlation process. Then, by using the error propagation method the uncertainties of data, i.e. errors, derived from that correlation can be calculated.

In the current study, the DIC technique is integrated into an SEM imaging system to measure the strain field at the surface of Zr-2 tensile samples. The strain measurement process comprises of several different stages; first, the investigated area must have enough features for correlation purposes; second, a reference point must be picked for each sample right at the beginning of each test so as to keep this point always in the center while deforming or capturing images. Keeping this point in the center certifies that images are captured from the same area at each loading step. Third, the user must bring the sample into focus every single time that capturing an image for DIC is intended. This is crucial especially when sample is deforming plastically as due to Poisson effects, it goes out of focus and causes fake strains in the DIC calculation. Once all images are captured, they can be used within commercial DIC packages for correlation calculations.

Reference List


