A Crystal Plasticity Model of Fatigue of Dissimilar Magnesium Alloy Bi-Crystals

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Abstract

A crystal plasticity finite element (CPFE) model was applied to the fatigue deformation of dissimilar Mg alloy bi-crystals. The mesoscopic stress-strain and microscopic slip and twinning behaviour of the model were first validated with experimental tension and compression data of pure Mg single crystals. High-cycle fatigue (HCF) simulations up to 1000 cycles were then used to systematically examine the effect of different textures on the cyclic deformation behavior of Mg AZ31-AZ80 bi-crystals at room-temperature. Fatigue behaviour was characterized in terms of the mesoscopic average stress-strain response and the evolution of the microscopic deformation (slip/twin activity). The model captures load asymmetry, cyclic hardening/softening and ratcheting. However, the model did not capture stress concentrations at the grain boundary (GB) for the grain shapes considered.

Either basal slip or tensile twinning was activated for any given orientation. When the soft AZ31 grain is oriented for basal slip almost all the shear strain is contained in that grain and has approximately ten times more accumulated shear strain than the other orientations. The results reveal there is a strong effect from orientation combinations on the cyclic deformation wherein a “hard” orientation shields a “soft” orientation from strain. When the AZ80 grain is oriented for basal slip and
the AZ31 grain is oriented for tensile twinning the bi-crystal is soft, but only in one direction since twinning is a polar mechanism. Approximately half as much accumulated shear strain occurs when both grains are oriented for twinning. The slip and twinning systems quickly harden in AZ31 in the first few hundred cycles and the shear strain amplitudes quickly devolve from values between $10^{-6} – 10^{-4}$ to around $10^{-7}$; values which would be difficult to resolve experimentally.

The results were then extended to the possible effects on the fatigue behaviour of an AZ31-AZ80 dissimilar weld idealized as an AZ31-AZ80 bi-crystal. It is predicted that the worst fatigue behaviour would occur when one grain is oriented for basal slip: AZ31 grain, results in strain localization; AZ80 grain, results in an increase in twin boundaries and irreversible deformation in an AZ31 grain.
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<th>Symbol</th>
<th>Description</th>
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<tbody>
<tr>
<td>CPFE</td>
<td>Crystal plasticity finite element</td>
</tr>
<tr>
<td>CRSS</td>
<td>Critically resolved shear stress</td>
</tr>
<tr>
<td>D</td>
<td>Strain rate tensor</td>
</tr>
<tr>
<td>De</td>
<td>Elastic part of the strain rate tensor</td>
</tr>
<tr>
<td>F</td>
<td>Deformation gradient</td>
</tr>
<tr>
<td>Fe</td>
<td>Elastic part of the deformation gradient</td>
</tr>
<tr>
<td>Fp</td>
<td>Plastic part of the deformation gradient</td>
</tr>
<tr>
<td>FCC</td>
<td>Face-centered cubic</td>
</tr>
<tr>
<td>FE</td>
<td>Finite Element</td>
</tr>
<tr>
<td>FSW</td>
<td>Friction stir weld</td>
</tr>
<tr>
<td>fβ</td>
<td>Twin volume fraction resulted from activity of twin system β</td>
</tr>
<tr>
<td>gα</td>
<td>Current strength of slip/twin system α</td>
</tr>
<tr>
<td>g0α</td>
<td>Critically resolved shear stress of slip/twin system α</td>
</tr>
<tr>
<td>g1α</td>
<td>Work hardening scaling stress</td>
</tr>
<tr>
<td>GB</td>
<td>Grain boundary</td>
</tr>
<tr>
<td>GP</td>
<td>Gauss point</td>
</tr>
<tr>
<td>hαβ</td>
<td>A parameter that describes interaction between slip/twin system α and β and is a function of the introduced hardening law</td>
</tr>
<tr>
<td>HCF</td>
<td>High-cycle fatigue</td>
</tr>
</tbody>
</table>
HCP  Hexagonal close-packed
L   Velocity gradient
Le  Elastic part of the velocity gradient
Lp  Plastic part of the velocity gradient
LCF Low-cycle fatigue
mα Slip direction of the slip/twin system α
M   Total number of slip and twin modes
n   Shear strain rate dependency exponent
nα Normal to the slip/twin plane α
N   Total number of slip and twin systems
pα Symmetric part of the Schmid tensor
PSB Persistent slip-band
PTR Predominant twinning reorientation
R   Rotation matrix from finite element solver
RSS Resolved shear stress
Sα  Schmid tensor
t   Time unit from the finite element solver
T   Cumulative shear strain amplitude
TVF Twin volume fraction
uik Displacement of point/edge/face k in direction i
UMAT User MATerial
γα Shear strain on slip/twin system α
\( \varepsilon \) strain

\( \theta_0^\alpha \) Initial hardening rate

\( \theta_1^\alpha \) Final slope of hardening curve

\( \sigma \) Cauchy stress tensor

\( \tau^\alpha \) Resolved shear stress on slip/twin system \( \alpha \)

\( \Gamma \) Accumulated plastic shear
Chapter 1 - Introduction

1.1 Motivation

In 2007 the United States congress passed the Energy Independence and Security Act. This legislation requires the combined fuel efficiency of America’s cars, light trucks and SUVs to have an average of 5 litres per 100 km (48 mpg) by 2025. This is a 50% increase from 2010 levels [1]. One of the most effective ways to increase fuel efficiency is to decrease the weight of the vehicle. Mg alloys are currently attracting interest as weight-saving components to improve fuel efficiency and reduce greenhouse gas emissions in automotive applications [2, 3].

Mg is the lightest structural metal currently available with a density of 64% of aluminum and 22% of iron. Mg and its alloys can offer the greatest strength and stiffness to weight ratios and high specific stiffness, which gives it potential for use in light-weight structural applications in automotive vehicles [4]. Modern light-weight production cars already incorporate Mg in die-cast parts such as steering wheel cores, engine head covers, and seat frames [5]. Compared to cast Mg alloys, wrought alloys show improved yield, tensile strength, formability and fatigue properties [4, 6]. However, applications of wrought Mg alloys are still restricted since their room temperature ductility is poor compared to other metallic alloys,
which limits crash-worthiness. Magnesium’s poor ductility is attributed to the complex plastic behavior due to its hexagonal-close-packed (HCP) crystal structure, which is inherently anisotropic and has a limited number of deformation systems available. In particular, mechanical twinning causes a strong tension/compression asymmetry.

Weight minimization can be optimized by using different materials; as a generalization, more than one type of material is used in a car. A specific example is a wheel which consists of a hub, spoke and rim. The unsprung mass of the car is transmitted to the road through the hub, spoke, rim, and tire. Most of the load is spread over the rim which can be made from a more ductile, lower strength, and less costly alloy than the hub. Tailoring multiple materials to a component is not new, but there are challenges in joining Mg alloys without further degrading its desirable materials properties.

It is difficult to weld Mg alloys by fusion welding processes without introducing defects since Mg is an extremely reactive metal. It has been shown that good welds can be made from Mg alloys, and even dissimilar Mg alloys, by friction stir welding (FSW) [7]. FSW is a solid state joining technique in which two pieces of metal are joined by a non-consumable rotating tool with a pin and shoulder that is inserted into the abutting edges of the pieces and moves along the line of the joint. However, the intense plastic deformation and heat input around the pin can cause
recrystallization and crystallographic texture modification as well as mixing of the different materials and therefore changes the mechanical behavior of the material. An idealization of a dissimilar Mg alloy FSW microstructure stressed in tension is shown in Fig. 1.1. Mg AZ31 is on the left and Mg AZ80 is on the right and a mixture of different alloy grains are in the weld zone. Two different grains on the interface are magnified showing the local stress field. In monotonic tensile deformation, yielding and subsequent strain localization occurs in the weld boundary [8]. Tsujikawa et al. have reported that FSW decreases the fatigue properties of Mg alloys in terms of endurance limit [9]. The decrease in fatigue strength could potentially be linked to the strong texture gradient across the weld boundary.

Fig. 1.1: Idealization of a Mg AZ31-AZ80 FSW, in tension, with two neighbor grains at the weld-base material interface magnified to show the local stress.
For structural car components undergoing dynamic loading, such as a wheel, which can see over ten million cycles in a lifetime, failure by fatigue damage becomes a concern. More than 90% of material failures during use are due to fatigue [10]. Improved understanding of the fatigue behavior of Mg requires realistic mathematical models that describe the relation between the cyclic deformation and key material attributes. The aim of this research is to use a crystal plasticity finite element (CPFE) code to better understand the effect of crystallographic texture on the high-cycle fatigue (HCF) behavior of dissimilar alloy welds. It will be used to give insight into the effect of texture gradients in the weld on local processes that can potentially result in fatigue performance drops in Mg FSW material in terms of both fatigue life and endurance limit.

1.2 Scope
The study presented herein focuses on the validation and application of a numerical model capable of simulating the elastic and plastic deformation of HCP materials. The scope of the research is:

1. Verification of the CPFE code using published macro- and microscopic deformation data for Mg, in regards to texture based anisotropy.

2. Capture the constitutive response of Mg alloys subjected to cyclic loading tests.
3. Assessment of the effect of texture on the fatigue properties of a Mg alloy FSW based on evidence from the literature.

1.3 Outline

The remainder of the thesis is organized as follows:

- Chapter 2 provides necessary background information about deformation in Mg and its alloys, fatigue phenomena and fatigue behavior in Mg and its alloys and crystal plasticity modeling;
- Chapter 3 details the formulation of the crystal plasticity finite element model including both the slip and twinning schemes;
- Chapter 4 details of the Mg single crystal monotonic tension/compression model methodology and presents the results of the simulations which are compared to current literature;
- Chapter 5 describes in detail the Mg alloy AZ31/AZ80 bi-crystal HCF model methodology and presents results of the simulations;
- Chapter 6 discusses, with reference to current literature, assessment of the model in describing fatigue, the HCF simulation results, application to FSW fatigue properties as well as limitations;
- Chapter 7 summarizes the present work and suggests work for the future.
Chapter 2 - Literature Review

2.1 Deformation Behaviour of Magnesium

Mg has a hexagonal (HCP) crystal structure with a close packed ABABA packing sequence. The primitive HCP unit cell has axes $a_1 = a_2 \neq c$ and the corresponding angles $\alpha = \beta = 90^\circ$ and $\gamma = 120^\circ$. The Mg unit cell has lattice spacing: $c = 5.200 \text{Å}$ and $a = 3.203 \text{Å}$. The c/a ratio is 1.624, which is near the ideally close-packed HCP lattice ratio of 1.633. The HCP unit cell is commonly illustrated by a hexagonal prism because of its symmetry. Fig. 2.1 shows both the primitive cell (heavy lines) and hexagonal prism cell. The prism cell directions and planes are described by the four axis Miller-Bravais crystallographic indices: \{ $a_1,a_2,a_3,c$ \}. Mg has a density of 1.74 g/cm$^3$ and a melting point of 650$^\circ$C.

In an HCP structure the common Burgers vectors are the $\frac{1}{3}(11\bar{2}0)$ $\text{<a>}$-vectors, which define the close-packed direction, and the $\frac{1}{3}(11\bar{2}3)$ $\text{<c+a>}$-vectors. The identified slip systems for HCP materials are summarized in Table 2.1. Slip in Mg has been observed on the basal, prism type I and pyramidal slip systems (Fig. 2.2). The first order pyramidal $\text{<a>}$ slip systems are crystallographically equivalent to a combination of cross-slip on the basal and prismatic slip modes, therefore the basal
and prismatic <a>-type slip systems account for 4 independent slip modes [11]. According to the Von Mises criteria five independent slip systems are necessary for arbitrary deformation in a polycrystalline material [12]. Deformation in the <c>-axis can be accommodated by pyramidal <c+a> slip. Deformation by twinning also plays a role in HCP materials as it can also accommodate shear in the <c>-axis [13].

![Hexagonal prism](image)

Fig. 2.1: The hexagonal prism. [13]

The activity of each deformation mode is controlled by the local stress on the slip or twin system. The resolved shear stress (RSS) on a slip/twin system is the component of the applied stress on the slip plane in the slip direction. An external uniaxial force can be related to the RSS through Schmid’s law:

$$\tau = \frac{F}{A} \cos \phi \cos \lambda$$  \hspace{1cm} (2.1)
where \( F \) is the applied force, \( A \) is the cross-sectional area, \( \phi \) is the angle between the loading axis and the slip plane normal and \( \lambda \) is the angle between the loading axis and the slip direction. The force mapping term \((\cos \phi \cos \lambda)\) is called the Schmid factor. Slip occurs when the RSS on the slip plane reaches the critical value for that particular system called the critical resolved shear stress (CRSS).

Table 2.1: Independent slip systems in HCP materials. [11]

<table>
<thead>
<tr>
<th>Slip system</th>
<th>Burgers vector type</th>
<th>Slip direction</th>
<th>Slip plane</th>
<th>No. of slip systems</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>( a )</td>
<td>( \langle 1\bar{1}2\rangle )</td>
<td>basal (0001)</td>
<td>3 2</td>
</tr>
<tr>
<td>2</td>
<td>( a )</td>
<td>( \langle 1\bar{1}2\rangle )</td>
<td>prism type I {10\bar{1}0}</td>
<td>3 2</td>
</tr>
<tr>
<td>3</td>
<td>( a )</td>
<td>( \langle 1\bar{1}2\rangle )</td>
<td>1st-order pyramidal type I {10\bar{1}1}</td>
<td>6 4</td>
</tr>
<tr>
<td>4</td>
<td>( c+a )</td>
<td>( \langle 1\bar{1}2\rangle )</td>
<td>2nd-order pyramidal type II {11\bar{2}2}</td>
<td>6 5</td>
</tr>
<tr>
<td>5</td>
<td>( c )</td>
<td>( \langle 0001\rangle )</td>
<td>prism type I {10\bar{1}0}</td>
<td>3 2</td>
</tr>
<tr>
<td>6</td>
<td>( c )</td>
<td>( \langle 0001\rangle )</td>
<td>prism type II {11\bar{2}0}</td>
<td>3 2</td>
</tr>
</tbody>
</table>

Magnesium’s observed anisotropic plastic properties are partly due to the stresses required for the movement of different dislocation types through the lattice. The basal slip systems correspond to the close-packed plane and direction. At room temperature the CRSS for basal slip is of the order of 1 MPa and is by far the easiest to activate [6]. Prism \(<a>-slip has been reported when using tension tests with the tensile axis parallel to the basal plane, and results in no RSS on the basal
planes. Investigations found that with increasing temperature, yield stress decreases and ductility increases [14, 15]. Pyramidal \(<c+a>-\)slip has been observed by TEM for Mg single crystals under c-axis compression at higher temperatures. CRSS for non-basal slip systems are temperature dependent [16, 17]. Fig. 2.3 shows the CRSS for the activation of different slip and twin systems in Mg at different temperatures. It can be seen that basal slip is temperature independent. At room temperature, tensile twinning has a CRSS similar to basal slip. Prismatic \(<a>-\)slip CRSS has an inverse relationship with temperature. Pyramidal \(<c+a>-\)slip CRSS has a more complicated temperature dependence where it actually starts increasing at room temperature and then decreases at 400K.

Fig. 2.2: Geometry of common slip planes in HCP Mg. [18]
Fig. 2.3: Temperature dependence of the CRSS for Mg. [19]

Twinning is an important deformation mode in HCP materials for the Von Mises criterion to be satisfied. However twinning is a polar mechanism; it allows shear in only one direction. For tension twinning, the shear strain is 0.129, and the amount of shear accommodation is proportional to the twin volume fraction (TVF) [11]. The maximum elongation that can be produced by complete twinning of a suitably oriented crystal of Mg is approximately 7% [20]. Unlike slip, twinning accommodates shear by lattice reorientation. The twinned region shares lattice points with the crystal on the twin plane. Like slip, the deformation can be described by a plane and a direction. Mg has two common twinning modes, \{10\overline{1}2\}\{10\overline{1}1\} tension twins and \{10\overline{1}1\}\{10\overline{1}2\} compression twins, which are shown in Fig. 2.4. When tension twinning is activated there is a lattice reorientation of 86.3° around the \(\langle 11\overline{2}0\rangle\) axis. For compression twinning there is a
lattice reorientation of 56.2° along the \(\langle1\bar{1}20\rangle\) axis. This reorientation of the crystal may enhance ductility because the twin lattice is oriented favourably to activate slip modes [21]. Tension twinning is very easily activated at room temperature as it has a CRSS close to basal slip [22].

Munroe and Tan [23] have attempted to consolidate work on the anisotropic deformation of different HCP single crystals to produce pole figures that map regions that correspond to favourable slip and twinning modes. The pole figure for Mg-type crystals is shown in Fig. 2.5. Based on tension tests, crystals orientated in region A deform primarily by prismatic or pyramidal slip. In region B twinning is most favourable. In region C double basal slip occurs and in region D single basal slip is the preferred mechanism. They found in compression, twinning occurs in region A; brittle fracture occurs with orientations in region B and the same deformation modes as crystals in tension are active in regions C and D.

Fig. 2.4: Geometry of tension and compression twinning systems in HCP structure materials. [24]
Kelley and Hosford [25] compared the compression deformation of Mg single crystals to highly textured and randomly oriented Mg polycrystals using plane-strain channel-die compression tests. They found that the anisotropic deformation behavior of single crystal Mg was similar to the deformation of textured polycrystals, but not for the random texture. The study revealed that even for orientations that suppressed basal slip there was still evidence that it occurred because its CRSS is so low any misalignment will result in enough RSS for basal slip. They also observed compression twinning followed by tension twinning and basal slip due to reorientation by the twinning process.

Fig. 2.5: Inverse pole figure representing the orientation dependence of different slip modes in Mg. [23]

Pure Mg cannot be used for structural applications due to its low strength and limited ductility and formability at low temperatures [26]. These properties can be improved upon by use of alloying elements. The main alloying elements for Mg are aluminum, zinc and manganese. Aluminum and zinc are used to increase
strength. Zinc is superior in improving strength compared to aluminum. However zinc decreases corrosion resistance, therefore a mixture of zinc and aluminum is preferred [26]. Magnesium alloys with aluminum and zinc elements are designated with two letters, AZ followed by two numbers referring to the nominal compositions of the alloying elements. Aluminum is the main alloying element, in AZ alloys up to 9 wt. %. Zinc is added up to 1 wt. %. Increasing the aluminum content in AZ series has the effect of increasing the material density to an average of 1.8 g/cm$^3$ and decreasing the melting point. Zinc is not known to change the c/a ratio while aluminum has been shown to increase it [27]. Akhtar and Teghtsoonian [27, 28] performed a study to investigate the effects of solid solution in the AZ series on basal and prism slip. They incrementally added small amounts of zinc and aluminum in solution and deformed single crystals oriented to favour basal and prism slip. They observed an increase in CRSS for basal slip for increasing both aluminum and zinc compared to pure Mg. For crystals oriented for prism slip, they found that at temperatures much below room temperature the CRSS decreased with increasing alloy in solid solution. At room temperature and above, the effect was opposite. These studies investigated the effects of very small amounts of alloying elements to preserve single crystals. The effect of alloy content on deformation becomes more complex with the addition of new phases.
There have been extensive investigations into the monotonic mechanical properties of Mg single crystals and alloys [29–32]. Extruded alloys develop a very strong fibre texture, i.e. basal planes parallel to extrusion direction. There are also some basal planes rotated in the transverse direction and almost none in the extrusion direction. When conducting tensile tests on different orientations of extruded Mg AZ31 it was reported that there was a strong anisotropy similar to polycrystalline pure Mg. Agnew and Duygulu [32] did TEM studies and found extensive non-basal slip which suggests that the ratio of prismatic and pyramidal slip to basal are lower in AZ31 than pure Mg. They found that the ratio of prismatic to basal CRSS to be 2-2.5 at room temperature. They also reported a strong temperature dependence on both flow stress and strain rate sensitivity, with flow stress decreasing with increasing temperature. AZ31 has a strain rate sensitivity of 0.02 at room temperature, which is texture dependent [33]. Above room temperature, the strain rate sensitivity increases due to temperature dependent recovery effects. Jain et al. [29] performed tension and compression tests on strongly and weakly textured Mg AZ80 between 77K and 293K. They also found evidence of non-basal slip traces at both temperatures.
2.1.1 Twinning Geometry and Morphology

A thorough review of the crystallography of twinning in HCP materials has been presented by Partridge [13] and Christian and Mahajan [34], and is summarized here. A twin is a region of a crystal in which one part of the lattice is a mirror image of the rest of the crystal with respect to the twinning plane [35]. Unlike plastic slip, which causes a gradual reorientation of the crystal toward an easy glide orientation, twinning causes a swift reorientation in part of the grain at inception with a gradual thickening of the twin with increasing plastic deformation. Fig. 2.6 shows the process of the formation of a twin in a crystal lattice.

![Fig. 2.6: Process of formation of twins. [36]](image)

The twinning shear can be described as the shape change that transforms a sphere into an ellipsoid due to a twinning shear, $s$, as shown in Fig. 2.7. The two lattices have specific crystallographic relationships and are characterized by the parameters $K_1$, $K_2$, $\eta_1$, and $\eta_2$ as depicted in Fig. 2.7. The twinning plane, $K_1$, is the first undistorted plane and the second undistorted plane is $K_2$. The direction of the
twinning shear, \( \eta_1 \) is contained on \( K_1 \) and does not move. The second characteristic direction \( \eta_2 \) is contained on \( K_2 \), which moves from \( \eta_2 \) to \( \eta_2' \) during shear as \( K_2 \) moves to \( K_2' \). A twinning mode is defined when \( K_1 \) and \( \eta_2 \) are fixed, or when \( K_2 \) and \( \eta_1 \) are fixed.

The twinning elements for the most commonly observed twin systems in HCP crystals are summarized in Table 2.2. In Mg and Mg alloys, \( \{10\bar{1}2\} \) c-axis tension twin and \( \{10\bar{1}1\} \) c-axis compression twin are usually observed. A schematic diagram showing the shape change produced by tension twinning in Mg and the twinning elements are shown in Fig. 2.8.

The twinning process can be divided into four stages. In stage one dislocations related to twinning accumulate and a twin zone forms in which a twin may or may not nucleate. In stage two the twin dislocations reach a critical point and a twin is

![Fig. 2.7: Conversion of a sphere into an ellipsoid by the twinning shear. The schematic reveals geometry relationships between twinning shear, s, and twinning parameters: \( K_1 \), \( K_2 \), \( \eta_1 \), and \( \eta_2 \). [13]](image_url)
nucleated. In stage three twins form with a lenticular shape, usually across a whole grain. Finally in stage four the twin thickens [37].

Table 2.2: Crystallographic elements and parameters of twin systems in HCP crystals. [11]

<table>
<thead>
<tr>
<th>$K_1$</th>
<th>$K_2$</th>
<th>$\eta_1$</th>
<th>$\eta_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>{1012}</td>
<td>{1012}</td>
<td>$\pm &lt;10 \bar{1} 1&gt;$</td>
<td>$\pm &lt;10 \bar{1} 1&gt;$</td>
</tr>
<tr>
<td>{1011}</td>
<td>{1013}</td>
<td>$&lt;10 \bar{1} 2&gt;$</td>
<td>$&lt;30 \bar{3} 2&gt;$</td>
</tr>
<tr>
<td>{1122}</td>
<td>{1124}</td>
<td>$\frac{1}{3} &lt;10 \bar{2} 3&gt;$</td>
<td>$\frac{1}{3} &lt;22 \bar{4} 3&gt;$</td>
</tr>
<tr>
<td>{1121}</td>
<td>(0002)</td>
<td>$\frac{1}{3} &lt;\bar{1} \bar{1} 26&gt;$</td>
<td>$\frac{1}{3} &lt;11 \bar{2} 0&gt;$</td>
</tr>
</tbody>
</table>

Fig. 2.8: The shape change produced by tension twinning in Mg. [13]

Studies have shown that the Schmid law applies to both slip and twinning [38–40]. However, other studies suggest that the Schmid factor is not the only factor involved in twin nucleation [37, 41]. Twin nucleation may be influenced by neighboring grains which causes twin nucleation to not follow the CRSS principle. When a twin is formed near a grain boundary (GB) the neighboring grain must
deform to accommodate the shape change. The neighboring grain, in turn, creates a back stress in both the parent and the twin.

2.2 Fatigue

Fatigue is a type of failure that occurs in materials subjected to dynamic and fluctuating stresses, such as cyclic tension/compression, bending or torsion stresses. This causes accumulation of small scale defects over a number of cycles. The micro-defects nucleate from plastic deformation in localized regions, which lead to the formation of micro-cracks or voids which grow and eventually lead to failure. In these circumstances it is possible for failure to occur at a stress level lower than the macroscopic yield strength in static loadings. Fatigue fractures “are responsible for up to 90 per cent of the mechanical failures which occur in service” [10]. Fatigue failure is brittle-like in nature, even in normally ductile metals [42].

Common methods of fatigue testing involve the characterization of total fatigue life, i.e. testing until failure. In these approaches the number of stress or strain cycles necessary to induce complete fatigue failure is measured under controlled amplitudes of cyclic stress or strain. Under high-cycle, low stress (HCF regime), fatigue situations the material deforms primarily elastically. These situations are usually characterized in terms of stress range. Under low-cycle, high stress, fatigue situations the stresses are generally high enough to cause appreciable plastic
deformation prior to failure. Under these circumstances the fatigue life is characterized in terms of the strain range [42].

Stress cycles can be classified into three types. The first type is called a fully-reversed stress cycle. It is a sinusoidal or triangular wave where the maximum and minimum stresses have the same absolute value. The second type is repeated stress cycle, which is also sinusoidal or triangular, where the maximum value and minimum value of stresses are asymmetric relative to zero stress level. In the final type of cyclic mode stress and frequency vary randomly. The three types of stress cycles and parameters used to characterize a cycle are shown below in Fig. 2.9. These cycles are defined by stress, but the parameters can also be applied to strain. The mean stress, $\sigma_m$, is the average of the maximum and minimum stress ($\sigma_{\text{max}}$, $\sigma_{\text{min}}$) in a cycle. The stress range, $\sigma_r$, is the difference between the maximum and minimum stress. The stress amplitude is half of the range and describes how high above or below the stress goes. The stress ratio, $R$, is the ratio of minimum and maximum stress amplitudes.

A common method of characterizing high-cycle fatigue life is through determining the S-N curve. An S-N curve is constructed by loading multiple samples of a material until fatigue failure under stress control. The stress amplitude is plotted against the number of cycles to failure. This test represents a way by which the fatigue life of a material tested under certain conditions can be easily characterized.
and compared to that of other materials and conditions. The curve allows determination of the endurance limit of the material, which is defined as the stress amplitude below which failure due to fatigue effectively never occurs. For some materials there is no well-defined endurance limit. In this case the limit is defined as the stress at which the material survives $10^7$ cycles without failure [43]. Examples of S-N curves with a well-defined and undefined fatigue limit are shown in Fig. 2.10.

A common method of characterizing low-cycle fatigue life is through cyclic stress-strain curves to observe the material’s cyclic deformation behavior. For many engineering materials, after a certain amount of plastic strain, the stress-strain behavior can be different in the reverse direction. This was first observed by Bauschinger performing uniaxial tension-compression tests on iron and steel [44]. It was found that the yield strength of the material was reduced when the load was reversed. This is known as the Bauschinger effect and is schematically shown in Fig. 2.11. Cyclic softening or hardening effects relate to the decreasing or increasing of resistance against material deformation under cyclic loading. The intensity of the effect usually saturates after a certain amount of cycles. Before saturation there is a continual change in dislocation substructure until a stable configuration is reached. The stable configuration is characterized by a closed hysteresis loop [42]. Transient responses by cyclic hardening/softening under
plastic strain control and stress control for uniaxial tests are schematically shown at the Fig. 2.12.

Fig. 2.9: Cyclic loading showing a) reversed stress cycle, b) repeated stress cycle, and c) random stress cycle. [10]

The cyclic deformation behavior is not always symmetric. When cyclic loading is done under stress-control, accumulation of axial plastic strain can occur if the
plastic deformation during the loading portion is not opposed by an equal amount of yielding in the reverse loading direction. This effect is called ratcheting and is shown in Fig. 2.13. It is a result of different nonlinear behaviour of the material in tension and compression. The accumulation of plastic strain in initial cycles depends on the cyclic hardening/softening behavior [45]. This effect usually occurs when applying a repeated cyclic load with a non-zero mean stress, but it can also occur under fully-revered loading, in materials in which pronounced yield anisotropy exists between tension and compression [42]. Ratcheting, which has stabilized is called shakedown i.e. accumulated elongation stops.

There have been many studies on the HCF of Mg alloys [46–51]. Nan and authors [47, 48] preformed studies on the HCF fatigue of extruded Mg AZ31 under stress-controlled rotating-bending fatigue conditions. The alloy formed a lamellar microstructure that was parallel to the extrusion direction. They found that the S-N curve had a well-defined fatigue limit of 120 MPa. This was due to crack propagation being blocked at phase boundaries. Ishihara et al. [46] investigated the effect of the microstructure on the HCF of extruded Mg AZ31. They performed fully reversed fatigue tests on samples parallel and perpendicular to the extrusion direction. They found that the endurance limit of the samples parallel to the extrusion direction was 120 MPa, which corroborates with Nan and authors [47,
The fatigue limit reduced to 90 MPa for the perpendicular orientation as cracks were not being blocked by phase boundaries.

Fig. 2.10: S-N curves for materials with a) defined fatigue limit and b) undefined fatigue limit. [10]

Fig. 2.11: Schematic illustration of the Bauschinger effect. [52]
Fig. 2.12: Uniaxial fatigue test material response: a) cyclic softening and b) cyclic hardening under plastic strain controlled loading and c) cyclic hardening and d) cyclic softening under stress controlled loading. [45]

Fig. 2.13: Schematic of uniaxial ratcheting and influence of hardening/softening behaviour. [45]
Investigations into the cyclic deformation and hardening of Mg single crystals using strain controlled fatigue tests at 0.9% and 0.18% found that the cyclic behavior was dependent on the strain amplitude [53]. At low plastic strain amplitudes of 0.18%, Mg cyclically deforms by single slip, much like a static tensile test, and the hardening rate is very low. At higher plastic strain amplitudes of 0.9% deformation is initially carried by single slip, but then duplex slip is activated and the hardening rate increases. Extensive twinning has been observed at the higher strains. Some evidence of de-twinning was observed, but only to a limited extent suggesting the CRSS for de-twinning is higher than slip. The twinning-detwinning-retwinning process has been observed in Mg single crystals that were oriented for twinning and strained at an amplitude of 0.5% [54]. This process resulted in an asymmetric hysteresis curve (low hardening in tension and high hardening in compression). With increasing cycles there was an accumulation of residual twins and a reduced activity of detwinning. A study by Li on cyclic deformation of Mg single crystals in compression-compression stress controlled tests from 19-97 MPa showed that orientation has a significant effect on cyclic deformation and ratcheting behavior [55]. For crystals oriented for twinning the strain range and ratcheting strain were very small compared to a crystal oriented for basal slip which had a ratcheting strain ten times larger. There was no cyclic
hardening or softening for the twin orientation, however there was cyclic hardening behavior for the basal oriented crystal.

Yu et. al. studied the low-cycle fatigue behavior of pure polycrystalline extruded Mg. Results from fully reversed strain-controlled tests in the extrusions direction of 1.0% and 0.12% strain amplitude [56] showed that, like single crystals, strain amplitude had an effect on cyclic hardening behavior. They reported that at the lower strain amplitude, there was marginal cyclic hardening and at the higher strain amplitude there was cyclic softening at the tensile peak stress and hardening at the peak compressive stress i.e. mean stress relaxation due to the Bauschinger effect. This disagrees with observations of cyclic hardening at the tensile peak in Mg alloys [57, 58]. However, in other similar studies of Mg alloys it was found that at strain amplitudes near 0.5% there was cyclic softening in the first few cycles and then hardening until failure [59–62]. Like single crystals it has been reported that twinning dominates at strain amplitudes above 0.5%. This coincides with cyclic hardening which is thought to be due to the formation and interaction of twins [57, 59, 60, 63]. The endurance limit of Mg alloys is texture dependent. Lv et al. [51] studied the direction dependence of fatigue for rolled Mg AZ31 and found that fatigue properties were slightly better in the TD direction, which had a fatigue limit of 90 MPa compared to 80 MPa in the RD direction. Wu et al. reported that the worst endurance limit was in the ND direction, which coincided with the pyramidal
slip as the dominant deformation mode as opposed to twinning [62]. The twinning-detwinning process has been observed in fatigue testing in the TD and RD directions [60, 61, 64]. This leads to asymmetric cyclic stress strain curves. However, a residual TVF remains after the first few cycles and gradually increases with the number of cycles, resulting in increasing cyclic hardening [57, 58]. Below cyclic strain amplitudes of 0.5% it has been shown that the hysteresis curves are symmetrical and there is no mean strain due to deformation being carried by slip mechanisms [57, 64]. Lin et al. studied the effect of cyclic loading on ratcheting and found that increasing stress amplitude or mean stress increases the ratcheting strain and increasing loading frequency decreases ratcheting strain [65].

Fatigue failure ultimately results from the initiation and propagation of cracks. Fatigue cracks are initiated as a result of local plastic deformation during cyclic loading [42, 66]. Even in materials without defects such as pores or inclusions, fatigue cracks can initiate as a result of persistent slip bands (PSBs). A schematic of a PSB in a polycrystal is shown in Fig. 2.14 [67]. PSBs result from the activity of irreversible dislocation glide during cyclic loading. Fatigue crack initiation can also occur at boundaries such as GBs or twin boundaries or even the boundary between PSBs and the grain matrix [42, 66]. Boundaries are areas of elastic and plastic incompatibility. This results in boundaries becoming areas of stress concentration, which can initiate cracks.
There is likely a connection with both basal slip and residual twins and fatigue fracture. Wu et al. [58] studied the LCF behavior of highly textured Mg ZK60. They found that at strain amplitudes of 1.2% there is a continuous cyclic hardening until failure which is most likely connected to the increasing number of residual twins which were measured using in-situ neutron diffraction. Yang et al. [49] studied extruded AZ31 in the ultra HCF regime. They found that even at very low cyclic stress amplitudes of 90 MPa, localized twinning was activated below the fracture surface and fatigue cracks were found along twin bands. Yu et al. studied the low cycle fatigue behavior of both single [54] and extruded polycrystalline [56] Mg. Slip, twin and crack activity was observed on specimens before failure using SEM. For single crystal fatigue testing they used a strain amplitude of 0.5% and for polycrystalline Mg they used 1% and 0.12%. It was found that in the single
crystals with the c-axis parallel to the loading axis the CRSS of twinning was 2.4 MPa, which is very close to the stress for basal slip, and micro-cracks were observed on both the residual twin boundaries and basal slip bands. The polycrystalline Mg loaded in the extrusion direction showed different behavior depending on the strain amplitude. At the high amplitude of 1% massive twins were formed during loading and cracks are formed along twin boundaries, however at the lower amplitude they reported that crack propagation was dominated by cleavage along slip planes.

2.3 Crystal Plasticity Modelling

The elastic-plastic deformation of crystalline materials is inherently anisotropic, and even more so in low symmetry crystal systems like HCP. Crystal plasticity provides a theoretical framework that links the macroscopic constitutive response to microstructural features to model the plastic anisotropy. Important structural features controlling deformation are the crystal structure and the crystal orientation relative to the deformation, which dictate the slip mechanisms. Grain size and temperature also have an effect. Crystal plasticity has as its origin in Schmid’s law observed in face centered crystals, which states that crystallographic slip is initiated when a CRSS is reached on a slip plane and slip direction [68]. Fig. 2.15
illustrates crystallographic slip in uniaxial tension. The RSS for the uniaxial tensile stress state can be expressed by Eqn. (2.1).

Fig. 2.15: Illustration of Schmid’s law for a uniaxial tensile test. [69]

Constitutive equations are developed from the physics of single crystal deformation and polycrystalline models are developed to capture the interaction of single crystal deformation at different length scales. The oldest crystal plasticity model was proposed by Sachs [70]. Sachs assumed that each grain had the same stress state as the applied macroscopic stress. In the Sachs model, slip will happen on the slip system which features the largest RSS so single slip is preferred. Under this assumption, the equilibrium conditions are satisfied, but the compatibility conditions are unsatisfied. This is known as the lower-bound model because it represents a lower bound on the averaged stress in the polycrystalline aggregate. In contrast, Taylor [71] proposed a model which strictly enforces compatibility by assuming that each grain experiences the same strain state as the macroscopic one.
With the Taylor model the equilibrium conditions are not satisfied. This leads to an upper bound on the average stress of the aggregate.

In crystalline materials, multiple slip systems can contribute to the total plastic deformation. Taylor proposed a time independent approach that assumed that between all possible combinations of slip systems, the set that minimizes plastic work rate is the one that contributes to deformation [71]. Problems arise in the solution when there is a non-unique choice for the set of active slip systems that contribute and therefore an ambiguous change to the lattice. This was solved by Bishop and Hill [72] who proposed a procedure where the maximized plastic work rate determines the stress-strain relationship. A second, time dependent, approach assumes there is no division between active and non-active sets of slip systems. Instead all slip systems are potentially active, depending on the current stress and hardening properties. Once the stress state is known, slipping rates on all possible slip systems are uniquely defined [73]. This physically more realistic scheme is used in the current research. The shear rates can be calculated as follows:

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

(2.2)

where \(\dot{\gamma}_0\) is the reference shear strain rate, \(n\) is the rate controlling exponent, \(\tau^\alpha\) is the RSS on the slip/twin system \(\alpha\) and \(g^\alpha\) is the strength of the system.
The kinematic formulation for the mechanics of crystals, used in the current research, was initially proposed by Rice and Hill [74–76]. In the kinematic equations it is assumed that deformation gradient can be decomposed into an elastic part, which contains reversible stretching and rotations, and a plastic part, which are the permanent deformations caused by slip and twinning (Fig. 2.16). The representative equations were written into a finite element (FE) framework by Asaro and Needleman [73, 77]. In the FE framework of the crystal plasticity problem both the displacement compatibility and the force equilibrium equations can be solved in the weak form at the same time.

![Diagram](image)

**Fig. 2.16**: Schematic illustrating the kinematics of the deformation of a crystalline solid deforming by slip. [77]

In the context of the rate-dependent scheme the strength of the system can evolve with the shear on each slip/twin system. There have been different empirical hardening laws proposed to model the evolution of these systems. The law proposed by Pierce et. al. [78] assumes the system strength is related to the secant
hyperbolic of the total shear strain on the system. The Bassani and Wu [79] hardening law improves upon the secant hyperbolic law by allowing the capture of Bauschinger effects. In the extended Voce hardening law the strength of each system is proportional to the total accumulated shear on all of the systems as follows:

\[
g^\alpha = g_0^\alpha + (g_1^\alpha + \theta_1^\alpha \Gamma) \left(1 - \exp\left(-\frac{\theta_0^\alpha \Gamma}{g_1^\alpha}\right)\right) \tag{2.3}
\]

where \(g^\alpha\) is the CRSS, \(g_0^\alpha\) is the initial CRSS, \(\Gamma\) is the accumulated shear on all slip/twin systems, \(\theta_0^\alpha\) is the initial hardening rate and \(\theta_1^\alpha\) and \(g_1^\alpha\) determine the asymptotic characteristics of hardening. The Voce law has been used successfully in many prior models [80] and therefore is the hardening model used in the proposed research as a first effort.

Unlike slip, deformation twinning causes rapid crystallographic reorientation. The orientation relationship between the matrix and twin region, \(R^{tw}\), is determined as follow:

\[
R^{tw} = 2n^{tw} \times m^{tw} - I \tag{2.4}
\]

where \(n^{tw}\) is the twinning direction and \(m^{tw}\) is the twin plane. The amount of shear on the twin system is correlated with TVF, \(f\), and a reference shear, \(\gamma_0^{tw}\), which is a
characteristic of the material. The above parameters must be incorporated to accurately model twinning.

Van Houtte was one of the first researchers to apply a twinning reorientation scheme in a crystal plasticity framework to brass deformation with the predominant twin reorientation (PTR) method [81]. In Van Houtte’s method, growth of the volume fractions of the twinned regions is tracked in each grain. Using a statistical criterion based on the volume fraction of the twinned regions in the grain and entire polycrystalline aggregate, the entire grain is reoriented into a dominant twin orientation. There are two weaknesses of this scheme. Firstly, for the statistical criterion to be meaningful a large number of grain orientations are necessary. Secondly, the grain is re-oriented based on the increment of TVF in the given time step, which is independent of the deformation history and may not represent the dominant twin system [82]. This scheme was improved upon by Tomé and coworkers [82, 83] with the volume fraction transfer (VFT) scheme. In this scheme the polycrystal is represented as a set of orientations with weights. The orientations remain fixed, but their volume fractions evolve during deformation i.e. the volume fraction of cell “n” in Euler space is transferred to neighbouring cell “m” during plastic deformation. This method results in fewer orientations that must be kept track of. The twinned parts of the grains are re-oriented at the end of each time step to account for multiple active twin systems. Both of these models treat
twins as a new grain that deforms similar to an untwinned grain. The disadvantage to this model is that the twinned region is treated as another grain which is allowed to further slip and twin, which is not physically realistic as twins are small lamellar structures and twinning is difficult [84]. Another model proposed by Kalidindi [84] for a finite element framework treats twinning as a deformation mode similar to slip. Fig. 2.17 shows the deformation gradient when Kalidindi’s twinning model is incorporated as a deformation mode. Plastic slip is considered in both the matrix and twin region. This formulation was successful in modeling texture development in studies carried out on both FCC and an HCP polycrystals [84, 85].

Staroselsky and Anand [86] proposed a rate-dependent approach to simulate the plastic deformation of AZ31B Mg alloy based on Van Houtte’s PTR method. They modified the evolution of the plastic part of the deformation gradient to try to account for grain-boundary sliding. The model was applied to simulate texture evolution and the average stress-strain behavior in Mg rods and plates. The prediction of the macroscopic stress-strain curves for AZ31B did not accurately match experimental data for some loading paths. Lévesque et al. [87] proposed a rate dependent model to study the formability of Mg AM30. The proposed model was successful in predicting the stress-strain curves as well as texture evolution for large strains. Abdolvand and Daymond [88] proposed a rate dependent model to study the effect of GB geometry and crystallographic texture on twinning in HCP
materials. In this model a new ‘child’ grain is nucleated in the ‘parent’ after a certain TVF is reached. Each parent can have multiple twin children. The children are allowed to grow as further twin activity takes place. Volume fraction is transferred from parent to child. With this model it was found that stress concentration at GBs was a controlling factor in twin inception. Zhang and Joshi [89] proposed a model to study Mg in a finite element framework where in twinning is treated as pseudo-slip until a critical TVF is reached and the entire grain or family of grains is reoriented, similar to Van Houtte’s PTR model. This model simulation results accurately matched the stress-strain behavior of channel-die compression tests for single crystal and polycrystal Mg, and consequently this twinning scheme is used in the current research.

Fig. 2.17: Decomposition of the total deformation gradient into the elastic and plastic parts including twinning. [84]
Due to the frequency of failure by fatigue it is important for models to capture the deformation phenomena associated with cyclic plasticity; in particular the Bauschinger effect. The Bauschinger effect can be described as translation of the yield surface which is known as kinematic hardening. An early non-linear kinematic law was introduced by Armstrong and Frederick [90] which allowed for formulation of the back stress tensor as follows:

$$d\alpha = C d\gamma - D\alpha |d\gamma|$$

(2.5)

where $\alpha$ is the back stress, C and D are material parameters and $\gamma$ is the shear strain. This type of model is used frequently as it has the advantage of being easy to implement. This type of model has been used to study the fatigue behavior of HCP materials. It has been validated with extensive comparison against experimental observations for HCF in titanium alloys [91, 92]. A comprehensive review of the capabilities of Armstrong-Frederick type cyclic plasticity models is presented by Jiang and Zhang [93]. Toth and authors [94, 95] reported that the Bauschinger effect can be captured even without a kinematic hardening law, because there was a constraint effect during loading and unloading that resulted in residual elastic stresses in the grains. Guillemer et al. [96] successfully recreated the macroscopic hysteresis curves of extruded pure Mg under small plastic strain control (0.1% and 0.4%) up to 100 cycles using crystal plasticity modelling.
showing the Bauschinger effect and cyclic hardening using an Armstrong-Frederick type relationship.

The twinning-detwinning phenomena has been modelled for HCP materials with an updated twinning scheme that treats twins as a new grain and includes constitutive equations for controlling both the expansion and the shrinking of nucleated twins [96–98]. Wang and authors [97–99] captured the hysteresis curve shape and instantaneous stress gradients associated with twinning and detwinning observed experimentally for extruded Mg AZ31 using strain-controlled simulations.

Cyclic ratcheting has been simulated using crystal plasticity simulations. Yu et al. [100] presented a model for residual twinning that compared well to experimental data for stress-controlled cyclic deformation of Mg single crystals and polycrystalline Mg AZ91. The authors were able to capture the stress rate and mean stress dependence on ratcheting.

In contrast to phenomenological constitutive models recent physics-based crystal plasticity models have attempted to incorporate internal variables. In the case of plasticity the most important microstructural state variable is the dislocation density as the dislocations are the carriers of plastic deformation. Dunne et al. [101] proposed an Orowan-based shear strain rate formulation as follows:
\[ \dot{\gamma}^\alpha = \rho_m^\alpha b \nu^\alpha \]  

(2.6)

where \( \rho_m^\alpha \) is the density of mobile dislocations, \( b \) is the Burgers vector and \( \nu \) is the average velocity of the mobile dislocations. In their study on Ti alloys they were able to look at how the combination of grain orientations influence local stress and accumulated slip distributions. The ‘worst’ combination occurred when a ‘hard’ orientation is beside a ‘soft’ orientation as the accumulation of slip is the highest. This model was extended to experimental observations of fatigue facet formation in titanium alloys. Hazeli et al. [102] used a physics-based model to investigate LCF of Mg AZ31. Their results corroborated the fact that the detwinning mechanism is responsible for the anisotropic hardening behavior during cyclic deformation [97, 98].

### 2.4 Objectives

Significant efforts have been made to evaluate the accuracy and applicability of crystal plasticity models to fatigue loading of Mg and Mg alloys. Models can reasonably capture cyclic deformation behavior in Mg in terms of phenomena such as the Bauschinger effect, hysteresis asymmetry, cyclic hardening and softening and ratcheting. Although there have been many successful studies on modeling fatigue, the literature on modelling fatigue in Mg and Mg alloys is limited and the vast majority are in the LCF regime, which does not accurately replicate the
loading conditions of many materials, cyclically loaded well below macroscopic yield. Therefore, this study represents a step in understanding the influence of microstructure and crystallographic texture on the HCF behavior of Mg alloys.

Studies about the crystal plasticity modelling of fatigue of Mg and Mg alloys were described in Chapter 2.3. Many authors have shown a microstructure dependence on fatigue behavior. However most studies focus on building and developing novel crystal plasticity methods to replicate experimental data and capture the fatigue behavior of materials that have gone through processes such as extrusion or rolling. There remains limited investigation on the variation of fatigue behavior at the meso- or microscopic scale for material that has undergone both complex plastic deformation and is comprised of different alloys, such as is possible with FSW processing and additive manufacturing. Such work would be beneficial to academics and industry as the connection between fatigue properties and microstructure and crystallographic texture would be better understood. The knowledge could be used to improve welding process design.

The purpose of this study is to use crystal plasticity modelling to study the meso- and micro-scale HCF fatigue deformation of a Mg AZ31/AZ80 weld, idealized as a dissimilar alloy bi-crystal. These AZ alloys could be implemented into a car wheel design. AZ31 is a common light weight AZ series alloy that could potentially form the hub. AZ80 is heavier but stronger and could be used for the rim. The model
used in the present study was initially codified by Abdolvand and Daymond [88, 37] to study the monotonic and tension and compression deformation of polycrystalline HCP materials, which includes contributions from both slip and twinning, and a strong focus on zircaloy-2. The model successfully captured macro- and micro-scale deformation such as stress-strain curves, texture evolution, lattice strains and twinning activity in zircaloy-2 under monotonic tension and compression. With the past success, the present study attempts to increase the application of the model to fatigue deformation of Mg bi-crystals. The objectives that outline the numerical targets of the research are:

1. Verify the CPFE code against single crystal monotonic tension and compression data at the meso- and micro-scale.

2. Assess the ability of the CPFE model to capture fatigue deformation behavior such as the Bauschinger effect, cyclic hardening/softening and ratcheting.

3. Capture the effect of crystal orientations on the HCF behaviour of joined dissimilar Mg alloy grains using the verified CPFE code. Specifically, the focus is on mesoscopic strain evolution and residual stress/strain development and microscopic slip/twin activity and shear strain evolution.

4. Assess how the texture would affect the fatigue properties in an actual dissimilar Mg alloy FSW using the fatigue model results.
A phenomenological-based crystal plasticity finite element code is developed to model elastic and plastic deformation, considering both slip and twinning, in HCP single and polycrystalline materials. Plastic deformation of the slip and twin systems is assumed to obey Schmid’s law. The rate-dependent finite element formulation described is capable of accurately capturing the influence of slip and twinning on deformation for low to medium strains.

The constitutive equations are implemented in an implicit finite element code (UMAT) executed in the ABAQUS finite element solver environment. Implicit refers to the finite element analysis where all of the state variables at time $t + \Delta t$ are calculated and updated at the same time. ABAQUS solves for stresses, strains and state variables incrementally. At the beginning of each time increment, ABAQUS provides the UMAT with the strain increment, $\Delta \varepsilon$, the rotation increment, $\Delta R$, and the time increment, $\Delta t$. The UMAT then updates the stress increment and state variables to their values at the end of the time increment. The state variables are the shear strain, shear stress, slip/twin system strength and slip/twin direction and plane normal vector. The UMAT also calculates the Jacobian matrix, which
describes the variation of the strain increment with respect to the variation of the stress increment. All the state variables are written based on the increment of shear strain. The non-linear equations are solved using a Newton-Raphson iterative solution, where an Euler method solution to the shear strain increment is used as an initial guess. An implicit solver is chosen over explicit, because it converges with larger time steps since the results are more stable compared to explicit.

The plastic deformation is assumed to be due solely to the crystallographic dislocation slip and twinning. Deformation by diffusion and GB sliding is not considered. The RSS on a slip or twin system, is assumed here to be the driving force for plastic deformation.

### 3.1 Code Formulation

In this section, the modeling framework used to determine deformation is summarized. The framework of the current model code was initially developed by Huang [103] to capture slip based plastic deformation in FCC polycrystals and updated to include slip and twinning in HCP materials by Abdolvand and Daymond [88].

In the current formulation the deformation gradient, F, can be decomposed into two components:
\[ F = F^e \cdot F^p \]  \hspace{1cm} (3.1) 

where \( F^e \) is the elastic part and \( F^p \) is the plastic part. The total spatial gradient of the velocity, \( L \), in the current state can be written based on \( F^e \) and \( F^p \) as follows:

\[ L = \dot{F}F^{-1} = \dot{F}^e\dot{F}^{-1}_e + \dot{F}^e\dot{F}^p\dot{F}^{-1}_p F^e^{-1} = L^e + F^eL^p F^e^{-1} \]  \hspace{1cm} (3.2)

The intermediate configuration plastic velocity gradient, \( L^p \), is defined as the sum of the crystalline shear displacement rates over all slip and twinning systems [84]:

\[ L^p = \left[ 1 - \sum_{\beta}^{N_{tw}} f_\beta \right] \sum_{\alpha}^{N_{pa}} S_\alpha \dot{\gamma}_\alpha + \sum_{\beta}^{N_{tw}} S_\beta f_\beta \dot{\gamma}_{0_{tw}} + \sum_{\beta}^{N_{tw}} f_\beta \sum_{\alpha}^{N_{ch}} S_\alpha \dot{\gamma}_\alpha \]  \hspace{1cm} (3.3)

where \( \dot{\gamma}_\alpha \) is the shear rate in slip system \( \alpha \), \( f_\beta \) is the contribution to the TVF of twin system \( \beta \), \( \dot{\gamma}_{0_{tw}} \) is the reference shear strain associated with twinning, \( S_\alpha \) and \( S_\beta \) are Schmid factors of slip and twinning systems, respectively. \( N_{pa} \) and \( N_{ch} \) are the number of slip systems available in the parent and child, respectively, and \( N_{tw} \) is the number of twinning variants available in the parent. There are three terms in the right hand side of Eqn. (3.3), the first term represents the contribution of plastic slip in the untwinned zone (parent), the second term represents twinning in the parent and the last term represents slip deformation in the twinned zone (child).

The average Cauchy stress tensor, \( \sigma \), at each material point due to parent and child is:
\[
\sigma = \left[ 1 - \sum_{\beta}^{N_{tw}} f_{\beta} \right] \sigma_m + \sum_{\beta}^{N_{tw}} f_{\beta} \sigma_{tw}^\beta
\] (3.4)

In the current model, the Asaro-Needleman rate dependent formulation is implemented by which all slip and twinning shear rates can be calculated following a power law [73]:

\[
\dot{\gamma}^\alpha = \dot{\gamma}_0 \left\| \frac{\tau^\alpha}{g^\alpha} \right\|^n \text{sign} \left( \frac{\tau^\alpha}{g^\alpha} \right)
\] (3.5)

where \(\dot{\gamma}_0\) is a reference shear rate, \(\tau^\alpha\) is the local resolved shear stress (RSS), \(g^\alpha\) is the current slip or twin system strength and \(n\) is the rate controlling exponent. Twinning is treated as a pseudo-slip system according to the model developed by Kalidindi [84]. The Asaro-Needleman equation has shown the ability to capture the influence of slip and twinning on deformation and texture evolution [73].

RSS, \(\tau^\alpha\), for both slip and twinning, is a function of the imposed stress and the Schmid factor [77]:

\[
\tau^\alpha = P^\alpha : \sigma
\] (3.6)

where \(P^\alpha\) is the symmetric part of the Schmid tensor. In the current model the elastic modulus is not updated. Instead the rotation of the lattice is considered in the stress calculation and in the determination of rate of deformation by updating the slip plane normal and slip direction [104]:
\[
\dot{m}^\alpha = m^\alpha (D^e + \Omega^e)
\]
\[
\dot{n}^\alpha = -n^\alpha (D^e + \Omega^e)
\]

(3.7)

where \(m^\alpha\) and \(n^\alpha\) are the slip or twinning direction and normal to slip/twinning plane, respectively. These vectors define the slip/twinning system \(\alpha\) in the reference state. \(D^e\) and \(\Omega^e\) are the elastic stretching and spin tensors, respectively.

An extended Voce hardening law is used to update the strength of each slip system:

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

(3.8)

where \(g^\alpha\) is the CRSS, \(g_0^\alpha\) is the initial CRSS, \(\Gamma\) is the accumulated shear strain on all slip/twin systems, \(\theta_0^\alpha\) is the initial hardening rate and \(\theta_1^\alpha\) and \(g_1^\alpha\) are the final slope of hardening curve and the scaling stress for work hardening, respectively.

This is a phenomenological hardening law that has been used successfully in many previous models [29, 80, 88, 105]. The evolution of the CRSS on slip/twin system is given by [37]:

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

(3.9)

\[
H_{\alpha\beta} = h_{\alpha\beta} q_{\alpha\beta}
\]
where $h_{\beta\beta}$ is the self-hardening and $h_{\alpha\beta}$ is the latent hardening tensors and $q_{\alpha\beta}$ are constants that allow the interaction of the different slip and twin systems to be taken into account.

### 3.2 Twinning Considerations

Two important aspects of twinning are included in the CPFE implementation to reproduce observed twinning effects: evolution of TVF and the lattice reorientation to reproduce the macroscopic deformation due to twinning. The TVF is related to the strain rate of the twinning systems, $\beta$ [84]:

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

$$
\dot{f}^{\beta} = 0, \quad \text{if } \tau^{\beta} < 0
$$

Eqn. (3.10) requires that the TVF never be negative, the twinned volume never greater than the parent, and no detwinning can occur. The TVF evolution is tracked for each twin system that is evaluated at each material point.

The transformation between the parent lattice and the twinned child lattice is given by the following:

$$
e^{ch}_{i} = R^{tw} e^{pa}_{i}
$$

(3.11)
where $e_{ch}^i$ is the new normal/slip vector in the child, $e_{pa}^i$ is the original vector in the parent and $R_{tw}$ is the twinning rotation tensor. Fig. 3.1 illustrates a grain with a twinned zone and the rotated slip direction and plane vectors [37].

![Fig. 3.1: Twinned and untwinned zone in a grain. [37]](image)

In Abdolvand and Daymond’s [88] original twinning code, the twin (child) and matrix (parent) were treated as separate entities. A twin nucleated after 0.2% TVF was reached at a Gauss point (GP). The initial stress in the new child grain is equal to that of the parent at the time of creation and then the RSS on each slip system is determined based on the new Schmid factors and stresses. In order to allow for relaxation in the child the initial strength and all of the plastic shear strains on all slip systems of the child are set to that of the parent. The new twin orientation is based on the PTR scheme.
This model succeeded in describing the stress-strain response, TVF and lattice strain evolution polycrystalline HCP materials in tension and compression based on matching experimental stress-strain curves.

Fig. 3.2: Schematic illustration of the twinning-induced reorientation process with a single finite element. [89]

In the present study, early attempts to simulate twinning in twin orientated Mg crystals, the twinning description failed. For unknown reasons, crystals oriented for twinning experienced massive hardening which result in unrealistic stress-strain curves. Handling of the twinned zone in the code was re-written in the current research to that proposed by Zhang et al. [89], which is based on the scheme proposed by Van Houtte [81]. Changing schemes resulted in more accurate stress-strain results. The lattice reorientation scheme in an individual element is shown in Fig. 3.2. At each GP the TVF for each twin system is updated every time
increment. When the total TVF of all the twin systems reaches a critical value, $f_{cr}$, the volume represented by that point is rotated from its original orientation to the twin orientation. A flow chart showing the steps through which the software solves the equations is shown in Fig. 3.3.
Fig. 3.3: Schematic diagram showing the steps of calculations that occur in the software when solving for deformation at a GP.
Chapter 4 - Single Crystal Monotonic Deformation Modelling

4.1 Introduction

The code described in Chapter 3 is implemented to model the monotonic deformation of Mg single crystals to verify whether it captures elastic and plastic deformation in Mg and its alloys. The results of the simulations are compared to digitized data extracted from the published tension and compression curves from the following literature on Mg single crystals: Kelley and Hosford [25], Reed-Hill and Robertson [14], and Bhattacharyya [35]. The model results are compared to the reported macroscopic stress-strain response and the underlying microscopic deformation activities are critically corroborated with experimental observations.

Kelley and Hosford [25] investigated the stress-strain behavior of pure Mg single crystals under plane strain compression conditions at room temperature for several different crystal orientations. Four of these orientations are shown in Fig. 4.1. In the figure a solid thick arrow indicates the loading direction, a thin solid line indicates the crystal extension direction and a thick open arrow indicates the plane strain constraints. The constitutive equation parameters from Eqns. (3.5), (3.6),
(3.9) and (3.10) were chosen by modeling these orientations and fitting the macroscopic stress-strain response with the Kelley and Hosford experiments.

Fig. 4.1: Single crystal orientations considered in plane-strain compression simulations. [25]

The experiments by Reed-Hill and Robertson [14] and Bhattacharyya [35] were tension tests, where the tensile axis was in a $\langle 10\overline{1}0 \rangle$ direction for the former, and with the c-axis $45^\circ$ to the tensile axis in the latter.

4.2 **The Model**

The elastic constants used for the simulation were taken from Slutsky and Garland [107] and are shown in Table 4.1. The active deformation modes included in the model are basal, prismatic $<$a$>$-type, pyramidal $<$c+a$>$-type slip and tensile twinning. The deformation due to the pyramidal $<$a$>$ can be reproduced with a
combination of basal and prismatic slip. Compression twinning is not included in the model as it is difficult to measure the CRSS due to brittle fracture and it was found that compression twins do not significantly contribute to c-axis deformation [25].

<table>
<thead>
<tr>
<th>Table 4.1: Mg Elastic Constants [107]</th>
</tr>
</thead>
<tbody>
<tr>
<td>C11 (MPa)</td>
</tr>
<tr>
<td>59400</td>
</tr>
</tbody>
</table>

The initial guesses for the parameter values for pure Mg were based on similar studies by Zhang and Joshi [89]. Final values were found through guess and check trials, wherein the hardening parameters of each system were manually changed incrementally until the stress-strain curves qualitatively matched visually. It was assumed that the self and latent hardening parameters were unity for each deformation mechanism. It was also assumed that each mechanism follows the same hardening rule, Eqns. (3.9) and (3.10). The reference twin shear was taken to be 0.129 [11]. The other model parameter values could be calibrated relatively easily as many of the orientations isolate single slip or twin systems. The most sensitive hardening parameter was the initial hardening rate, \( \theta_0 \), which describes the initial slope of the stress-strain curve at yield. The final values are shown in Table 4.2 and are very close to the parameters found in the work by Zhang and Joshi [89]. The critical TVF, \( f_{cr} \), was found to be 90%. 

54
Table 4.2: Mg Plasticity Parameters

<table>
<thead>
<tr>
<th>Mode</th>
<th>n</th>
<th>$\gamma_0$ (s$^{-1}$)</th>
<th>$g_0$ (MPa)</th>
<th>$g_1$ (MPa)</th>
<th>$\theta_0$ (MPa)</th>
<th>$\theta_1$ (MPa)</th>
<th>$q_{0\beta}$*</th>
</tr>
</thead>
<tbody>
<tr>
<td>Basal</td>
<td>50</td>
<td>0.001</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>Prism</td>
<td>50</td>
<td>0.001</td>
<td>15</td>
<td>75</td>
<td>2000</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>Pyramidal</td>
<td>50</td>
<td>0.001</td>
<td>40</td>
<td>115</td>
<td>3000</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>Twinning</td>
<td>50</td>
<td>0.001</td>
<td>3.5</td>
<td>20</td>
<td>100</td>
<td>0</td>
<td>1</td>
</tr>
</tbody>
</table>

*The latent hardening parameter describes the added hardening that the slip/twin systems experience due to twinning. All other values are set to unity.

The microscopic deformation activities are measured by $\bar{r}^\alpha$, which is the relative activity on slip or twin system $\alpha$, defined as [89]:

$$\bar{r}^\alpha = \frac{1}{V} \int r^\alpha dv$$ (4.1)

where $r^\alpha$ is the relative activity of deformation system $\alpha$ at each GP and $V$ is the total sample volume. The relative activity at each material point, $r^\alpha$, is the ratio of total shear activity of the slip or twin system to the total shear sum on all slip and twin systems at a given time increment. This formulation is shown in Eqn. (4.2) [89]:

$$r^\alpha = \frac{\sum_{i=1}^{N} |\Delta\gamma_{i}^\alpha|}{\sum_{\alpha}^{M} \sum_{i=1}^{N} \Delta\gamma_{i}^\alpha}$$ (4.2)

where $M$ is the total number of slip (3) and twin (1) modes, which is 4, $N$ is the total number of systems in a given slip or twin mode, and $\Delta\gamma_{i}^\alpha$ is the shear strain increment on the slip/twin system $i$ in the mode $\alpha$. 55
4.3 Applied Boundary Conditions

For all of the single crystal tension and compression simulations, orientations were assigned to a cube of 2×2×2 first-order eight-noded elements (C3D8) to permit some stress variation inside of the crystal. The cube of elements representing the single crystal is shown in Fig. 4.2. The following constraints were imposed to suppress rigid body motion and allow for rotations when the crystal is oriented for basal slip:

\[
\begin{align*}
  u_i^E &= 0 \text{ where } i = x, y \\
  u_i^{EFGH} &= 0 \text{ where } i = z
\end{align*}
\]  

(4.3)

where \( u_i^k \) is the displacement of a point/edge/face \( k \), described in Fig. 4.2, in direction \( i \). The elements were loaded on the face in the positive \( z \)-direction. When modelling the Kelley and Hosford experiments [25] the die-channel walls were modelled as surface node displacement constraints as follows:

\[
  u_i^{ABEF} = u_i^{CDGH} = 0 \text{ where } i = x
\]  

(4.4)

For each crystal the loading was controlled by uniaxial strain that was applied on the positive \( z \)-direction face.
Fig. 4.2: The cube of elements representing the Mg single crystals.

4.4 Results and Discussion

4.4.1 Kelley and Hosford [25]

Fig. 4.3 shows the comparison between the Kelley and Hosford [25] average true stress-true strain data and the simulated results. The simulated and experimental data match well. Fig. 4.4 shows the evolution of the relative activities of the slip and twin systems with strain for each orientation. Generally acceptable results were achieved by using the parameters in Table 4.2. The stress-strain curves compared fairly closely; however it is clear that some disparities exist.
Fig. 4.3: Comparison of stress-strain responses from plane-strain compression simulations (solid lines) with Kelley and Hosford experiments (symbols).

In the following sections the results of the macroscopic stress-strain responses and the microscopic deformation activities are discussed for each orientation.
Fig. 4.4: Orientation-dependent relative activities of slip and twin modes versus strain corresponding to the macroscopic responses in Fig. 4.3. Zero system activity is not shown for clarity.

4.4.1.1 Case A (Compression along the c-axis)

Trends that were captured by the model for orientation A were the high yield stress and strong hardening. It can be seen that in the model there is a slight overestimation of the tensile modulus. Fig. 4.4(a) demonstrates that only pyramidal \(<c+a>\) slip, the strongest slip system, accommodated the c-axis compression. This is in agreement with both Zhang and Joshi [89] and Graff et al. [107] who also compared crystal plasticity simulations to the Kelley and Hosford study. Pyramidal \(<c+a>\) slip has also been experimentally observed by Obara et al. [16] for c-axis compression. Kelley and Hosford [25] remarked that the hardening was due to basal slip attributed to a specimen misalignment. It should be noted that Kelley and
Hosford [25] observed some compression twinning, which is neglected in this study, just before specimen fracture.

4.4.1.2 Case B (Compression perpendicular to the constrained c-axis)

Trends that were captured by the model for orientation B were the lower yield stress, compared to orientation A, strong hardening and hardening saturation at about 6% strain. It can be seen that in the model there is a slight underestimation of hardening before the major bend in the stress-strain curve and slight overestimation of hardening after. Fig. 4.4B demonstrates that deformation was initially accommodated by tensile twinning but was then quickly dominated by prismatic slip. In this orientation the Schmid factor for twinning is higher, but is not allowed due to the constraints. This could explain the observed ductility. This result is again in agreement with Zhang and Joshi [89] and Graff et al. [107]. In contrast to the simulations Kelley and Hosford found no traces of prismatic slip for this orientation. They were surprised by these results and reported that this result was likely due to the experimental limitations of the die-channel in constraining tensile twin activation.
4.4.1.3  Case C (Compression perpendicular to the un-constrained c-axis)

Case C had a very low yield stress with initially weak linear hardening at strains below 6%, followed by a sudden increase in stress. The twin induced 90° reorientation activates mostly pyramidal slip to further accommodate deformation and results in a sharp increase of macroscopic stress which is shown in Fig. 4.4C. This is again in agreement with Zhang and Joshi [89] and Graff et al. [107]. The sudden increase in stress is due to the total reorientation of the entire crystal as each GP reaches $f_{cr}$ at the same time due to a homogeneous stress state. This would not be the case in real specimens which have internal heterogeneities and would result in gradual elastic-plastic transition. Kelley and Hosford reported that after the reorientation the deformation characteristics were almost identical to A, which is reproduced in the simulated stress-strain curve. Pyramidal slip is dominant as in orientation A, but there is some prismatic slip which is due to the crystal rotating less than 90° so the constraint is weaker on the prismatic system.

4.4.1.4  Case D (Basal Slip)

Case D had the lowest yield stress and very small linear hardening. Fig. 4.4D demonstrates that basal slip is active over the strain range. Basal is very easily activated in Mg and for orientation D the Schmid factor is the highest. This is
again in agreement with Zhang and Joshi [89] and Graff et al. [107] and only basal slip was reported by Kelley and Hosford [25]. Phenomenologically, basal slip is related to good ductility but low strength.

4.4.2 Reed-Hill and Robertson [14]

Fig. 4.5 shows the comparison between the Reed-Hill and Robertson [14] stress versus elongation data at room temperature and the simulated results. The simulation captures the important trends of Reed-Hill and Robertson’s results and matches generally well. Similar to the Kelley and Hosford stress-strain curve for orientation B, there is a slight underestimation of hardening before hardening saturation and a slight overestimation after.

Fig. 4.6 shows the evolution of the relative activities of the slip and twin systems with deformation of the single crystal. Prismatic slip was the only active system over the strain range. The simulated stress-strain curve is similar to orientation B in Fig. 4.3, which is also dominated by prismatic slip. Reed-Hill and Robertson [14] reported that at room temperature they found evidence of prismatic duplex slip as the dominant slip mode.
Fig. 4.5: Comparison of stress versus elongation responses from a tension simulation with the tensile axis in a (10\overline{1}0) direction (solid lines) with Reed-Hill and Robertson experiments (symbols). [14]

Fig. 4.6: Relative activities of slip and twin modes versus elongation corresponding to the macroscopic responses in Fig. 4.5. Zero system activity is not shown for clarity.

4.4.3 Bhattacharyya [35]

Fig. 4.7 shows the comparison between the Bhattacharyya [35] stress vs strain data and the simulated results. The simulated results again overestimated the tensile
modulus; however, the CRSS of basal slip is so low and so easily activated that non-uniform deformation can occur, and the apparent experimental tensile modulus can actually represent the non-uniform elastic-plastic transition. It can be seen that the simulated results match closely with that of Bhattacharyya up until \( \approx 15\% \) strain after yield. At this point the rate of hardening of the material rises significantly until the model breaks down at \( \approx 27\% \) strain. Fig. 4.8 shows the evolution of the relative activities of the slip and twin systems with strain of the single crystal. Basal slip was the only active slip system over the strain range. This is in agreement with Bhattacharyya [35]. When the c-axis is 45° to the tensile axis the Schmid factor for basal slip is at the maximum of 0.5.

![Graph showing stress-strain response](image)

**Fig. 4.7:** Comparison of stress–strain responses from tension simulation with the tensile axis 45° to the c-axis (solid lines) with Bhattacharyya experiments (symbols). [35]
Fig. 4.8: Relative activities of slip and twin modes versus strain corresponding to the macroscopic responses in Fig. 4.7. Zero system activity is not shown for clarity.

Increasing the number of elements up to 4x4x4 or increasing the order of elements (C3D20) did not affect the point at which there is a strong increase in the hardening rate, which suggests the difference between the hardening in the simulation compared to experiment is either an artifact from the hardening law used, or the model did not fully replicate the experimental conditions. The model breaks down at ≈27% strain. The model is specified for low to medium strains so this point may represent the capability limit of this model [103]. In the literature it has been reported that with saturation type hardening laws, such as Voce hardening, there is a maximum rotation angle before there are no solutions possible [108]. For this crystal there was a rotation of approximately 35°, which could represent the rotation limit. This suggests that a more complex, perhaps dislocation based model, is needed to describe the hardening behavior at such large strain.
4.5 Summary

A phenomenological CPFE model has been used to study the deformation mechanisms of single crystal pure Mg incorporating hardening laws for key slip and twin modes, the parameters of which are derived from experimental observations. Twinning was modeled as an additional slip system. The crystallographic reorientation of the twinned volume was taken into account based on the PTR method after a critical TVF is reached.

The results of simulations of channel-die compression tests and uniaxial tension tests of different orientations have been evaluated and show that, while there are some discrepancies between the model and experimental data when comparing the stress strain behavior, they compare well, both macroscopically and microscopically to experimental results. In the future the hardening parameters could be optimized more rigorously. The results verified that the experimentally observed anisotropy phenomena of Mg, and its alloys can be captured by the CPFE formulation by considering four deformation mechanisms: basal, prismatic and pyramidal slip systems and tensile twinning. This evidence greatly increases the confidence that the model can be successfully applied to more complicated loading conditions in Mg and Mg alloy models.
Chapter 5 - Bi-Crystal Fatigue Modelling

5.1 Model

The purpose of the study is to systematically examine the effects of crystal orientation on the HCF behavior of a dissimilar Mg alloy bi-crystal. The FE fatigue model input consists of two cubic-shaped grains with properties of Mg AZ31 and Mg AZ80 joined together with a flat, planar interface, as shown in Fig. 5.1. The model is deformed cyclically in the z-axis and the orientations are denoted by the angle between the load axis and crystal c-axis. Nine simulations were done using combinations of crystals oriented at 0°, 45° and 90°, as shown in Fig. 5.2. These orientations represent the weakest and strongest orientations, depending on whether the crystal is in tension or compression, and these orientations also readily activate basal slip (45°) and tensile twinning (0°, 90°). Basal slip and twinning have been reported to be the cause of fatigue damage at low stress amplitudes [49, 54, 56, 58]. Combining these orientations could elucidate local behavior that could be detrimental to fatigue performance in a FSW Mg alloy. From here on these bi-crystals orientations will be referred to as the ‘perfect orientations’. Two other simulations were done on bi-crystals with orientations off of these high Schmid factor angles, which were chosen to activate double slip during monotonic
deformation. These cases will be referred to, from here on, as the ‘imperfect orientations’. The imperfect bi-crystal orientations are: AZ31(80°)-AZ80(155°) and AZ31(25°)-AZ80(100°). The present research characterizes both the monotonic and fatigue deformation in terms of mesoscopic and microscopic deformation behavior of the bi-crystals.

Fig. 5.1: FE bi-crystal input: The red grain (left) is AZ31 and the blue grain (right) is AZ80.

Fig. 5.2: Crystal orientations used in simulations. Black arrows represent the loading axis. The orientations are described by the angle of the c-axis and load axis: a) 0° b) 45° c) 90°.
5.2 Simulation Conditions

The constitutive framework used in this section is the same as described in Chapter 3. The current formulation contains a Voce saturation type hardening law, an isotropic hardening law, meaning that the yield surface expands during deformation, but does not translate. A combination of isotropic and kinematic hardening laws is usually necessary to model cyclic deformation phenomena where there is a difference in hardening behavior when the loading path is reversed [93]. Isotropic hardening laws will not properly capture cyclic loading behavior because when the load is reversed the expanded yield surface will not be reached and the material will act elastically. For many cyclic plasticity models the cyclic effects are captured by a kinematic formulation in the hardening law, usually in the form of the Armstrong-Frederick relation for back stress [109, 110]. With the present choice of boundary conditions (BCs) the bi-crystal is constrained in such a way that type-II accommodation stresses are created during loading. These stresses act to translate the yield surface resulting in apparent kinematic hardening [94]. The following constraints were imposed on the bi-crystal surfaces:

\[ u_{ABEF}^x = u_{ADEH}^y = u_{EFGH}^z = 0 \]
\[ u_{CDGH}^x - u_x^H = u_{BCFG}^y - u_y^E = u_{ABCD}^z - u_z^A = 0 \]  \( (5.1) \)
The chosen BCs are representative of the bi-crystal being a unit cell in an infinite medium, which give the bi-crystal the representation of two neighbor grains in a bulk material.

As described above, the load axis is in the z-direction. Fully reversed fatigue loading, $R=-1$, was used for all simulations. The perfect orientation simulations were performed using stress controlled loading with an amplitude of 58 MPa. Stress control is difficult to model for materials with low hardening characteristics due to the nature of the calculations. When ABAQUS calculates values at the start of the time increment it uses an algorithm which outputs an approximation, and the N-R iteration in the UMAT is used to minimize the error. For materials with a low hardening rate, a small increase in stress can result in very large plastic strains. The approximation by ABAQUS will be near the upper bound and errors can accumulate. The error is minimized using small time steps and a Newton-Raphson (N-R) iteration scheme for solving the state variables. A time step convergence study was undertaken where the time step was set at 0.00001 s and raised incrementally until solution convergence no longer occurred, which were steps larger than 0.001 s. Below this step size there were no changes in the shear strain evolution. The present study uses a frequency of 10 Hz, a minimum time step of 0.00001 s, a max time step of 0.001 s and an N-R residual error value of $10^{-10}$. In terms of average stress-strain, convergent results were achieved with each crystal.
having 6x6x6 linear brick elements (C3D8). A strain controlled fatigue simulation of the 90°-45° bi-crystal was carried out, at an amplitude near to that of the stress controlled simulation, and the results were similar, and therefore it is concluded that the stress controlled simulations are stable.

Table 5.1 and Table 5.2 show the single crystal properties used, which were taken from Jain et al. [29] who used similar constitutive equations to compare AZ31 and AZ80 sheet deformation behaviour. The rate sensitivity exponent, n, that is reported is 20 compared to 50 used in the single crystal simulations. The real value from precise mechanical testing of Mg alloys is highly alloy, strain, temperature and orientation dependent and can vary from 10 to 500 [111]. Since the effective shear strain rate for the fatigue simulations is approximately 0.0001/s, and in the quasi-static strain rate range of the monotonic test rates, this difference in n should not noticeably affect the slip rate predictions. The single crystal elastic constants are the same as those used for the single crystal tensile and compression simulations.

For HCF loading the material deforms primarily elastically and fatigue experiments are usually performed below the yield stress under stress control. Modelling in the HCF regime was chosen to more realistically reproduce the approximate loading of an idealized structural component like a car wheel [112].
The 58 MPa stress amplitude used represents an average of 0.9σ_y in the weakest load direction of all the perfect orientation combinations. These values are listed in Table 5.3. The yield strength was calculated using a 0.05% offset method using the stress-strain results from tension and compression simulations on the bi-crystals up to 5% strain. This amplitude was chosen so that the stress level was near the mesoscopic yield point for each perfect orientation bi-crystal, and therefore remains in the HCF regime, yet there would still be microscopic deformation as the stress is above the CRSS of basal slip and tensile twinning. The imperfect orientation bi-crystals are stronger and were loaded with a stress amplitude of 78 MPa. The 0.9σ_y values for these bi-crystals are shown in Table 5.4. A study by Stevenson and Vander Sande suggested detwinning is negligible during fatigue tests [53] while some authors report that TVF steadily increases after approximately 100 cycles under LCF [54, 56, 57, 64]. Loading was done for 1000 cycles to move beyond the regime that detwinning affects fatigue, i.e. the number of cycles beyond which TVF constantly increases.

The study is restricted to the small deformation context by assuming small strain/small rotation plasticity. Using small deformation theory also has the advantage of allowing for larger time steps as compared to finite deformation theory which require much smaller time steps to achieve convergence. The disadvantage of small deformation is that texture changes cannot be captured;
however as the stress amplitude is very near the yield stress of the bi-crystal restricting to small deformation theory is appropriate.

<table>
<thead>
<tr>
<th>Table 5.1: Plasticity parameters for AZ31 [29]</th>
</tr>
</thead>
<tbody>
<tr>
<td>n</td>
</tr>
<tr>
<td>Basal</td>
</tr>
<tr>
<td>Prism</td>
</tr>
<tr>
<td>Pyramidal</td>
</tr>
<tr>
<td>Twinning</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Table 5.2: Plasticity parameters for AZ80 [29]</th>
</tr>
</thead>
<tbody>
<tr>
<td>n</td>
</tr>
<tr>
<td>Basal</td>
</tr>
<tr>
<td>Prism</td>
</tr>
<tr>
<td>Pyramidal</td>
</tr>
<tr>
<td>Twinning</td>
</tr>
</tbody>
</table>

Simulations were run on a Suze Linux 10.1 computer with eight Intel Xeon processors (2.33GHz) and 40 GB of ram. Each 1000 cycle bi-crystal fatigue experiment took approximately 24 hours to complete.

## 5.3 Results

### 5.3.1 Tension/Compression Simulations

Each bi-crystal was loaded in both tension and compression up to 5% strain. The average stress-strain curves for each bi-crystal combination are shown in Appendix A. Single and bi-crystal experimental data for Mg AZ31 and Mg AZ80 are not
available, but the results were reasonable when compared to studies of the stress-strain response of AZ31 and AZ80 sheet material [29]. As expected for HCP materials, there is a strong anisotropy between deformation in tension and compression. Slip and twin activities were also analyzed. The relative activities, of both crystals, after 5% strain are shown below in Table 5.5. In the orientations column the orientation of AZ31 is the first angle and the orientation of AZ80 is the second angle. It should be noted that from here on when orientation combinations are described they will follow this nomenclature. Activity in the AZ31 and AZ80 grains are highlighted in red and blue, respectively. If the slip/twin system is active in both it is marked in green.

<table>
<thead>
<tr>
<th>Orientations</th>
<th>0°-0°</th>
<th>0°-45°</th>
<th>0°-90°</th>
<th>90°-0°</th>
<th>90°-45°</th>
<th>90°-90°</th>
<th>-45°-0°</th>
<th>-45°-45°</th>
<th>-45°-90°</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.9σ_{y,t} (MPa)</td>
<td>62</td>
<td>57</td>
<td>60</td>
<td>80</td>
<td>79</td>
<td>275</td>
<td>56</td>
<td>52</td>
<td>59</td>
</tr>
<tr>
<td>0.9σ_{t,c} (MPa)</td>
<td>380</td>
<td>77</td>
<td>89</td>
<td>66</td>
<td>58</td>
<td>66</td>
<td>60</td>
<td>52</td>
<td>56</td>
</tr>
</tbody>
</table>

Table 5.4: Tensile and compressive yield strengths, 90% σ_{y,t,c}, of the imperfect bicrystal orientations (AZ31 angle-AZ80 angle)

<table>
<thead>
<tr>
<th>Orientations</th>
<th>25°-100°</th>
<th>80°-155°</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.9σ_{y,t} (MPa)</td>
<td>72</td>
<td>106</td>
</tr>
<tr>
<td>0.9σ_{t,c} (MPa)</td>
<td>75</td>
<td>88</td>
</tr>
</tbody>
</table>
Non-uniform deformation was observed in the tension/compression simulations. This has been previously reported in bi-crystals by Lemonds et al. [113] due to strain incompatibilities between crystals. The non-uniform deformation can activate deformation modes with initially smaller Schmid factors. For example, in the 90°-45° bi-crystal tension twinning is activated in the AZ80 grain, which is orientated most favourably for basal slip, and basal slip is activated in the AZ31 crystal that is oriented most favourably for prismatic slip. More double slip/twinning was activated in the 25°-100° and 80°-155° bi-crystals as the orientations do not have a maximum Schmid factor for a single slip or twinning mode. This behavior is also reflected in the yield strengths (Table 5.3, Table 5.4).

<table>
<thead>
<tr>
<th>Orientations</th>
<th>Tension Basal</th>
<th>Tension Prism</th>
<th>Tension Pyr</th>
<th>Tension Twin</th>
<th>Compression Basal</th>
<th>Compression Prism</th>
<th>Compression Pyr</th>
<th>Compression Twin</th>
</tr>
</thead>
<tbody>
<tr>
<td>0°-0°</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>0°-45°</td>
<td>0.5</td>
<td>0</td>
<td>0</td>
<td>0.5</td>
<td>0</td>
<td>0.04</td>
<td>0.48</td>
<td>0</td>
</tr>
<tr>
<td>0°-90°</td>
<td>0</td>
<td>0.4</td>
<td>0.02</td>
<td>0.58</td>
<td>0</td>
<td>0.08</td>
<td>0.48</td>
<td>0.44</td>
</tr>
<tr>
<td>90°-0°</td>
<td>0</td>
<td>0.43</td>
<td>0.04</td>
<td>0.53</td>
<td>0</td>
<td>0.15</td>
<td>0.43</td>
<td>0.42</td>
</tr>
<tr>
<td>90°-45°</td>
<td>0.31</td>
<td>0.38</td>
<td>0.1</td>
<td>0.21</td>
<td>0.5</td>
<td>0</td>
<td>0</td>
<td>0.5</td>
</tr>
<tr>
<td>90°-90°</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>-45°-0°</td>
<td>0.5</td>
<td>0.4</td>
<td>0.094</td>
<td>0.21</td>
<td>0.44</td>
<td>0.06</td>
<td>0.5</td>
<td>0</td>
</tr>
<tr>
<td>-45°-45°</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>-45°-90°</td>
<td>0.24</td>
<td>0.55</td>
<td>0.01</td>
<td>0.2</td>
<td>0.44</td>
<td>0.06</td>
<td>0.5</td>
<td>0</td>
</tr>
<tr>
<td>25°-100°</td>
<td>0.35</td>
<td>0.37</td>
<td>0</td>
<td>0.28</td>
<td>0.65</td>
<td>0.08</td>
<td>0.09</td>
<td>0.18</td>
</tr>
<tr>
<td>80°-155°</td>
<td>0.17</td>
<td>0.82</td>
<td>0.01</td>
<td>0</td>
<td>0.43</td>
<td>0</td>
<td>0</td>
<td>0.57</td>
</tr>
</tbody>
</table>
5.3.2 Fatigue Simulations

5.3.2.1 Average stress/strain

The average axial stress-strain graphs for both the AZ31 and AZ80 grains after 1000 cycles are all shown in Appendix B. Both curves begin at the origin and the AZ80 curve is recorded on top of the AZ31 curve. The average axial stress-strain response is shown for AZ31 at 0° in Fig. 5.3(a)-(c). It can be seen that for all combinations there is a mean positive strain in both crystals; however the ratcheting strain in each cycle is so small the curves appear as a solid band. A Mg crystal loaded in tension parallel to the c-axis is favourably oriented to activate tensile twinning. The positive strain in the AZ31 grain is due to the polar nature of the twins. It can be seen in Fig. 5.3 that the magnitude of the strain accumulation in both grains is dependent on the orientation of the AZ80 grain. The accumulation effect is over twice as strong when AZ80 is at 45°; also there is positive accumulation in the AZ80 grain even when the crystal is oriented for basal slip. Similar trends are observed when AZ31 is 90° except there is compressive accumulated strain. The average stress-strain response curves in the bi-crystals when AZ31 is -45° to the loading axis, all appear practically identical. The average axial stress-strain graphs in AZ31 of the -45°-0° bi-crystal after 1 and 10 cycles is
shown in Fig. 5.4(a) and (b), respectively. Mesoscopic yielding occurs for this group of bi-crystals, which allows for the visualization of the Bauschinger effect.

Fig. 5.3: Average axial stress vs axial strain in AZ31 (blue) and AZ80 (red) after 1000 cycles when AZ31 is 0° to loading axis and AZ80 is: a) 0°, b) 45° and c) 90°.
The strain accumulation can be more easily viewed in terms of the mean strain versus the number of cycles. The mean strain evolution in the different AZ31 grains is shown in Fig. 5.5. The mean strain evolution in AZ31 at 0° and 90° are almost mirror images of each other. The magnitude of the accumulation is slightly lower for 90° because the twin variants are constrained differently. When the c-axis is aligned with the loading axis all twin systems are almost equally constrained and are allowed to activate under tension. When the load is applied perpendicularly to the c-axis the twin variants are constrained in the load axis and the extension is in the y-axis, whose surfaces are constrained by the neighboring grain. Fig. 5.5(c) shows the mean strain in AZ31 when it is at -45°. There is some directional accumulation, which is different depending on the orientation of the AZ80: positive when AZ80 is 0° and negative at 90°, but it is very small compared to the other AZ31 orientations. The 25°-100° bi-crystal also shows little directional
accumulation of strain. The 80°-155° bi-crystal shows some negative accumulation of strain.

Fig. 5.5: Effect of bi-crystal orientations on the mean strain evolution in the AZ31 grains as the orientation in AZ80 is changed for AZ31 at a) 0°, b) 90° and c) -45°.

The final mean strain after 1000 cycles for the perfect and imperfect orientations is listed in Table 5.6 and Table 5.7, respectively. The maximum magnitude of accumulated strain is 0.12% when the bi-crystal is 0°-45°. The next highest is 0.078% for 90°-45°. When the AZ80 is off of 45° the mean strain is approximately half. The mean strain when AZ31 is -45° is 100 orders smaller, which is essentially
negligible. For the 25°-100° bi-crystal there is a small positive mean strain of 3.7E-3% in AZ31 and 1.1E-3% in AZ80. The 80°-155° has net negative mean strain of 0.016% in AZ31 and 0.012% in AZ80. Most bi-crystal orientations demonstrate marginal cyclic hardening in both grains i.e. changes in strain amplitude on the order of microstrain; however, the AZ80 grain in the 90°-45° and 80°-155° orientation show cyclic softening and then marginal hardening. After 1000 cycles the strain amplitude is almost constant for all perfect orientations with an amplitude of approximately 0.115%. When AZ31 is -45° there is practically no hardening, on the order of nanostrain, after the first 50 cycles. This behavior is similar for the 25°-100° bi-crystal. The hardening curve for the 0°-0° bi-crystal is shown in Fig. 5.6. All other mesoscopic hardening curves are shown in Appendix B. The final strain amplitudes of the imperfect orientation bi-crystals are slightly higher around 0.149%. The change in strain amplitude from highest to lowest, in all bi-crystals, is only a difference of a few microstrain. Low hardening is consistent with previous studies on Mg alloys [59, 60, 61, 62] where the hardening is low at low strain amplitudes below 0.5%.
5.3.2.2 Microscopic deformation

The fatigue behavior was also characterized in terms of the microscopic deformation of the individual slip and twin system activities. The simulations were consistent with the literature in that at low strain amplitudes shear is carried by single slip, as expected for the perfect orientations, in this case basal slip and tensile twinning at room temperature. Due to the formulation of the shear strain
rate equation, there is shear on all slip and twin systems even if the system is too hard to activate in reality, though the shear on these hard systems is very small, on the order of $10^{-20} - 10^{-15}$. These systems are defined as inactive.

As mentioned in Chapter 2.2, fatigue fracture is due to accumulated damage from local slip and twinning deformation. A nominal measure of damage accumulation under cyclic loads is cumulative shear amplitude, $T$, which is defined as [42]:

$$T = 4 \sum_{i}^{N} \gamma_{a,i}$$  \hspace{1cm} (5.2)

where $\gamma_{a,i}$ is the shear strain amplitude at cycle $i$ and $N$ is the total number of cycles. Figures 5.7 - 5.10 show the effect of bi-crystal orientations on the evolution of the total cyclic damage in each grain. For the perfect orientations only either basal slip (45°) or tensile twinning (0°, 90°) was activated in either grain. It can be seen in Fig. 5.7 and Fig. 5.8 that the orientation of one grain can have a strong effect on the microscopic cyclic deformation on the other.

Figure 5.7 shows the cumulative shear curves in the AZ31 and AZ80 grains when AZ31 is at 0° and the AZ80 orientation changes. For these combinations shear is always greater in the AZ31 grain. This is to be expected as AZ31 is the weaker material therefore strain will be highest in this grain.
Fig. 5.7: Effect of bi-crystal orientations on the evolution of the total accumulated shear strain amplitude in the AZ31 and AZ80 grains with orientation of AZ31 at 0° and orientation of AZ80 at a) 0°, b) 90° and c) 45°.

When AZ31 is 0° the least amount of cumulative damage occurs in the 0°-90° bi-crystal (Fig. 5.7(b)), with a value of 2.3E-03. For this bi-crystal the damage rate in the AZ31 grain decreases with increasing cycles, demonstrating that cyclic hardening is occurring. Relative to AZ31, there is very little shear strain occurring in the AZ80 grain. For the 0°-0° bi-crystal (Fig. 5.7(a)) the evolution of the hardening behavior is similar in the AZ31 grain until approximately cycle 700 wherein the grain starts to soften. This corresponds with softening and shear
damage accumulation in the AZ80 grain. After 1000 cycles the cumulative shear amplitude damage in AZ31 was 2.6E-03 and was 0.46E-03 in AZ80. Relative to the other bi-crystals, approximately twice as much shear damage accumulates in the AZ31 grain for the 0°-45° combination (Fig. 5.7(c)). The AZ80 grain softens immediately and the rate of shear amplitude accumulation, T, is on the same order as the AZ31 grain.

The trends for the evolution of shear amplitude damage accumulation for AZ31 at 90° (Fig. 5.8) are similar to those when AZ31 is 0°, which is to be expected as twinning is the active deformation mode in AZ31 for both of these orientations. However, there are two main differences. Firstly, the magnitude of the shear damage accumulation is less. Secondly, the AZ80 grain only starts to shear after 500 cycles for the 90°-90° bi-crystal. Like the mesoscopic deformation, these results can be accounted for by the difference in constraints on the twin systems. Tensile twins in Mg and its alloys have six different variants. All six variants are equally active for crystals oriented 0° to the load axis. In comparison, crystals oriented 90° to the load axis have two active variants, [01̅12](0̅111) and [0̅1̅12](01̅11) with all other variants inactive. As only two variants are allowed to accommodate shear in this case this creates a stiffer crystal. Similar to the 0°-45° bi-crystal, as fatigue loading continues the fatigue behavior in the 90°-45° grains
change wherein the AZ31 grain becomes harder while the AZ80 becomes softer. The shear damage accumulation in fact becomes greater in the AZ80 grain compared to the AZ31 grain after 450 cycles.

Fig. 5.8: Effect of bi-crystal orientations on the evolution of the total accumulated shear strain amplitude in the AZ31 and AZ80 grains with orientation of AZ31 at 90° and orientation of AZ80 at a) 0°, b) 90° and c) 45°.
Fig. 5.9: Effect of bi-crystal orientations on the evolution of the total accumulated shear strain amplitude in the AZ31 and AZ80 grains with orientation of AZ31 at \(-45^\circ\) and orientation of AZ80 at a) \(0^\circ\), b) \(90^\circ\) and c) \(45^\circ\).

Fig. 5.10: Effect of bi-crystal orientations on the evolution of the total accumulated shear strain amplitude in each grain in the a) \(25^\circ\)-\(100^\circ\) and b) \(80^\circ\)-\(155^\circ\) bi-crystal.
When AZ31 is at -45° the cyclic shear damage accumulation in AZ31 is not affected by the orientation of the other grain. There is also ten times more shear in these grains than the previous orientation pairs. This is a combination of the softest slip system and the weakest material. There is almost negligible shear in the AZ80 grain for -45°-0° and -45°-90°. Some shear accumulation in AZ80 does occur for -45°-45° after 300 cycles.

The cumulative shear amplitude cyclic damage results can be related to the evolution of the shear strain amplitudes in each grain. Fig. 5.11 shows the evolution of the shear strain amplitude in each grain when AZ31 is at 0°. The other shear strain amplitude curves are shown in Appendix B. When AZ80 is the same orientation as AZ31, 0°, there is softening in AZ80 until the shear amplitudes are similar. For AZ80 at 45° the AZ31 grain actually becomes softer in terms of shear amplitude. The shear strain amplitude in the AZ80 grain becomes higher than the AZ31 grain. When AZ80 is 90° the shear strain amplitude is very small. Final shear strain amplitudes of both grains are higher when AZ80 is a softer orientation. The shear strain amplitude after 1000 cycles in each grain for the perfect orientations is listed in Table 5.8. Shear damage accumulation for each perfect orientation combination is listed in Table 5.9.
Table 5.8: Cyclic shear amplitude in the perfect orientation bi-crystals after 1000 Cycles

<table>
<thead>
<tr>
<th>Orientation</th>
<th>0°-0°</th>
<th>0°-45°</th>
<th>0°-90°</th>
<th>90°-0°</th>
<th>90°-45°</th>
<th>90°-90°</th>
<th>-45°-0°</th>
<th>-45°-45°</th>
<th>-45°-90°</th>
</tr>
</thead>
<tbody>
<tr>
<td>AZ31 (E-7)</td>
<td>2.30</td>
<td>8.65</td>
<td>1.40</td>
<td>0.93</td>
<td>7.25</td>
<td>1.11</td>
<td>58.5</td>
<td>58.0</td>
<td>58.5</td>
</tr>
<tr>
<td>AZ80 (E-7)</td>
<td>1.72</td>
<td>9.45</td>
<td>6.65E-4</td>
<td>0.02</td>
<td>9.00</td>
<td>0.43</td>
<td>1.19</td>
<td>5.90</td>
<td>0.06</td>
</tr>
</tbody>
</table>

Table 5.9: Cyclic shear damage accumulation, T, in the perfect orientation bi-crystals after 1000 Cycles

<table>
<thead>
<tr>
<th>Orientation</th>
<th>0°-0°</th>
<th>0°-45°</th>
<th>0°-90°</th>
<th>90°-0°</th>
<th>90°-45°</th>
<th>90°-90°</th>
<th>-45°-0°</th>
<th>-45°-45°</th>
<th>-45°-90°</th>
</tr>
</thead>
<tbody>
<tr>
<td>T, AZ31 (E-3)</td>
<td>2.61</td>
<td>4.92</td>
<td>2.30</td>
<td>1.31</td>
<td>3.23</td>
<td>1.40</td>
<td>91.6</td>
<td>91.5</td>
<td>91.6</td>
</tr>
<tr>
<td>T, AZ80 (E-3)</td>
<td>0.46</td>
<td>4.10</td>
<td>1.1E-3</td>
<td>1.12E-2</td>
<td>3.60</td>
<td>0.11</td>
<td>7.5E-2</td>
<td>2.52</td>
<td>2.30E-2</td>
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</table>

Fig. 5.11: Effect of bi-crystal orientations on the evolution of shear strain amplitude in the AZ31 and AZ80 grains with orientation of AZ31 at 0° and orientation of AZ80 at a) 0°, b) 90° and c) 45°.
The cyclic shear damage accumulation curves for the imperfect orientation bi-crystals are shown in Fig. 5.10. Like 90°-45°, the AZ80 grain becomes softer than AZ31 in 80°-155°, and similar to 45°-90°, all damage appears to occur in AZ31 for 25°-100° only it does it much quicker in the 80°-155° bi-crystal. The cyclic shear amplitudes after 1000 cycles are shown in Table 5.10. For these bi-crystals both slip and tensile twinning is activated in each grain, however one deformation mode contributes vastly more to the total deformation. Table 5.11 shows the contribution to total cumulative shear amplitude damage from basal and twinning modes in each grain. For the 25°-100° bi-crystal basal slip is mostly activated in AZ31, and tensile twinning in AZ80. For the 80°-155° bi-crystal twinning is mostly activated in AZ31, and basal slip in AZ80.

<table>
<thead>
<tr>
<th>Orientations</th>
<th>25°-100°</th>
<th>80°-155°</th>
</tr>
</thead>
<tbody>
<tr>
<td>AZ31 (E-7)</td>
<td>58.0</td>
<td>1.07</td>
</tr>
<tr>
<td>AZ80 (E-7)</td>
<td>1.59E-2</td>
<td>5.10</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Orientation</th>
<th>Basal</th>
<th>Twinning</th>
</tr>
</thead>
<tbody>
<tr>
<td>T, 25°-100° (E-3)</td>
<td>87.2</td>
<td>0.24</td>
</tr>
<tr>
<td>T, 80°-155° (E-3)</td>
<td>1.72E-04</td>
<td>1.01</td>
</tr>
</tbody>
</table>
As discussed in Chapter 2.2 there is a connection between twinning and fatigue fracture. Table 5.12 and Table 5.13 list the TVF after 1000 cycles for each perfect orientation and imperfect orientation bi-crystal, respectively. The highest TVFs are in AZ31 for the 0°-45° and 90°-45° combinations with 1.9% and 1.3%, respectively, which is to be expected as these bi-crystals had the highest shear accumulation due to twinning. Changing the orientation from 45° cuts the TVF to about half of that value. Very little twinning occurs in the AZ80 grain. Basal slip may dominate in AZ31 for the 25°-100° bi-crystal but there is still a non-negligible TVF, 0.093%, after 1000 cycles. For the 80°-155° there is approximately 3 times less TVF in AZ31; however it is difficult to compare final values as the stress amplitudes are different.

<table>
<thead>
<tr>
<th>Orientation</th>
<th>0°-0°</th>
<th>0°-45°</th>
<th>0°-90°</th>
<th>90°-0°</th>
<th>90°-45°</th>
<th>90°-90°</th>
<th>-45°-0°</th>
<th>-45°-45°</th>
<th>-45°-90°</th>
</tr>
</thead>
<tbody>
<tr>
<td>TVF, AZ31 (%)</td>
<td>1</td>
<td>1.9</td>
<td>0.91</td>
<td>0.49</td>
<td>1.3</td>
<td>0.51</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>TVF, AZ80 (%)</td>
<td>0.18</td>
<td>0</td>
<td>4E-4</td>
<td>4E-3</td>
<td>0</td>
<td>0.04</td>
<td>0.015</td>
<td>0</td>
<td>0.005</td>
</tr>
</tbody>
</table>

Table 5.13: TVF in the imperfect orientations after 1000 Cycles

<table>
<thead>
<tr>
<th>Orientations</th>
<th>25°-100°</th>
<th>80°-155°</th>
</tr>
</thead>
<tbody>
<tr>
<td>TVF, AZ31 (%)</td>
<td>0.093</td>
<td>0.34</td>
</tr>
<tr>
<td>TVF, AZ80 (%)</td>
<td>0.001</td>
<td>7.3E-3</td>
</tr>
</tbody>
</table>
Chapter 6 - Discussion

6.1 Model

The crystal plasticity code of Abdolvand and Daymond [37, 88] was originally developed to describe monotonic loading in HCP metals. In Chapter 4 it was demonstrated that the code achieves generally acceptable results in the modelling of monotonic deformation of Mg single crystals by comparing well with single crystal tension and compression experiments. The present study assessed the model’s ability to simulate fatigue. Successful modelling formulations for uniaxial fatigue loading must capture the following cyclic deformation behavior: the Bauschinger effect, cyclic hardening/softening and ratcheting. It can be seen in Fig. 5.4, Fig. 5.6 and in Appendix B that cyclic hardening and the Bauschinger effect is captured. However, the cyclic hardening is very low and the shear strain amplitudes quickly evolve towards negligible values. This suggests that the bi-crystals deform almost elastically. This may be due to the constraints used, which represent the two grains being unit cells in the bulk, being more stiff compared to constraints representing a more realistic polycrystalline material. However, again, significant shear strain is not expected at a low stress amplitude. In strain controlled studies of polycrystalline Mg alloys, at strain amplitudes of around
0.1%, the hysteresis curves are small or even appear elastic and hardening is marginal [53, 56, 57]. However, it is difficult to conclude whether this model accurately captures true Mg alloy cyclic behavior as the author is unaware of any experimental or modelling literature which reports on the cyclic hardening or evolution of the shear strain damage under stress control. There have been models which have matched macroscopic cyclic deformation in extruded Mg [96], although this was in an LCF regime only up to 100 cycles. Further fatigue studies need to be done with the model and compared to experimental fatigue studies to further verify and elucidate the capabilities of the crystal plasticity code.

Monotonic and cyclic loading have inherently different hardening behaviors. The hardening parameters for AZ31 and AZ80 were taken from monotonic experiments and therefore the cyclic behavior will most likely be quantitatively different. Although the absolute value of the results cannot be verified with experimental data this study demonstrates that the current formulation can capture cyclic deformation phenomena and therefore the results can provide some insight into local cyclic deformation behavior of dissimilar Mg alloys.

In future studies the bi-crystal could be constrained by a layer of elements that represent the average material properties. This would be a more realistic representation. However, the disadvantage to both of these constraint schemes is that surface effects cannot be modelled. Surface roughness has a strong effect on
fatigue as PSBs move to the surface and create steps which cause stress concentrations. Even freeing one surface can potentially change the type-II stresses and the cyclic deformation phenomena may be lost. The Armstrong-Frederick relation is a non-linear kinematic hardening model that is based on a mechanism of strain hardening and dynamic recovery, through the inclusion of a back stress term, and has been used in many cyclic loading models to capture the fatigue phenomena [93]. It is possible that if an Armstrong-Frederick relation was included in the model formulation, the cyclic deformation response could be tailored to match those observed in experiment in a way that changing the surface constraints cannot. A back-stress term would model kinematic hardening without the need of surface constraints, which would allow the study of free surface effects on fatigue.

6.2 Perfect Orientations

Ratcheting effects at the mesoscopic level occur due to tensile twinning. Twinning is activated in grains oriented with components of the c-axis either parallel or perpendicular to the loading axis. Tensile twinning causes an apparent ratcheting effect due to its polar nature, wherein they only increase in the positive direction. It has been reported in polycrystalline Mg alloys that there is no observable macroscopic mean strain in the hysteresis curves below 0.5% strain amplitude [57,
In this study the strain amplitude was approximately 0.155%, well below this value, yet there was significant mesoscopic ratcheting. This is most likely due to the perfect orientation bi-crystal grains being oriented for the twinning systems to have the highest Schmid factor where the c-axis is perfectly parallel or perpendicular. In a polycrystalline material the majority of grains will not be perfectly aligned for twinning and therefore the ratcheting effect will be weakened. Ratcheting could also be affected by the twinning-detwinning effect. Detwinning is not included in the present model; however, the stress amplitude in this study is low and only activates single slip and twinning, which have similar CRSS. The CRSS to activate detwinning is unknown; however it has been reported that the stress to activate detwinning is higher than twinning and therefore de-twinning may not be activated in the bi-crystals [53].

It can be seen from the monotonic stress-strain curves in Appendix A that two yield events occur due to a neighboring grain effect. The first yield event represents yield from the weakest orientation. Hardening after the first event is dependent on the deformation behavior of the neighbor grain. From Table 5.5 it can be seen that when there is only twinning and/or basal slip the material yields relatively quickly and there is limited hardening. This is to be expected as these systems have the lowest CRSS and limited hardening, which is derived from the hardening parameters in Table 5.1 and Table 5.2. When the neighbor grain is in a
harder orientation, which activates prismatic or pyramidal slip there is initial yield and then relatively strong hardening since both grains are constrained to deform together. The second yield event represents yield of the harder orientation. This neighbor effect, wherein the harder grain shields the weaker grain, has a significant effect on the fatigue deformation behavior of the bi-crystals in terms of the amount of shear strain that occurs when loading is in a certain direction.

The results show that the amount of ratcheting depends on the combination of bi-crystal orientations even if one of the grains remains in the same orientation i.e. the ratcheting is stronger in 0°-45° than 0°-0°. It is also seen that ratcheting occurs even in a 45° orientation, which would not normally show ratcheting, if the neighboring crystal is oriented for twinning. This is due to the neighbor effect that was seen in the monotonic bi-crystal simulations. For this purpose, the change in ratcheting behavior when AZ31 is 0° is considered. When the 0°-45° combination is in tension both grains are soft as twinning is activated in AZ31 and has a similar CRSS to basal slip in AZ80, which are 31 and 33 MPa, respectively. For two soft orientations lots of twinning can occur in AZ31 and there is a strong ratcheting effect. In the 0°-0° or 0°-90° the AZ80 grain is relatively stronger and the neighbor grain hardens AZ31 which leads to less twinning. Ratcheting is higher in 0°-0° where both grains are oriented for tensile twinning, and since strain is not recovered in one of the directions, the AZ80 grain eventually softens. Ratcheting
also occurs in the AZ80 grain even when it is orientated for basal slip, which
deforms isotropically, independent of the load direction. This can be explained by
the anisotropy of the neighbor grain. In the compression direction, twinning cannot
be activated in AZ31 when it is 0°. The Schmid factor is largest on the pyramidal
system which has a CRSS of 163 MPa, much larger than the CRSS for twinning.
Therefore, there is strain shielding of the AZ80 grain and the positive strain cannot
be totally recovered. Ratcheting occurs even when there is no apparent
microscopic deformation, i.e. AZ80 grain in 0°-90° bi-crystal. The AZ80 grain has
a shear strain amplitude of effectively 0. Since strain cannot be recovered due to
twinning in AZ31, and there is no deformation for compressive loading, this is an
elastic strain due to AZ31 “pulling” on the neighboring grain.

Hardening effects due to neighbors are also manifested in the microscopic
deformation. The cyclic cumulative shear damage curves (Fig. 5.7 - Fig. 5.9) show
a pattern wherein there is more overall deformation when both grains have weak
orientations compared to when there is a combination of weak and hard
orientations. The “hard” grain causes the “soft” grain to harden, which is usually
AZ80 and AZ31, respectfully. However, this effect also works vice versa where
the “soft” grain softens the hard grain. This hardening/softening effect can be seen
in the evolution of the shear strain amplitudes of the bi-crystal when AZ31 is 0°
(Fig. 5.11) and Appendix B. For the 0°-45° and 90°-45° combinations the shear
strain amplitude actually becomes higher in the AZ80 grain than the AZ31 grain. This effect may be due to the relative CRSS of twinning and basal in each grain, the microscopic hardening behavior of twinning that is unrecoverable, or a combination of both. It remains beyond the scope of the present study to fully explain this phenomenon. For some of the bi-crystals, like AZ31 at -45°, no softening is observed in the AZ80 grain, suggesting that if the difference in strengths in the grains is too large softening will not occur in the harder grain. Fig. 5.6 and Appendix B suggest the microscopic deformation in the grains of all bi-crystals occurs in such a way as for both grains to evolve toward similar mesoscopic strain amplitudes.

The cyclic cumulative shear amplitude damage, T, curves are a nominal measure of the global damage due to fatigue shear. It does not necessarily accurately portray fatigue damage, because at small strain amplitudes a significant fraction of dislocation motion is reversible [42]. This is not the case with twins as they are polar in nature. Significant T values were observed in AZ80 when AZ31 is oriented for twinning and AZ80 is oriented for basal slip. Shear in the AZ80 grain does not represent reversible slip, for these orientations, as strain is not recovered due to the hardening from the AZ31 grain during loading in the reverse direction. The highest cumulative shear amplitude values are achieved in AZ31 when it is oriented for basal slip. This slip is reversible and therefore these values may not
accurately describe fatigue damage. What the cumulative shear strain amplitude curves do show is that shear strain localization occurs in this group of bi-crystals, where almost all of the strain occurs in the AZ31 grain. This is similar to the 0°-90° and 90°-0° bi-crystals.

As mentioned in Chapter 2.2 the local mechanisms for crack initiation, which ultimately cause fatigue failure, are PSBs, twin boundaries and GBs. These act as stress concentration sites due to elastic and plastic strain incompatibility. PSBs and twin boundary formulations are not explicitly defined in this model. The reorientation of the matrix due to twinning would essentially create a boundary, as a twin reorientation would essentially represent a new grain. A reorientation event only occurs when a TVF of 90% is achieved; however, only a maximum TVF of less than 2% is achieved in the present study. The GB is represented by the interface between elements of different orientations. It was found in this study that no apparent stress concentrations were formed at the GB. The axial stress and axial strain for the bi-crystals with the most shear deformation (0°-45° and -45°-45°) after 1000 cycles are shown in Fig. 6.1. There are some stress concentrations but they are concentrated at the constrained surface, in the corners, and not particularly at the GB. The concentrations are due to the basal planes want to shear and rotate but are not allowed due to the surface constraints. No areas of stress concentration occur when the grain is oriented for twinning. The areas of stress concentration are
very small, on the order of $5 \times 10^{-3}$, in either tension or compression. The areas of stress concentration is residual stress caused by the BCs and is created after the first cycle, which essentially integrates them into the BCs. When the stress is at a peak or trough there is no appreciable effect on the bi-crystal stress state. The average stress without surface concentrations was measured in the $-45^\circ -45^\circ$, as it had the highest stress concentrations, by not including the surface nodes when calculating the bi-crystal stress state. When the bi-crystal is in an unloaded state, at the end of a cycle, the surfaces cause a 100% increase in the average residual axial stress; however, since the stress values are on the order of kPa and would be unable to activate any slip or twin system.

For $0^\circ -45^\circ$ the strain appears homogeneous throughout each crystal. For $-45^\circ -45^\circ$ there are small strain gradients, but these are also at the surface and not the GB. This may mean that the present model is inappropriate to capture this behavior, however the stress amplitude used in the simulation is low and possibly below the fatigue limit, meaning that failure would occur only after $10^6$ cycles. Strain controlled experiments on pure polycrystalline Mg found that at amplitudes of 0.12%, close to 0.115% reported here, damage could not be resolved until 70% of total fatigue life which is approximately 10000 cycles [56]; however, it was found that after 10000 cycles that, while there was a linear increase in shear strain, there still were no apparent changes in the contour plot for the $90^\circ -45^\circ$ bi-crystal.
Different damage criterions may need to be included in the constitutive formulation for HCF damage mechanisms.

Fig. 6.1: The axial stress in a) 0°-45° c) -45°-45° and axial strain in b) 0°-45° d) -45°-45° after 1000 cycles. Stress units are in MPa.

Although stress gradients do not appear in the model, trends in the macroscopic deformation can be used to assess what orientations could be the most susceptible to crack initiation events, and therefore which orientations have a poor fatigue endurance limit in a dissimilar Mg alloy FSW. In extruded Mg alloys with strong basal texture, tensile twinning is the major deformation mode under HCF in the extruded direction, and cracks have been observed along twin bands. When there is
a random texture, basal slip has been reported at the surface during HCF [114]. FSW results in a mixing of material chemistry as well as significant texture changes. Texture affects the activation of different deformation modes. Strain localizes quickly in the interfaces at yield during tensile deformation, which implies that the texture change across an interface has a strong effect on deformation [8]. The texture change may increase basal slip. The orientations in this study are those that activate these deformation modes and may have a strong effect on fatigue life and endurance limit. However deformation under fatigue loading is much more complicated than under monotonic loading due to the inherent anisotropic nature of HCP materials.

Tensile twinning shear is highest in AZ31 at 0° or 90° when the AZ80 grain is oriented for slip at 45°. This bi-crystal can develop twice as much TVF compared to different orientations of AZ80. While 1.3-1.9% TVF appears low, it is a reasonable value at strain amplitudes of 0.155% [115]. However, this amount of TVF would be difficult to resolve in an experiment due to the heterogeneous nature of the deformation. A significant amount of twins and twin boundaries could be formed which could result in poorer fatigue life. It was also found that for these bi-crystals, basal slip was not wholly reversible. Irreversible slip results in PSBs which are areas of stress concentration. PSBs also cause strain incompatibility when they interact with GBs. For these reasons it is predicted that grains that are
0°-45° or 90°-45° to the load axis are detrimental to fatigue performance. Bi-
crystals with AZ31 oriented for basal slip may also be detrimental to fatigue
performance. When AZ31 is oriented for basal slip almost 100% of the
microscopic deformation is contained in that grain and had the most amount of
strain amplitude damage. This could cause high strain incompatibility with the
neighboring grain, and hence the GB between AZ31 and AZ80 would be an area
for high stress concentration and therefore a site for crack nucleation.

6.3 Imperfect Orientations
After FSW the resulting textures in the grain-grain interface will mostly consist of
imperfect orientations. The imperfect orientations elucidate how the fatigue
behavior changes as the Schmid factor on the slip and twin systems changes.
Macroscopically it can be seen from Table 5.3 and Table 5.4 that rotating the
orientation slightly away from the ideal angle increases the 0.9σy significantly
when compared to the perfect orientations which are closest to them (45°-90° and
90°-45°). In either tension or compression to medium strains in the imperfect
orientations, both tensile twinning and basal slip occur in AZ31 and AZ80 in fairly
equal amounts. However, for the stress amplitude near the yield point, one system
is much stronger than any of the others and single slip or twinning occurs similarly
as to the perfect orientations. The 25°-100° bi-crystal suggests that since basal slip
in Mg is activated so easily, there is a certain orientation in which it will become
the dominate deformation mode, which will cause the 25°-100° to behave similarly
to 45°-90°. Further studies would be needed to see at which orientation basal slip
begins to dominate. The fatigue behavior of the 80°-155° bi-crystal behaves
similarly to the 90°-45° bi-crystal. Similar to the 90°-45° bi-crystal, the AZ80
grain becomes softer in terms of the evolution of the shear strain amplitude as seen
in Appendix B and Fig. 5.10(b). The change in orientations acts to increase the
difference in the relative level of hardening between AZ31 and AZ80 compared to
90°-45°, which is likely due to AZ31 showing less twin accumulation at 80°
compared to 90°. The final shear amplitude in each grain in the 80°-155° grain is
1.07E-7(AZ31) and 5.10E-7(AZ80) compared to 7.25E-7(AZ31) and 9.00E-
7(AZ80) in the 90°-45°. While 80°-155° is a stronger bi-crystal, it is difficult to
determine whether it would result in better fatigue properties as there are two
competing fatigue mechanisms. There is a smaller rate of increasing TVF in AZ31;
however deformation could potentially localize in the AZ80 grain causing strain
incompatibilities or basal PSBs.

6.4 Modelling Limitations

Crystal plasticity models can be used to understand the contribution of material
properties on fatigue deformation at different length scales. However, it is difficult
to capture every phenomenon. The model used in this study is no exception. For fatigue deformation, detwinning has been observed in many studies [54, 58, 62]. De-twinning is not included in the formulation. Although as previously mentioned, de-twinning may be negligible for the stress amplitudes used in this study as the CRSS may be too high to activate. For uniaxial simulations the effect would most likely also be negligible as this phenomenon has mostly been observed for experiments with strain path changes [105]. A detwinning scheme is necessary to fully capture cyclic deformation of Mg at higher stresses, which causes an asymmetric hysteresis curve. This has been implemented in other crystal plasticity models [97, 98] and could be added to the present code for future studies.

Twinning itself is not wholly understood and as discussed in Chapter 2.3 there have been many proposals to model the effects of twinning [81, 82, 84, 86, 88, 89]. The scheme in the present research is that proposed by Zhang and Joshi [89] wherein twinning is treated as pseudo-slip and rotation occurs after a critical amount of TVF. This scheme was chosen because it recreated the macro and microscopic deformation of an Mg single crystal in plain-strain compression oriented for twinning and was therefore concluded as an appropriate scheme. It captures an average value of stress relaxation due to twinning and evolution of TVF; however, it is a wholly simplistic view of twinning. This scheme does not realistically describe twin nucleation, growth or structure. In the current scheme,
twin boundaries arise during reorientation of a discrete volume represented by a GP after a TVF of 90% is reached. Twins nucleate as a small lenticular structure and grow with more deformation. The initial scheme implemented by Abdolvand and Daymond [88] in their polycrystalline model included twin nucleation and growth, but broke down when applied to single crystals. Further work should be done on implementing a more realistic twin scheme that can properly capture twinning effects in Mg.

In the HCF regime, fatigue fracture is dominated by crack initiation [92]. To accurately capture this phenomenon crack initiation criteria must be included in the model formulation. While the microscopic deformation obtained from the present model may be used to infer fatigue performance, a crack initiation criterion would allow for fatigue life studies. The model could be further improved by accounting for size effects (Hall-Petch effects), which could be significant for heterogeneous twinning reorientation events because of the creation of new grains. Temperature dependence of the deformation modes would also be an important extension as the model could then be applied to study the temperature effects on fatigue. The activities of the slip and twin modes are controlled firstly by the CRSS of each system and secondly by the hardening of the systems. It has been suggested that the self and latent hardening parameters of Mg slip and twin systems most likely evolve during deformation [116], therefore the Voce hardening law, Eqn. (3.9),
and/or evolution of the hardening, Eqn. (3.10), may be too simple to wholly describe the fatigue behavior.

The model in the present research is used to study the meso- and microscale fatigue deformation of a dissimilar alloy bi-crystal. Even with modern techniques, it is difficult to impossible to resolve mesoscale microstructure changes and grain scale stress-strain states in the bulk material. Modern microscopy techniques can study in-situ changes of microstructure during fatigue loading at the surface or near surface, i.e. SEM, but not within the bulk material. In-situ neutron diffraction has been used to analyze the statistical nature of twinning and detwinning in a bulk volume across many grains [54]. However, no real time microstructure changes can be observed. The model is limited as the microscopic fatigue deformation results cannot be compared to experimental data. The model results can be correlated to experiment by matching macroscopic deformation data such as stress-strain curves and crystallographic texture changes.
Chapter 7 - Conclusions and Future Work

7.1 Conclusions

A rate-dependent CPFE code, originally developed to describe the monotonic deformation of polycrystalline HCP materials with a strong focus on Zircaloy-2, was applied to the fatigue of a dissimilar Mg alloy bi-crystal. Slip and twinning were the two major deformation modes accounted for in the model, at room temperature. The basal, prismatic and pyramidal \(<c+a>\) slip and tension twinning systems were considered. Twinning was treated as pseudo-slip as described by Kalidindi [84]. The evolution of the strength of each slip and twin systems was described by a Voce hardening law [80]. A PTR scheme was used to describe twinning reorientation wherein the volume represented by a GP was reoriented based on the most active twin system after a critical value of 0.9 TVF accumulates, as described by Zhang and Joshi [89]. This modification was implemented after it was found that the scheme implemented by Abdolvand and Daymond [88], wherein twins nucleated after 0.02 TVF and grew with increasing deformation, resulted in unrealistically large hardening in the stress-strain curve after twin nucleation in Mg single crystals.
The major goal of this research was to investigate the deformation of Mg and Mg alloys using the CPFE code. Firstly, verification of the code to describe the mesoscopic and microscopic deformation of Mg was conducted. By using available single crystal tension and compression data for pure Mg in the literature, the parameters for the time-dependent strain rate and hardening rate equations were calibrated for the CPFE code using a guess and check trial method. It is observed that the current code is suitable for modeling Mg deformation as it achieved generally acceptable results when comparing the stress-strain data, although with some limitations and issues. The tensile modulus was sometimes overestimated and when prismatic slip dominated the hardening rate was slightly lower before saturation and slightly higher after saturation. At higher strains when there is high crystal rotation, the Voce hardening law no longer accurately describes hardening. The microscopic deformation activities were accurately captured in the model when compared to experimental observations. The code was concluded to be appropriate for simulating deformation in single and bi-crystal Mg and Mg alloys.

The CPFE code was used to investigate the meso- and microscopic fatigue behavior of Mg AZ31-AZ80 alloy bi-crystals up to 1000 cycles. Eleven orientation combinations were studied: bi-crystals with combinations of 0°, 90° and 45° and a 25°-100° and 80°-155° bi-crystal. The material parameters used in the code were taken from Jain et al. [29] who used similar constitutive equations to study Mg
AZ80 and AZ31 polycrystalline sheet deformation. The fatigue loading simulations were used to: (a) assess the ability of the code to capture fatigue deformation, and (b) systematically study the effect of crystal orientation on the HCF behavior of the bi-crystals. Based on the simulation results, the CPFE is capable of simulating fatigue behavior as it captured the following cyclic deformation phenomena: the Bauschinger effect, cyclic hardening, and ratcheting. The following are the general conclusions of this bi-crystal fatigue study using the CPFE code:

- At stress amplitudes near the yield point either basal or twinning is activated as they both have similarly low CRSS values, which is consistent with the literature.

- There is a strong neighbor effect when the AZ31 grain is oriented for twinning due to the surface constraints. Approximately twice as much twinning occurs in AZ31 when AZ80 is oriented for basal slip.

- The most cyclic deformation occurs when the AZ31 grain is oriented for basal slip. All deformation is localized in this grain regardless of the orientation in the AZ80 grain. The accumulated shear amplitude damage, T, in AZ31 is 0.0915 when AZ31 is oriented for basal slip compared to the second highest value of 0.00492 in the 0°-45° bi-crystal.
During cyclic loading the softer AZ31 grain hardens and the stronger AZ80 softens in terms of microscopic deformation. The microscopic deformation evolves in such a way as to lead to the mesoscopic strain amplitude in each grain to become similar.

Each perfect orientation bi-crystal had mesoscopic strain amplitude of approximately 0.115%. After 1000 cycles the shear strain amplitude approaches 1E-08 to 1E-07. These values would be difficult to resolve experimentally although limited hardening for strain amplitudes of 0.1% - 0.2% is consistent with the literature.

The yield increases for orientations away from the highest Schmid factor, but the cyclic deformation behavior near yield is comparable to the highest Schmid factor orientations.

The results of this study were also applied to assess the potential effects on fatigue performance of a possible FSW of dissimilar materials. The FSW process creates a misoriented interface, which was simplistically replicated in this study using bi-crystals. Fatigue damage in the HCF regime is carried by basal slip and twinning in AZ31 and AZ80 Mg alloys. Therefore, orientation combinations which result in the most basal and twinning deformation would be expected to have the worst fatigue properties, i.e. orientations near 0°-45°, 90°-45° and when AZ31 is 45°.
7.2 Future Work

The following tasks are suggested for future research:

- There is no available experimental research on the mesoscopic HCF behavior of Mg alloys in the bulk. More experimental fatigue studies of grains in the bulk are required to validate the results of this study. The model can be expanded to describe larger numbers of grains in a polycrystal.
- There have been experimental studies of bi-crystal deformation for special orientations in other metal systems but very few fatigue studies. Given the difficulty in growing such crystals particularly for Mg alloys, it is difficult to push anyone to do so, but coupled with predictions from computational approaches, specific orientation combinations should be investigated.
- A bi-crystal is a simplification of bulk material. To obtain results which would better model structural materials a more realistic microstructure and crystallographic texture should be modelled which could be taken from electron back-scattered diffraction, or neutron diffraction measurements.
- The twinning scheme used in this research is simplistic and does not account for observed twinning phenomena such as nucleation, growth and detwinning. A more advanced twinning model should be implemented in the code.
- Free surface behavior has a strong effect on fatigue performance. For fatigue studies, kinematic hardening, such as an Armstrong-Frederick relation, should be implemented in the future to capture cyclic deformation phenomenon. This will allow the freeing of constraints on the material surfaces.

- The current CPFE code does not account for crack initiation or growth. Employing this model to simulate fatigue life studies will require crack initiation and growth criteria. The code is a general crystal plasticity model and can be used to study different phenomena not studied in the present research such as texture evolution, grain size effects and temperature effects.
 References


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[37] H. Abdolvand, "Multi-scale modeling and experimental study of deformation twinning in
hexagonal close-packed materials," Queen's University, Kingston, 2012.


Appendix A - Monotonic tension and compression stress-strain

The monotonic tension/compression stress-strain plots for the bi-crystal orientations discussed in Chapter 5 follow here.
Fig. A.1: AZ31/AZ80 bi-crystal axial stress-strain curves until 0.05 strain tension (smooth line) / compression (dashed line) simulations: a) 0°-0° b) 0°-90° c) 0°-45° d) 90°-0° e) 90°-90° f) 90°-45° g) -45°-0° h) -45°-90° i) -45°-45°.

Fig. A.2: AZ31/AZ80 bi-crystal axial stress-strain curves until 0.05 strain tension (smooth line) / compression (dashed line) simulations: a) 25°-100° b) 80°-155°.
Appendix B  -  Fatigue deformation

The fatigue deformation plots for the bi-crystal orientations discussed in Chapter 5 follow here. For the stress-strain curves the AZ80 curve is on top of the AZ31 curve and both start at the origin.
Fig. B.1: AZ31/AZ80 bi-crystal axial stress-strain curves for fatigue simulations after 1000 cycles in the AZ31 grain(Blue) and AZ80 grain(Red): a) 0°-0° b) 0°-90° c) 0°-45° d) 90°-0° e) 90°-90° f) 90°-45° g) -45°-0° h) -45°-90° i) -45°-45°.

Fig. B.2: AZ31/AZ80 bi-crystal axial stress-strain curves for fatigue simulations after 1000 cycles in the AZ31 grain(Blue) and AZ80 grain(Red): a) 25°-100° b) 80°-155°.
Fig. B.3: AZ31/AZ80 bi-crystal axial strain amplitude evolution for fatigue simulations up to 1000 cycles in the AZ31 grain (smooth line) and AZ80 grain (dashed line): a) 0°-0° b) 0°-90° c) 0°-45° d) 90°-0° e) 90°-90° f) 90°-45° g) -45°-0° h) -45°-90° i) -45°-45°.

Fig. B.4: AZ31/AZ80 bi-crystal axial strain amplitude evolution for fatigue simulations up to 1000 cycles in the AZ31 grain (smooth line) and AZ80 grain (dashed line): a) 25°-100° and b) 80°-155° bi-crystal.
Fig. B.5: AZ31/AZ80 bi-crystal shear strain amplitude evolution for fatigue simulations up to 1000 cycles in the AZ31 grain (smooth line) and AZ80 grain (dashed line): a) 0°-0° b) 0°-90° c) 0°-45° d) 90°-0° e) 90°-90° f) 90°-45° g) -45°-0° h) -45°-90° i) -45°-45°.

Fig. B.6: AZ31/AZ80 bi-crystal shear strain amplitude evolution for fatigue simulations up to 1000 cycles in the AZ31 grain (smooth line) and AZ80 grain (dashed line): a) 25°-100° b) 80°-155°.
Fig. B.7: AZ31/AZ80 bi-crystal axial stress and axial strain contour plots for fatigue simulations after 1000 cycles when AZ31 is 0°. Axial stress plots: a) 0°-0° c) 0°-90° e) 0°-45°. Axial strain plots: b) 0°-0° d) 0°-90° f) 0°-45°.
Fig. B.8: AZ31/AZ80 bi-crystal axial stress and axial strain contour plots for fatigue simulations after 1000 cycles when AZ31 is 90°. Axial stress plots: a) 90°-0° c) 90°-90° e) 90°-45°. Axial strain plots: b) 90°-0° d) 90°-90° f) 90°-45°.
Fig. B.9: AZ31/AZ80 bi-crystal axial stress and axial strain contour plots for fatigue simulations after 1000 cycles when AZ31 is -45°. Axial stress plots: a) -45°-0° c) -45°-90° e) -45°-45°. Axial strain plots: b) -45°-0° d) -45°-90° f) -45°-45°.