Microstructural fracture mechanics: stored energy density at fatigue cracks

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Abstract

This paper addresses the mechanistic drivers of short fatigue crack growth using theory, computational crystal plasticity and experimental test and characterisation. The asymptotic theory shows that the crack tip stored energy density is non-singular and finite and can be related to stress intensity, but unlike the latter, it depends on the crystal Burgers vector and intrinsic slip strength. The computational methods allow the stored energy to be calculated accurately at crack tips and show that good agreement is obtained for static cracks with the theory. The experiments allow the crack tip stored energy to be measured, demonstrating intimate microstructural sensitivity, direct correlation with experimental crack growth variations and good quantitative agreement with both asymptotic theory and computational modelling. Hence a new microstructurally-sensitive fracture mechanics **has been presented in the context of short cracks within crystalline materials.**

Keywords: short crack growth; stored energy; microstructure; fracture mechanics

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21 1 Introduction

22 Fatigue of ductile alloys continues to be the life-limiting failure mechanism in almost
23 all safety-critical engineering structures in existence and remains profoundly
24 important to understand. A very significant fraction of life may be taken up by short
25 crack growth; that is, the stage of crack propagation during which the rate of growth
26 and the crack path are very dependent on microstructure (Ghonem, 2010; Irving and
27 Beevers, 1974).

28 Many experimental studies (Briffod et al., 2019; Gao et al., 2007; Kumar and Curtin,
29 2007; Sangid et al., 2011; Schäfer et al., 2013; Texier et al., 2019; Wan and Dunne, 2020;
30 Zhai et al., 2000) have sought to explain the role of microstructure in determining
31 crack path and propagation rate. **Because the crack path taken also determines the
32 local microstructure which controls the local propagation rate, the overall short crack
33 growth rate therefore depends upon both. Hence any quantitative microstructural
34 fracture mechanics must capture the mechanisms controlling both the path and rate
35 of short crack propagation.**

36 Classical fracture mechanics of ductile metals assumes that a crack exists in a
37 homogeneous, isotropic and elastic-plastic medium, and thereby does not explicitly
38 recognise microstructure. Pioneering methodologies include the Griffith fracture
39 energy (Griffith, 1921), the stress intensity factor (SIF) (Irwin, 1957), and the J-integral
40 (Rice, 1968) which have been extensively applied to predict crack growth at the macro-
41 scale (Suresh, 2012). But they reflect neither the characteristic length scale, nor the
42 mechanistic crack tip drivers when the crack length is in the scale of 1-10 grains.

43 In fatigue, the stress intensity range ΔK is taken to be the primary driving force in Paris
44 law (Paris and Erdogan, 1963), but for low ΔK reflecting short cracks, experimentally
45 observed rates of growth can vary greatly with crack length (Shademan and Soboyejo,
46 2002) which Paris law does not capture. This again results from the microstructural
47 sensitivity of short cracks where the crack tip grows within a continuously changing
48 environment. Hence fatigue indicator parameters (Rovinelli et al., 2017; Rovinelli et
49 al., 2015) have been assessed to attempt to quantify this response. However, unlike
50 the classical driving forces (such as ΔK), these measures are singular quantities which
51 become undefined at the (sharp) crack tip.

52 A related, but nevertheless very different microstructure-sensitive driving force,
53 namely the stored energy density, has recently been introduced which is predicated
54 on the idea that local partially reversed slip under fatigue gives rise to dislocation
55 interaction and the establishment of dislocation structures over a length scale
56 determined by the dislocation density (Wan et al., 2014; Zheng et al., 2019). This
57 elastically stored energy density has been shown to be dominated by the
58 geometrically necessary dislocation (GND) density (Zheng et al., 2019), thereby giving
59 a measure of the energy stored in lattice curvature potentially available to drive the
60 generation of new surfaces in the form of crack growth (Wilson et al., 2018). Recent
61 results show that tortuous short crack growth paths and the effects of crystallography
62 and grain boundaries on growth rate in FCC, BCC and HCP alloys are captured (Wilson
63 and Dunne, 2019; Wilson et al., 2019).

64 This paper addresses the fracture mechanics of short fatigue crack growth which is
65 microstructurally sensitive. A computational methodology, reported before, is first

employed to determine crack tip stored energy density and cyclic stored energy density rates for two differing single crystal orientations with edge cracks, and offers pragmatic evidence of the non-singularity of stored energy unlike stress and dissipated energy. A new theory is then introduced for a blocked slip line emanating from a crack tip, giving rise to quantifiable GND density and consequently stored energy density. It is shown for the first time that the latter is a non-singular and finite quantity, thereby justifying its use as a mechanistically-based crack driving force that uniquely captures microstructural sensitivity. In addition, it is shown for the first time that it is related to the classical stress intensity thus showing consistency with, and linkage to classical fracture mechanics, but with the unique merit of being microstructurally sensitive. This is followed by in-situ high resolution digital image correlation (DIC) and electron backscattered detection characterisation of growing fatigue cracks in Zircaloy-4 alloy and, for the first time, the experimental measurement of crack tip stored energy density and an assessment of its microstructural sensitivity. The results from the three complementary methods are then discussed and contextualised.

2 Methods

2.1 Crystal plasticity finite element modelling

A strain-rate dependent, dislocation-based crystal plasticity finite element (CPFE) framework is adopted for the material description in this study. Only a summary is given here, and full details of the framework can be found in (Dunne et al., 2007).

The plastic strain rate $\dot{\epsilon}^p$ is determined from the shear rate $\dot{\gamma}^{(i)}$ along all active slip systems, which gives:

$$\dot{\boldsymbol{\varepsilon}}^p = \sum_{i=1}^M \dot{\gamma}^{(i)} \mathbf{s}^{(i)} \otimes \mathbf{n}^{(i)} \quad (1)$$

where M is the total number of active slip systems (up to 32 for a Hexagonal Closed Packed (HCP) crystal), and $\mathbf{s}^{(i)}$ and $\mathbf{n}^{(i)}$ are the slip direction and normal direction vectors of the i^{th} slip system, respectively. The slip rate $\dot{\gamma}^{(i)}$ along the i^{th} slip system is governed by thermally activated dislocation escape from obstacles (such as lattice defect, impurities, inclusions, etc), which is given by

$$\dot{\gamma}^{(i)} = \rho_{ssdm} b^2 v_D \exp\left(-\frac{\Delta H}{k\theta}\right) \sinh\left(\frac{\Delta V}{k\theta} \left|\tau^{(i)} - \tau_c^{(i)}\right|\right) \quad (2)$$

where ρ_{ssdm} is the mobile statistically stored dislocation (SSD) density, b the Burgers vector, v_D the frequency of attempted dislocation jump over obstacles, ΔH the activation energy with associated activation volume ΔV , k the Boltzmann constant, θ the temperature, and $\tau^{(i)}$ and $\tau_c^{(i)}$ are the resolved shear stress and critical resolved shear stress on the i^{th} slip system, respectively. The critical resolved shear stress, or intrinsic slip system strength, $\tau_c^{(i)}$ evolves with both SSD and geometrically necessary dislocation (GND) density, where the former is related to the plastic strain evolution and the latter to lattice curvature resulting from plastic strain gradients. The strain rate sensitivity (SRS) of a slip system is governed by the combination of ΔH and ΔV (Dunne et al., 2007).

A Taylor-based hardening law is adopted for the evolution of shear resistance along the i^{th} slip system:

$$\tau_c^{(i)} = \tau_{c0}^{(i)} + Gb\sqrt{\rho_{ssd} + \rho_{gnd}} \quad (3)$$

106 where $\tau_{c0}^{(i)}$ is the intrinsic critical resolved shear stress, G the shear modulus, and ρ_{ssd}
 107 and ρ_{gnd} are the density of statistically stored and geometry necessary dislocations
 108 respectively. The evolution of SSD density for simplicity is related only to the effective
 109 plastic strain p :

$$\dot{\rho}_{SSD} = \lambda \dot{p} \quad (4)$$

110 where the coefficient λ controls the slip system isotropic hardening rate. The effective
 111 plastic strain rate $\dot{p}$ is given by:

$$\dot{p} = \sqrt{\frac{2}{3} \dot{\boldsymbol{\epsilon}}^p : \dot{\boldsymbol{\epsilon}}^p} \quad (5)$$

112 where $\boldsymbol{\epsilon}^p$ is the plastic strain tensor.

113 The components of the GND density tensor are calculated from Nye's dislocation
 114 tensor (Nye, 1953) $\boldsymbol{\Lambda}$ that originates from the lattice curvatures given by the curl of
 115 the plastic deformation gradient $\boldsymbol{F}^p$:

$$\boldsymbol{\Lambda} = \nabla \times \boldsymbol{F}^p = \sum_{i=1}^M \rho_{Gs}^i \boldsymbol{b}^i \otimes \boldsymbol{s}^i + \rho_{Get}^i \boldsymbol{b}^i \otimes \boldsymbol{t}^i + \rho_{Gen}^i \boldsymbol{b}^i \otimes \boldsymbol{n}^i \quad (6)$$

116 where ρ_{Gs}^i is the screw component, ρ_{Get}^i and ρ_{Gen}^i the edge components, $\boldsymbol{b}^i$ the
 117 Burgers vector, $\boldsymbol{s}^i$, $\boldsymbol{t}^i$ and $\boldsymbol{n}^i$ the unit vectors on the i th slip system, respectively.

118 The full form of solving the GND density tensor $\boldsymbol{\rho}_G$ is hence given by:

$$\boldsymbol{A} \boldsymbol{\rho}_G = \bar{\boldsymbol{\Lambda}} \quad (7)$$

119 where $\bar{\boldsymbol{\Lambda}}$ is the vectorized Nye dislocation tensor, $\boldsymbol{A}$ is a $9 \times (3 \times 32)$ matrix containing
 120 the coefficients of the $\boldsymbol{b}^i \otimes \boldsymbol{s}^i$, $\boldsymbol{b}^i \otimes \boldsymbol{t}^i$ and $\boldsymbol{b}^i \otimes \boldsymbol{n}^i$ terms. The 96 independent GND
 121 components cannot be uniquely solved with the nine equations alone from the term
 122 $\boldsymbol{\Lambda}$. The scalar GND density is hence determined by the by L_2 -norm minimization of the

edge and screw dislocation density components of Nye's tensor (Cheng and Ghosh, 2015):

$$\rho_{gnd} = \sqrt{\sum_{i=1}^M (\rho_{Gs}^i)^2 + (\rho_{Get}^i)^2 + (\rho_{Gen}^i)^2} \quad (8)$$

The dissipated energy density U is given by:

$$U = \int \boldsymbol{\sigma} : d\boldsymbol{\varepsilon}^p \quad (9)$$

and the stored energy density G (Wan et al., 2014) is given as:

$$G = \frac{U\Delta V_s}{\Delta A_s} = \int \frac{\xi \boldsymbol{\sigma} : d\boldsymbol{\varepsilon}^p}{\sqrt{\rho_{ssd} + \rho_{gnd}}} \quad (10)$$

where ΔV_s and ΔA_s are the dislocation storage volume and area over which the dislocation lines penetrate the surface, respectively, and ξ is the fraction of plastic work stored as dislocation structures and estimated to be ~ 0.05 (Kamlah and Haupt, 1997). The zircaloy-4 single crystal material properties used in the CPFE modelling are given in Table 1 and taken from (Wilson et al., 2018).

Table 1. Material properties for (HCP) zircaloy-4.

E_{11} (GPa)	E_{33} (GPa)	ν_{12}	ν_{13}	G_{12} (GPa)	G_{13} (GPa)
98	123	0.40	0.24	35	32
b (nm)	ρ_{ssdm} (μm^{-2})	λ (μm^{-2})	k (JK $^{-1}$)	ΔH (eV)	ΔV
0.32	0.01	0	1.38×10^{-23}	0.31	$18.8b^3$
$\tau_{c0}^{(a)}$ (MPa)-prism		$\tau_{c0}^{(a)}$ (MPa)-basal		$\tau_{c0}^{(c+a)}$ (MPa)-pyramidal	
153		204		532	

A Zr single crystal with an edge crack subject to Mode I loading is modelled using the above CPFE formulation, and is shown in Figure 1. The specimen has dimensions $4500\mu m \times 1500\mu m \times 150\mu m$ and contains a $270\mu m$ edge crack, and is loaded along the

x-direction under stress control, as shown in Figure 1(a). Various crystal orientations are assigned to the single crystal to understand the microstructure sensitivity of the material response near the crack tip. Both of the front and back faces of the specimen are constrained to give conditions of plane strain in (b), relevant for fracture studies. Both monotonic and cyclic (stress ratio $R=0$ and period $T=20s$) stress-controlled remote loading is imposed, with peak applied stress intensity factor $K_{max} = 12.4MPa\sqrt{m}^{0.5}$ illustrated in (c). A highly focused and refined mesh is configured in the vicinity (within a radius of half of the crack length) of the crack tip, which is denoted by the red dot in (d), while the surrounding region is assigned a coarser mesh to reduce the computational expense. Continuum 3D hexahedral second order elements (ABAQUS type C3D20R), with reduced integration, are chosen to discretise the whole specimen.

Figure 1. The crystal plasticity finite element model for the edge crack problem showing (a) the dimensions and loading direction, (b) boundary conditions, (c) the cyclic loading history, and (d) the mesh local to the edge crack.

2.2 Experimental procedure

Two edge-notched Zircaloy-4 beam samples (Sample AZ and BY) with large-grain polycrystal microstructures shown in Figure 2 were cyclically loaded in three-point bend testing under force-controlled loading with R-ratio of zero (*i.e.* zero to peak to zero load in any one cycle). They share approximately the same geometries and loading conditions to peak applied stress intensity factor of $12.4 \text{ MPam}^{-0.5}$.

Figure 2. SEM images showing notch geometries and crack paths in (a) Sample AZ and (b) Sample BY and (c) IPFZ of Sample AZ; (d) IPFY of Sample BY.

In situ optical DIC strain measurement fatigue testing was carried out with overall set up shown in Figure 3(a) which included a Questar Microscope Lens (QM-100), a QIclick versatile scientific CCD camera, the three-point bend testing rig and a three-axis sliding supporting stage. The three-point bend test setup was mounted on a Shimadzu universal testing machine. The Questar Microscope is connected to the camera with a C-mount adaptor and Faber Optic Illuminator supplying coaxial illumination. The lens is mounted on a supporting stage which allows sliding along three orthogonal directions, and the camera is supported by a screwed metal cylinder

attached to the supporting stage to avoid motion. The Questar Microscope has a nominal highest resolution of $1\mu\text{m}$ and is able to recognize the sprayed sample surface silica speckles with size of $1\mu\text{m}$ with a working distance of about 150 mm in Figure 3(b) and (c).

Figure 3. (a) In-situ micro-scale optical Digital Image Correlation set-up, (b) OM image and (c) SEM image showing the distributed $1\mu\text{m}$ silica speckles on the sample surface for DIC measurement.

A succession of speckle images were captured by the camera in-situ during fatigue testing with a time interval of 0.5s during cyclic three-point bend testing such that the speckle displacements were recorded throughout individual cycles and over many cycles in-situ. Images of 1392×1040 pixels were captured. After testing, the images were processed to determine surface total strain components using in-house cross-correlation Matlab code (Jiang et al., 2016) at both peak and fully unloaded instants within cycles, as well as intermediate points. In the (second pass) cross-correlation analysis a window size of 64×64 pixels ROI with 95% overlapping was used such that the spatial resolution of strain measurement achieved was less than approximately $3\mu\text{m}$.

The in-situ DIC measurements included total strains at the unloaded condition and at peak load in a full cycle. The strains obtained in the unloaded condition give an approximate measure of the plastic strains, provided the residual elastic strains are

190 small. The zero R-ratio loading makes this a reasonable assumption, minimising any
 191 reversed plasticity on unload. The total strains $\boldsymbol{\varepsilon}^t$ at the cycle peak load may be written
 192 as the sum of elastic $\boldsymbol{\varepsilon}^e$ and plastic $\boldsymbol{\varepsilon}^p$ strains. Thus the elastic strain can be extracted
 193 approximately from the difference between total strain and plastic strain

$$\boldsymbol{\varepsilon}^e = \boldsymbol{\varepsilon}^t - \boldsymbol{\varepsilon}^p \quad (11)$$

194 From Hooke's law, the stress is given by

$$\boldsymbol{\sigma} = \mathbf{D}\boldsymbol{\varepsilon}^e \text{ or } \boldsymbol{\varepsilon}^e = \mathbf{C}\boldsymbol{\sigma} \quad (12)$$

195 where $\mathbf{D}$ is the (global) anisotropic stiffness matrix after rotation to account for
 196 crystallographic orientation, $\mathbf{C}$ the (global) compliance matrix after rotation where $\mathbf{C} =$
 197 $\mathbf{D}^{-1}$. The rotation matrix is determined from Euler angles obtained from EBSD
 198 characterisation. In 3D,

$$\begin{pmatrix} \varepsilon_{xx}^e \\ \varepsilon_{yy}^e \\ \varepsilon_{zz}^e \\ \gamma_{xy}^e \\ \gamma_{yz}^e \\ \gamma_{zx}^e \end{pmatrix} = \begin{pmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ & & C_{33} & C_{34} & C_{35} & C_{36} \\ & & & C_{44} & C_{45} & C_{46} \\ & & & & C_{55} & C_{56} \\ & & & & & C_{66} \end{pmatrix} \begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{xy} \\ \sigma_{yz} \\ \sigma_{zx} \end{pmatrix} \quad (13)$$

199 Under plane stress conditions relevant to the front free surface of the sample,
 200 $\sigma_{zz}=\sigma_{yz}=\tau_{xz}=0$. Thus eq.(13) is reduced to

$$\begin{pmatrix} \varepsilon_{xx}^e \\ \varepsilon_{yy}^e \\ \gamma_{xy}^e \end{pmatrix} = \begin{pmatrix} C_{11} & C_{12} & C_{14} \\ C_{12} & C_{22} & C_{24} \\ C_{14} & C_{24} & C_{44} \end{pmatrix} \begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{xy} \end{pmatrix} \quad (14)$$

201 The stress tensor becomes

$$202 \quad \boldsymbol{\sigma} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & 0 \\ \sigma_{xy} & \sigma_{yy} & 0 \\ 0 & 0 & 0 \end{pmatrix} \text{ or } \boldsymbol{\sigma} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} \\ \sigma_{xy} & \sigma_{yy} \end{pmatrix} \text{ in plane stress.}$$

203 The two-dimensional strain field in the sample unloaded condition gives
 204 approximately the plastic strains with the elastic part relaxed. This gives

$$\boldsymbol{\varepsilon}^p = \boldsymbol{\varepsilon}^{Unload} = [\varepsilon_{xx}^p \quad \varepsilon_{yy}^p \quad \varepsilon_{xy}^p]^T \quad (15)$$

205 GNDs carry the lattice curvature when the material is deformed plastically and
 206 heterogeneously. Previous studies (Ashby, 2006) have provided a one-dimensional
 207 estimation of the GND density along a single slip plane, which is given by:

$$\rho_{gnd} = \frac{1}{b} \frac{\partial \gamma}{\partial s} \quad (16)$$

208 where b is the slip system Burgers vector, γ the shear strain and s the position in the
 209 slip direction coordinate axis. Eq.(16) is generalised into two-dimensions, which gives

$$\boldsymbol{\rho}_{gnd} = \frac{1}{b} (\nabla \times \boldsymbol{\varepsilon}^p) \quad (17)$$

210 or in index notation

$$(\boldsymbol{\rho}_{gnd})_{ij} = \frac{1}{b} (\boldsymbol{\varepsilon}^p)_{i,j} \quad (18)$$

211 The full form of eq. (18) gives

$$\begin{bmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \\ \rho_{31} & \rho_{32} \end{bmatrix} = \frac{1}{b} \begin{bmatrix} \frac{\partial \varepsilon_{xx}^p}{\partial x} & \frac{\partial \varepsilon_{xx}^p}{\partial y} \\ \frac{\partial \varepsilon_{yy}^p}{\partial x} & \frac{\partial \varepsilon_{yy}^p}{\partial y} \\ \frac{\partial \varepsilon_{xy}^p}{\partial x} & \frac{\partial \varepsilon_{xy}^p}{\partial y} \end{bmatrix} \quad (19)$$

212 Through minimizing the dislocation energy, a scalar GND density is given as the sum
 213 of the 2nd order norm of its components

$$\rho_{gnd} = \left(\sum_{j=1}^2 \sum_{i=1}^3 \rho_{ij}^2 \right)^{1/2} \quad (20)$$

214 The algorithm for determining GND density assumes the DIC region covers a single
 215 phase, single crystal microstructure, and all activated slip systems share the same
 216 Burgers vector. In particular, the <a>-prismatic slip Burgers vector ($b = 0.32\text{nm}$) is
 217 utilised for Sample AZ and the <c+a>-pyramidal slip Burgers vector ($b = 0.52\text{nm}$) for
 218 Sample BY.

219 Figure 4(a) shows a schematic of crack growth from cycle $i-k$ to cycle i with a crack
 220 advance Δa represented by the dashed arrow, such that the crack-tip advances by Δa
 221 in k cycles. The location of the ROI (marked as the rectangular region) is adjacent to
 222 the crack-tip at cycle i but at a distance Δa from the crack-tip at cycle $i-k$, such that the
 223 stored energy difference calculation is made with respect to the very same ROI.

224 For any point (x, y) in the ROI, the plastic strain tensor is obtained from DIC. Therefore,
 225 the plastic strain difference during k cycles can be obtained from the plastic strain at
 226 cycle i and that at cycle $i-k$. The stress tensor at peak load for any point (x, y) is obtained
 227 as outlined above, such that the stored energy from cycle $i-k$ to cycle i everywhere
 228 within the ROI, $U(x, y)$, can be integrated up as illustrated in the schematic in Figure
 229 4(b) with knowledge of the peak stresses and their variation with cycles

$$U(x, y) = \int_{i-k}^i \boldsymbol{\sigma}(x, y) : d\boldsymbol{\epsilon}^p(x, y) = \frac{1}{2} (\boldsymbol{\sigma}_i + \boldsymbol{\sigma}_{i-k}) : (\boldsymbol{\epsilon}_i^p - \boldsymbol{\epsilon}_{i-k}^p) \quad (21)$$

230 It is argued that at the crack tip area, $\rho_{\text{gnd}} \gg \rho_{\text{ssd}}$ with large lattice distortion near the
 231 crack-tip such that the contribution of ρ_{ssd} to the total dislocation density can be
 232 neglected. Hence the *cyclic stored energy density* can be obtained from

$$\dot{G}(x, y) = \frac{\xi \dot{U}(x, y)}{\sqrt{\rho_{\text{gnd}}}} \quad (22)$$

Figure 4. Schematic of cyclic energy calculation: (a) the crack growth from cycle $i-k$ to cycle i with a crack advance Δa ; (b) the stress at peak load versus accumulated plastic strain in the ROI.

3 Results

The results of computational crystal plasticity analyses of single crystal edge cracks under monotonic and cyclic loading are presented first in particular to address the role of crystallographic orientation on crack tip stored energy density and hence its dependence on microstructure and evolution with fatigue cycles. This is followed by the presentation of new asymptotic theory for stored energy density, providing direct comparisons with the computational results, and demonstrating that the stored energy density is non-singular and finite at crack tips. Lastly, the in-situ DIC-measured crack tip strains are used to estimate the crack tip stored energy density for differing microstructures during short crack growth. We demonstrate its intimate sensitivity to microstructure, including crystal orientation and key features of the microstructure, reflecting experimentally observed crack growth rates. The results of the three methods are then compared and discussed.

3.1 Crystal plasticity computational stored energy density at edge cracks

A dislocation-based, rate-dependent crystal plasticity finite element (CPFE) formulation described above is adopted to determine key field quantities, including stored energy density, near an edge crack tip in single crystals of (HCP) Zircaloy-4 alloy. The crystal and material properties are given in Table 1. The specimen is subjected (initially) to remote monotonic loading under conditions of plane strain up to remote stress $\sigma_0=320\text{MPa}$, giving a peak applied stress intensity factor of $12.4\text{MPa}\sqrt{\text{m}}^{0.5}$. The HCP crystal orientation selected, with its c-axis out of plane in this case, is shown in Figure 5(a). The plastic strain field developed near the crack tip is shown in Figure 5(b), where the two significant slip bands emanating from the crack tip develop because of the activation of the symmetrical $\langle a \rangle$ -prismatic slip systems. Various finite element sizes are utilised near the crack tip, in order to investigate the mesh sensitivity of the stress, plastic strain, and geometrically necessary dislocation (GND) density at the crack tip as shown in Figure 5(c), and the dissipated energy and stored energy density in Figure 5(d). The GND field arises from the highly localized strain gradients established at the crack tip (Xia and Hutchinson, 1996). The stress, plastic strain, GND density and dissipated energy decrease rapidly as the crack tip element size is increased, as anticipated, and demonstrate the well-known result that the finer the FE mesh at the crack tip, so the stress increases as a result of the (elastic) singularity at the crack tip. Because the dissipated energy is directly related to stress and plastic strain, it too becomes large at the crack tip, and these quantities depend upon the finite element meshing local to the crack tip, confirming that they are not rigorously appropriate for use as crack driving forces. In contrast, Figure 5(d) indicates that the stored energy density attains a finite magnitude at the crack tip of $\sim 3\text{Jm}^{-2}$, even as the

element sizes near to the crack tip are diminished down to $2\mu\text{m}$ (0.7% of the crack length), so that this quantity appears to be non-singular at the crack tip. A sharp crack in an elastic medium leads to the singularity of stress at the crack tip. In the CP modelling reported here, of course, the material undergoes slip thereby eliminating the elastic singularity but elasto-plastic FE analyses at sharp cracks also show a strong mesh dependence with increasing element size tending to reduce the stress magnitude. This is discussed further in the context of the theoretical result and experimental measurements in Section 4.

Figure 5. Single crystal HCP zircaloy-4 with edge crack under monotonic loading showing (a) schematic of the model single crystal with orientation shown and subject to Mode I loading, (b) the distribution of xx-component of the plastic strain field near the crack (crack tip element size $2\mu\text{m}$), (c) crack tip stress, plastic strain and GND density and (d) crack tip dissipated energy and stored energy density at the crack tip versus (tip) element size.

Figure 6 examines the predicted microstructure sensitivity of the stored energy density from the CPFE study in monotonic and cyclic (fatigue) loading. Figure 6(a) shows schematically two edge-cracked single HCP crystal orientations, namely P and Q. The nominal crack plane is the crystal (10-10) plane for both P and Q. Figure 6(b)

shows the spatial distributions of stored energy density ahead of the crack tip for a highly refined FE mesh with minimum element size of $2\mu\text{m}$. The stored energy density distribution for Type P shows two diffused bands reflecting the $\langle a \rangle$ -prism slip near the crack tip, while that for Q shows a more concentrated distribution due to $\langle c+a \rangle$ -pyramidal slip activation combined with additional $\langle a \rangle$ -slip arising from the stress triaxiality near the crack tip, which destroys the symmetry. The stored energy variations along the paths (indicated in (b)) are compared in Figure 6(c) for the two single crystals at peak load subject to monotonic loading. The stored energy for Type Q is systematically higher than that for Type P all along the path, which demonstrates the stored energy at the crack tip is strongly influenced by the local microstructure. The stored energies at the crack tip are estimated to be 6.3 Jm^{-2} and 2.9 Jm^{-2} for crystals Q and P respectively such that the stored energy density for Q is 2.2 times that for P. The microstructural dependence comes from both anisotropy of elasticity (via modulus) and the plasticity (via slip strength, Burgers vector and slip direction), which is addressed in the following theory section. The computationally predicted stored energy evolutions with fatigue cycles (stress ratio $R=0$ and period 20s) for static edge cracks are shown in Figure 6(d) for crystals P and Q over the first 10 cycles. The rate of evolution of crack tip stored energy density per cycle for crystal Q is predicted to be 1.8 times that for crystal P for a static (non-growing) crack. This demonstrates that the cyclic stored energy density accumulated per cycle, which has been associated with short fatigue crack growth rate (Wilson et al., 2019), is clearly dependent on the crystallographic orientation near the crack tip. The dependence of the cyclic stored energy density on microstructure is assessed later by comparison with experimental quantitative characterisation.

Figure 6. The CPFE-predicted plane strain stored energy density for two edge cracked single crystal orientations showing (a) schematic diagrams of the two crystal orientations P and Q with respect to the edge crack, (b) stored energy distributions for the two crystals under monotonic loading (and path definitions), (c) stored energy density (rolling average) along the two paths as indicated in (b), and (d) the evolution of (static) crack tip stored energy density at the unloaded instants with cycles for the two crystals. This set of results is obtained in the CPFE simulation with mesh element size of $2\mu m$.

3.2 Theoretical analysis of stored energy density at edge cracks and relationship to classical fracture mechanics

An edge-cracked single crystal is shown schematically in Figure 7(a) which is subjected to remote mode I type loading resulting in stress intensity K . The stresses at the crack tip are assumed to activate slip when the resolved shear stress τ , on any given slip system achieves the critical resolved shear stress (CRSS) τ_c for that system. Note that in HCP zircaloy-4, $\langle a \rangle$ -type basal, prismatic and pyramidal, as well as $\langle c+a \rangle$ pyramidal slip are possible but all have independent CRSSs (see Table 1). Hence the single crystal orientation influences which systems are activated.

Figure 7. Schematic of (a) edge-cracked single crystal with bands of slip emanating from the crack tip under remote mode I loading σ_0 and a sub-region showing (b) crystal orientation P with an activated slip line aligned parallel to an $\langle a \rangle$ -prismatic plane, and (c) crystal orientation Q with slip line aligned parallel to $\langle c+a \rangle$ -pyramidal slip. In (b) and (c), slip γ^p has been activated and dislocation glide blocked resulting in shear stress τ orientated at θ to the horizontal axis.

In Figure 7(b), prism slip is indicated whereas in (c), it is $\langle c+a \rangle$ -pyramidal. For simplicity and insight in this study, we address only shear on an individual identified slip system and argue that there is substantive evidence, particularly for zircaloy-4 (Wan and

345 Dunne, 2020; Wilson et al., 2019), but for other crystal systems also (Wilson et al.,
 346 2019), that fatigue crack growth is crystallographic in nature. Figure 7(b) shows the
 347 activated prismatic slip line orientated at θ to the x-axis, of length l_s from the crack
 348 tip. Dislocations are nucleated at the crack tip, and the high resulting local curvature
 349 because of strong plastic strain gradients results in a high density of GNDs but that
 350 along the length of the slip line, dislocations glide but are ultimately terminated by
 351 reducing resolved shear stress and the plastic-elastic boundary. Hence we argue that
 352 it is reasonable to consider this scenario to be a blocked slip system along which the
 353 total slip may be decomposed into elastic and plastic parts:

$$\gamma = \gamma^e + \gamma^p \quad (23)$$

354 but for which there is no slip step, such that $\gamma = 0$, so that

$$\gamma^p = -\gamma^e \quad (24)$$

355 At the first onset of slip on this system, the resolved shear stress must achieve the
 356 CRSS such that

$$\tau = \tau_c \quad (25)$$

357 The local resolved shear stress and hence elastic shear strain can be obtained from
 358 the elastic solution at the crack tip in polar coordinate system (r, θ) given by

$$\gamma^e = \frac{K_\theta}{\mu(2\pi)^{1/2}} r^{-\frac{1}{2}} \quad (26)$$

359 where K_θ is the orientation-dependent stress intensity factor, μ the shear modulus, r
 360 the radial distance from the crack tip, and the polar angle term is determined by the
 361 slip system orientation such that

$$K_{\theta} = \frac{1}{4} \left(\sin \frac{\theta}{2} + \sin \frac{3\theta}{2} \right) K \quad (27)$$

so the plastic shear is given by

$$\gamma^p = -\frac{K_{\theta}}{\mu(2\pi)^{1/2}} r^{-\frac{1}{2}} \quad (28)$$

Differentiating the plastic strain term γ^p with respect to r gives

$$d\gamma^p = \frac{K_{\theta}}{2\mu(2\pi)^{1/2}} r^{-\frac{3}{2}} dr \quad (29)$$

which is needed subsequently. The GND density may be determined considering the radial plastic strain gradient given by (Ashby, 2006)

$$\rho_{\text{gnd}} = \frac{1}{b} \frac{\partial \gamma^p}{\partial r} = \frac{K_{\theta}}{2b\mu(2\pi)^{1/2}} r^{-\frac{3}{2}} \quad (30)$$

where b is Burgers vector along the slip direction. Note that $\sigma_{r\theta}$, γ^p and ρ_{gnd} are all singular as $r \rightarrow 0$ but diminish to zero as $r \rightarrow \infty$ away from the crack tip as anticipated. The stored energy density (Wan et al., 2014; Zheng et al., 2019) G at the crack tip resulting from the slip line emanating from it in this instance is then given by

$$G = \int_0^{l_s} \frac{\tau d\gamma^p}{\sqrt{\rho_{\text{gnd}}}} = \int_0^{l_s} \frac{\tau_c \frac{K_{\theta}}{2\mu(2\pi)^{1/2}} r^{-\frac{3}{2}} dr}{\left[\frac{K_{\theta}}{2b\mu(2\pi)^{1/2}} r^{-\frac{3}{2}} \right]^{1/2}} = \int_0^{l_s} \tau_c \left[\frac{K_{\theta} b}{2\mu(2\pi)^{1/2}} \right]^{\frac{1}{2}} r^{-\frac{3}{4}} dr \quad (31)$$

where l_s is the slip line length. Note that the integrand $\frac{\tau d\gamma^p}{\sqrt{\rho_{\text{gnd}}}} \sim r^{-\frac{3}{4}}$ so as $r \rightarrow \infty$, so

$\frac{\tau d\gamma^p}{\sqrt{\rho_{\text{gnd}}}} \rightarrow 0$ away from the crack tip. Also, in Equation (32), (middle expression), while each of the numerator (dissipated energy) and denominator (GND density rooted) in their own rights tend to zero as the distance from the crack tip increases, the integral to give the stored energy density transpires to be finite. The consequences of this in

375 the context of CP modelling and experimental results are discussed further in section

376 4. This then results in a stored energy density of

$$G = \left[\frac{8\tau_c^2 b K_\theta l_s^{1/2}}{\mu(2\pi)^{1/2}} \right]^{\frac{1}{2}} \quad (33)$$

377 In order only to seek further comparisons with classical fracture mechanics, we
378 consider the plastic zone size r_p which is classically expressed approximately for
379 conditions of plane strain to be

$$r_p = \frac{(1 - 2\nu)}{2\pi} \left(\frac{K}{\sigma_y} \right)^2 \quad (34)$$

380 where σ_y is the yield stress. Equation (34) is therefore re-written to relate the slip line
381 length, l_s , in terms of the appropriate crystal quantities for plane strain as

$$l_s = \frac{(1 - 2\nu)}{2\pi} \left(\frac{K_\theta}{\tau_c} \right)^2 \quad (35)$$

382 and combined with eq. gives the approximate plane strain relationship

$$G = \left[\frac{4\tau_c b K_\theta^2 (1 - 2\nu)}{\pi\mu} \right]^{\frac{1}{2}} \quad (36)$$

383 where $K_\theta = \frac{1}{4} \left(\sin \frac{\theta}{2} + \sin \frac{3\theta}{2} \right)$ is the stress intensity factor in terms of slip line
384 orientation shown in Figure 7(a), τ_c the slip system critical resolved shear stress, b the
385 slip system Burgers vector, and μ and ν the in-plane (elastically anisotropic) shear
386 modulus and Poisson's ratio respectively. Firstly, it transpires that the stored energy
387 density (which has units of Jm^{-2}) as defined is finite and non-singular at the crack tip.
388 Second, it is related to the classical stress intensity K (and in turn, the Griffith fracture
389 energy) and shear modulus, but is modified by microstructural properties b , the

390 Burgers vector which introduces a crystal length scale, and the intrinsic slip system
391 strength, the critical resolved shear stress, τ_c , and the slip plane orientation to loading,
392 θ . It is therefore in contrast to the quantities stress, strain and dissipated energy, all
393 of which are singular at crack tips.

394 We note that the relationship given in equation (36) is approximate, since in general
395 multi-slip occurs under stress, with the activation of multiple differing slip systems
396 (particularly basal and prism slip systems typically with much lower intrinsic strengths
397 than those for the $\langle c+a \rangle$ types). In addition, under activation, slip systems harden (not
398 just from GND contributions but also from statistically stored dislocation evolution).
399 Further, the form of equation (36) is obtained after simplifying equation (33) to
400 approximate the slip length. This is why the computational approach presented earlier
401 is important and provides a much more general methodology. However, it is
402 important to compare the stored energy densities obtained from the theoretical
403 relationship in equation (36) with the computational method presented earlier,
404 particularly for the crystal and edge crack configurations P and Q. Later in the paper,
405 we will also compare these energies with those obtained from direct measurement at
406 crack tips in experiments on zircaloy-4.

407 Zircaloy-4 material properties are given in Table 1 (Section 2.1), and the stored energy
408 density computed from equation (36) for P and Q orientations respectively are found
409 to be $G^P=2.77 \text{ Jm}^{-2}$ and $G^Q=7.50 \text{ Jm}^{-2}$ for applied monotonic loading of $K=12.4 \text{ MPam}^{-0.5}$. These are quite different for the two crystallographic orientations considered
410 $(G^P/G^Q=2.7)$ because of the differing slip system Burgers vectors and strengths, the
411 differing slip system orientations with respect to the mode I loading direction, and the

relevant in-plane (anisotropic) elastic properties. Crystal orientation and edge crack Q configuration is intuitively more resistant to slip (for a given applied stress) along $\langle c+a \rangle$ planes than orientation P where the corresponding prism slip is easily activated. Hence the stored energy density in Q is more localised and as a consequence, gives rise to higher energy density for given loading. These theoretical results are very close to those obtained from the previous computational approach and are discussed further together with experimental results in the next section. The full comparisons between stored energies predicted by eq.(36), from the computational crystal plasticity analysis, and from experimental results are presented in Table 2 in the Discussion section.

Finally, we note that eq. (36) relates stored energy density G to stress intensity K . The critical stress intensity, measured at a macro length scale which ignores microstructure, provides the fracture stress with knowledge of the crack length. Previous computational work has related a critical stored energy density G_c to both critical stress intensity K_c and the critical J-integral (Wilson et al., 2018) energy and showed that the differing critical stress intensities resulting from edge cracks in different single crystal orientations (and textures in the case of polycrystals) could be predicted. Hence eq. (35) similarly enables critical stress intensity to be predicted for edge cracks in differently orientated single crystals.

3.3 Experimental observation of the correlation between the stored energy and crack growth rate

Cyclic three-point bend tests with stress ratio $R = 0$ were carried out on two strongly textured Zircaloy-4 (HCP) edge-notched beam samples AZ and BY whose microstructures are shown in Figure 2, together with corresponding inverse pole

436 figures (IPFs). Sample AZ has a texture representative of the crack and crystal
437 orientation of Type P considered above; that is, the crack growth occurs along in-plane
438 prism directions and the crystal c-axes are normal to crack growth direction and the
439 y-direction (horizontal). Sample BY has a Type Q texture so that the crystal c-axes
440 predominantly lie approximately parallel to the y-axis in Figure 2.

441 Representative results of DIC-measured crack tip strain accumulation for sample AZ,
442 dominated by prism slip, as the crack grows with increasing fatigue cycles, is shown in
443 Figure 8. The bands of approximately symmetrical strain emanating from the crack tip
444 are of the form shown by the CPFE results in Figure 5 and the strain magnitude
445 increases as the crack grows from 410 to 550 μm . A full summary of the instantaneous
446 distributions of the crack tip total strain (from DIC), stress (see Methods), GND density
447 (see Methods) are shown in Figure 9 (c)-(e) and (g)-(i) for Samples AZ (Type P) and BY
448 (Type Q) respectively, when both samples have an effective crack length of
449 approximately 500 μm . Sample AZ (P) generally shows more diffused strain patterns at
450 the developing crack tip compared to Sample BY (Q), for which they are more localised,
451 originating from the predominant activation of $\langle a \rangle$ -prism systems and $\langle c+a \rangle$ -
452 pyramidal systems in samples AZ and BY respectively (Clouet et al., 2015; Gong et al.,
453 2015; Wilson et al., 2019). Using these data, the stored energy density is calculated at
454 a given fatigue cycle from the measurements of stress (elastic strain and anisotropic
455 elastic stiffness, with the former estimated as the difference of total strain minus
456 plastic strain), plastic strain (from DIC measurements at the fully unloaded state) and
457 GND density (from plastic strain gradients calculated from DIC plastic strain
458 measurements) as outlined in Section 2.2.

Figure 8. Evolution of crack tip total strain (xx) distribution of Sample AZ (P) in the unloaded condition with increasing crack length (from cycles 1000 to 2400) corresponding to effective crack lengths of (a) 410 μm to (h) 550 μm . The black arrows locate the crack tip.

The cyclic stored energy density (*i.e.* energy per cycle) near the crack tip is obtained by calculating differences of stored energy density (using eq.(22)) over intervals of cycles, ensuring the very same region of interest is used ahead of the crack tip and at earlier cycles before the crack tip has arrived) and is compared in Figure 9(f) and (j) for the two P and Q samples. It is calculated indicatively and locally at the crack tip by averaging over the defined region shown in Figure 9. This methodology is discussed in the context of the non-singular analytical and the CP calculation methods in Section 4. The cyclic stored energy density near the crack tip in Sample BY (Q) is considerably higher than that in Sample AZ (P), reflecting its microstructural sensitivity.

Figure 9. Experimental observations of the field quantities near short cracks (indicated by black arrow heads) for samples AZ (Type P) and BY (Type Q) in force-controlled fatigue tests. (a) Sample AZ features the Type P crystal orientation (i.e. crack perpendicular to c-axis) and (b) sample BY the Type Q crystal orientation (i.e. crack parallel to c-axis). The distributions of plastic strain, stress, GND density and cyclic stored energy density are shown for sample AZ in (c)-(f) and for sample BY in (g)-(j) for a crack length of $\sim 500\mu\text{m}$.

The measured crack growth rates with evolving crack length are shown in Figure 10(a) for the two samples. For Sample BY (Type Q microstructure), growth rate is systematically higher than that of Sample AZ (Type P microstructure) for all effective crack lengths. For both microstructures, crack growth rate increases with crack length as anticipated because of (macroscopically) increasing stress intensity ($\sim \sigma_0 \sqrt{\pi a}$). The strong difference in rates of growth for P and Q suggests that it is governed by the local microstructure, but particularly, the dominant differing crystallographic orientations near the crack tip. For the case of crack growth related to $\langle c+a \rangle$ -pyramidal slip (Type Q), considerably higher growth rates occur than for $\langle a \rangle$ -prism slip growth (Type P). These differing crack growth rates are consistent with other recent

491 studies (Wan and Dunne, 2020). The corresponding cyclic stored energy densities
492 determined from measurements in the experiments are shown in Figure 10(b) against
493 crack length. They also exhibit strong dependence on the sample crystallographic
494 orientations at the cracks, revealing that Type Q orientation leads to considerably
495 higher crack tip stored energies than Type P. This is important because it makes clear
496 that despite the same remote loading and geometry, the differing crystallographic
497 orientations give rise to quite different rates of crack growth and that these are
498 directly reflected in the crack tip stored energies, with higher energies associated with
499 higher growth rates. It provides evidence that the stored energy density is
500 microstructurally sensitive and able to differentiate the crack growth behaviours in
501 contrast to, for example, the stress intensity.

502 An interesting variation in crack growth rates is apparent in Figure 10(a) over crack
503 lengths between 400-500 μ m for Sample BY (Q). With reference to Figure 10 (c), as the
504 crack approaches a triple junction, its growth rate increases (labelled Event e_1 in Figure
505 10 (a) and (c)) but on traversing the grain boundary, retards to below the previous
506 average (Event e_2) until completely clear of the triple junction and grain boundary and
507 recovers to the trend rate (Event e_3). Figure 10 (b) makes clear that all the features of
508 the growth rate excursions resulting from the local microstructural effects are
509 similarly picked up, and followed reasonably closely. This provides further evidence
510 that the growth rates are related to the stored energy density, with the details of the
511 measured crack growth rates intimately reflected by the stored energy density rates.
512 The latter also reinforce that higher growth rates correspond to a higher crack tip
513 stored energy.

Figure 10. (a) Crack growth rates, and (b) cyclic stored energy densities versus crack length for the two samples AZ and BY featuring two distinct crystallographic orientations P and Q. (c) The events of the interaction between crack tip and its microstructure as indicated by e_1 , e_2 and e_3 in (a) for Type Q.

4 Discussion

In the theory section, it was shown that the crack tip stored energy density was obtained by spatially integrating over the non-zero slip field ahead of the crack tip for a single active slip system. The integration was carried out over the slip line length since beyond this region, there would be no plasticity, nor GND density and hence no contribution to stored energy. While the integrand in Equation (31) tends to zero with distance from the crack tip, as do the dissipated plastic energy and the GND density

individually, the stored energy density remains finite and non-singular. In fact, an integration to infinity would be the same for the reason already given. Thus the theoretical solution gives the total stored energy generated *by* the crack tip, which may, in principle, be slightly different to the stored energy determined by CP modelling and experiment *at* the crack tip. In the CP modelling, the finite element discretisation means that a strictly crack-tip value is influenced by the finite element mesh used, with smaller elements tending to give more accurate results for the local value which should converge to a unique value since the analytical solution demonstrates that it is finite and non-singular. However, if the stress were to be determined for the edge crack in an elastic medium, then of course a singularity would exist and the stress extracted then simply increases as the element size decreases. This is moderated, of course, if plasticity is allowed at the crack tip, but it is widely recognised that the resulting stress calculation becomes strongly mesh dependent. The stored energy, however, for the reasons explained, converges, and the finite element value at the crack tip is selected in this work. In the experiment, the spatial resolution of strain measurement using DIC (at best, this is of order $\sim 5\mu\text{m}$) at the crack tip is key since this determines the precision of the calculated stress, GND density and stored energy density. The determination of these quantities from the DIC strain measurements *at* the crack tip doesn't strictly have meaning in this context, so an average stored energy density local to the crack tip is determined instead. Hence the discussion which follows is contextualised by the constraints imposed from the three independent methodologies just discussed.

The results obtained from the computational analyses, the theoretical solution and the experiments are summarised in Table 2. For the experimental results, the crack

550 growth rates and cyclic stored energy density rates are determined at a crack length
551 of $\sim 500\mu\text{m}$ for which the cracks are growing within the bulk of their respective grains,
552 and with limited impact, therefore, from surrounding boundaries and microstructural
553 features. As a consequence, the comparisons with single crystal computations and the
554 theory are reasonable to make.

555 We note that the ratio of experimental crack growth rates for Q/P at this crack length
556 is 2.8 and that the experimental cyclic stored energy density rate ratio is 2.5. The
557 corresponding CP model computed stored energy density rate Q/P ratio is 1.8. In
558 addition, the static (at peak loading) ratio of stored energy density is 2.2 and the
559 equivalent theory predicted ratio is 2.7, giving remarkable consistency and agreement
560 throughout. It is correspondingly argued that stored energy density is
561 microstructurally sensitive, that it correctly captures crystal orientation effects on
562 crack growth rates, and in addition that it correctly captures complex microstructural
563 feature interactions with cracks corresponding to retardations and accelerations of
564 growth rates. Further, it is a quantity which is non-singular at the crack tip so is a
565 rigorous and appropriate driving force for short crack growth. In addition, it has been
566 shown to be related to classical macroscale fracture mechanics drivers including the
567 stress intensity. Other studies also carried out in zircaloy-4 (and other alloys) have also
568 shown that tortuous (and otherwise) short crack paths are captured (Wilson and
569 Dunne, 2019; Wilson et al., 2019) with computed stored energy density and
570 crystallographically determined directions.

571 Table 2. Summary of computed, analytical and experimental crack tip stored energy
572 densities and their cyclic rates for crystal orientations P and Q for crack length $\sim$
573 $500\mu\text{m}$.

Sample	Stored energy CP Model	Stored energy Non-singular solution	Experiment/ Characterization
P	2.87 Jm ⁻²	2.77 Jm ⁻²	$da/dN = 0.1\mu\text{m} / \text{cycle}$ $dG/dN = 0.5 \times 10^{-3} \text{Jm}^{-2} / \text{cycle}$
Q	6.32 Jm ⁻²	7.50 Jm ⁻²	$da/dN = 0.28\mu\text{m} / \text{cycle}$ $dG/dN = 1.25 \times 10^{-3} \text{Jm}^{-2} / \text{cycle}$
Q/P	$G^Q/G^P = 2.2$ $\frac{(dG/dN)^Q}{(dG/dN)^P} = 1.8$	$G^Q/G^Q = 2.7$	$\frac{(da/dN)^Q}{(da/dN)^P} = 2.8$ $\frac{(dG/dN)^Q}{(dG/dN)^P} = 2.5$

574

575 The relationship between stress intensity K and stored energy density G in equation
576 (33) may be rearranged to give the stress intensity. In the context of single crystal
577 fatigue, as the crack grows, it is not unreasonable to argue that the microstructural
578 sensitivity diminishes such that the macroscale mode I critical stress intensity K_c
579 determines unstable crack growth and failure. We argue that this is also characterised
580 by a critical stored energy density (Wilson et al, 2018) when $G = G_c$, where G is
581 calculated at the local microstructural level and, as demonstrated above, is
582 microstructurally sensitive. Equation (36) then gives

$$K_c = \left[\frac{\pi\mu}{4(1-2\nu)\tau_c b} \right]^{\frac{1}{2}} G_c \quad (37)$$

583 Using the zircaloy property data in Table 1 of Section 2.1, this gives for crystal
584 orientations P and Q that $K_c^P = 13.6 \times 10^6 \left(G_c/2 \right) = 6.8 \times 10^6 G_c$ and $K_c^Q = 2 \times$
585 $10^6 G_c$ or that $K_c^Q/K_c^P = 0.3$ so that an edge cracked single crystal with c-axis parallel
586 to the crack (crystal orientation Q) is less tough than the edge cracked crystal with c-
587 axis normal to the crack with in-plane basal (orientation P). There is no data for single

crystal zircaloy-4 in the literature but there is for very strongly textured polycrystal samples (Cockeram and Chan, 2013) of zircaloy-2 with relevant orientations which makes clear that the fracture toughness of a single crystal with c-axis parallel to crack direction is less tough (~ 0.7) than that with c-axes orientated away from crack direction.

Finally, the microstructure sensitivity revealed in this study is also found to be quantitatively consistent with single crystal Ti_3Al (Umakoshi et al., 1996) (HCP) where the $\langle c+a \rangle$ fracture toughness is about twice of that of $\langle a \rangle$ and strongly textured Ti-6Al-4V (HCP) alloy (Bowen, 1978) toughness testing shows the same ratio. This is qualitatively in line with low-scale discrete dislocation plasticity simulation on Zn (Olarinrithinun et al., 2013) (HCP).

5 Conclusions

Crack tip stored energy density has been proposed as an appropriate driving force for microstructurally-sensitive short crack growth. Integrated theory, computational crystal plasticity and experimental/characterisation studies have been carried out with the following concluding remarks:

- Crack tip stored energy density is non-singular providing a rigorous measure for crack growth driving force which is related to classical stress intensity together with intrinsic slip strength and length scale given by the crystal Burgers vector.
- The stored energy density has been demonstrated to be microstructure-governed, and quantitatively reflects experimental observations of both

610 crystal orientation-dependent crack growth rates and the influence of
611 microstructure (grain boundaries, triple junctions). The microstructure
612 sensitivity is reflected consistently by the analytical solution, the
613 computational CP analysis and the experimental observations.

- 614 • A critical stored energy density at which unstable crack growth occurs enables
615 classical fracture toughness to be predicted analytically for simple single
616 crystal cracks and, potentially, computationally for more complex
617 microstructures.

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