



On the mechanistic driving force for short fatigue crack path

Daniel J. Long^{*}, Fionn P.E. Dunne

Department of Materials, Royal School of Mines, Imperial College London, SW7 2AZ United Kingdom

ABSTRACT

The growth of fatigue cracks at the microstructural level is significant for many engineering industries. The multifarious nature of crack propagation at microstructure length scales necessitates the use of advanced modelling techniques to predict fatigue life accurately. A key contributor to this is the path of the crack, which also remains challenging to predict; the maximum slip criterion has been used widely in the literature but is not fully adequate. This paper tests the hypothesis that for short crystallographic cracks, there is some other factor responsible for guiding their extension on a particular plane. With this, using a crystal plasticity finite element modelling framework, two new energy-based methods are developed: a microstructure-sensitive maximum energy release rate criterion, and a maximum normal stored energy density criterion. Results demonstrate, for the two cases studied, both methods offer a significant improvement over the maximum slip criterion when applied to real microstructures. In particular, the maximum normal stored energy method gives closest agreement with experiments, while maximum energy release rate offers new insights into a mechanism for crack bifurcation.

1. Introduction

Short crack paths in polycrystalline microstructures can strongly influence crack growth rate but cannot be easily predicted. This paper presents a critical appraisal of three microstructure-sensitive criteria for crack path. Experimental evidence suggests that short or stage I cracking is controlled by crystallographic slip (Miao et al., 2012; Texier et al., 2019; Waddell et al., 2020; Rice and Thomson, 1974). Laird (1967) first highlighted observations of short cracks following paths inclined at 45° to the loading direction, compared with 90° for long cracks. Naturally, for an idealised single crystal with orientation such that slip planes are orientated at 45° (relative to the remote loading direction), slip is maximised due to increased shear stress. Neumann (Neumann, 1974; Neumann, 1969) later added refinement to this observation by demonstrating the proclivity for very short cracks to oscillate between visibly active slip systems. An in-situ SEM study by Zhang et al. (2019) of crack initiation and short propagation in single crystal nickel showed that crack nucleation occurred within shear bands containing multiple octahedral slip traces. The tortuous short cracks which followed were controlled by the same phenomenon. Similar observations were recorded by Carroll et al. (2013). Recent work by Rovinelli et al. (2018) used high resolution 3D short crack path data in combination with crystal plasticity modelling to establish correlations between candidate mechanistic crack path drivers and experimental path. Bayesian networks were used to analyse the data and identify two high-correlation drivers in the order: (i) misalignment between the principal stress axis and the slip direction and (ii) maximum resolved shear stress, which corresponds somewhat with the historically documented maximum slip driver (Laird, 1967). However, (iii) maximum accumulated shear strain was also analysed and showed lower correlation with the experimental crack path. Nevertheless, maximum accumulated shear strain was shown to be strongly linked with crack growth rate. Similar investigations were carried out by Pierson et al. (2018) using a large 3D crack path dataset. While no micromechanical field variable was shown to definitively predict short fatigue crack path, both stress and strain gradients were implicated as important factors.

With the use of numerical modelling methods to predict short crack growth, there has been near consensus on the use of the

^{*} Corresponding author.

E-mail address: d.long20@imperial.ac.uk (D.J. Long).

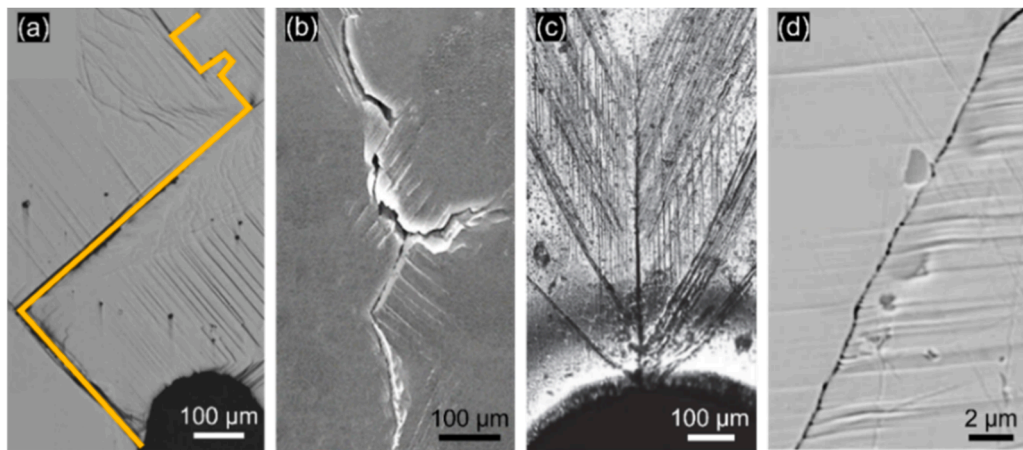


Fig. 1. Experimental evidence for short fatigue crack propagation in a range of metallic materials where the crack direction is visibly different to slip trace directions corresponding to high slip activity. (a) Microstructurally short fatigue crack growth in a Ni-based superalloy (Otsuka et al., 2018). The crack path is controlled by octahedral planes. There is clearly preferential activation of a single octahedral slip system, despite the tortuous crack path following several planes. (b) An experimental crack path in a polycrystalline Al alloy (Li et al., 2016). The crack path is partly controlled by grain boundary decohesion (intergranular) and intragranular crystallographic cracking. There are several examples of slip activity with traces orthogonal to the crack path. (c) A straight basal fatigue crack path in a Mg single crystal (Lu et al., 2022). There are clear basal slip traces, but also microcracking and high slip parallel to pyramidal planes. (d) A high magnification image of the end of a fatigue crack path in a Zr alloy (Wan, 2020). The crack path is parallel to a prismatic plane, but higher levels of slip are observed on another plane.

maximum slip criterion (Zhang et al., 2020; Lin et al., 2011; Karamitros et al., 2022; Guo et al., 2023). Lin et al. (2011) were amongst the first to use the maximum slip criterion for short crack path within crystal plasticity finite element (CPFE) models, which showed strong microstructure-sensitivity in polycrystalline materials. However, intragranular variations in crack path were not captured since the local stress state was not updated according to the crack tip position. Building on this, (Zhang et al., 2020) simulated crack growth in single crystal nickel using CPFE modelling combined with the eXtended Finite Element Method (XFEM) (Belytschko and Black, 1999). Maximum slip was used as the criterion for crack path and was shown to capture experimental phenomena such as tortuosity, but the overall segment lengths and oscillation frequencies disaccorded with experiments. There is also a range of experimental evidence which demonstrates crystallographic fatigue crack growth along planes which show less slip activity than others (see Fig. 1). (Farukh et al., 2016) used a maximum principal strain criterion (non-crystallographic) to predict crack direction in a polycrystalline nickel superalloy for comparison with experiment. Despite the application of crystal plasticity, the simulated crack path was essentially orthogonal to the remote loading direction and was in poor agreement with the experimental path. Several energy-based criteria for crack path have also been proposed (Srivastava et al., 2021; Chang et al., 2006; Wang, 1996). However, implementation of such criteria is often at the continuum level and lacks microstructure-sensitivity. Methods such as maximum energy release rate (Sun and Jin, 2012) were developed based on Griffith theory (Griffith, 1921) from classical continuum fracture mechanics but have not yet been investigated in the context of short fatigue crack paths. There is experimental evidence in the literature, presented in Fig. 1, which suggests that maximum slip may not be the exclusive determinant for short fatigue crack path. Ravi et al. (2021) have also shown experimentally that both mode I and II mechanisms contribute to the opening of short fatigue cracks, demonstrating the importance of crack tip stress. Thus, there is a need to explore new and alternative predictive methods.

In this paper, it is hypothesised that short crack paths are controlled partially, but not entirely by crystallographic slip (it is not disputed, however, that crack nucleation (*small cracks*) is dominated by slip activity (Hémerly et al., 2021)). According to McDowell (1996), *small cracks* differ from *short cracks* by their ratio of crack length to the characteristic microstructure length scale, i.e., grain size for most metallic materials. Microstructurally *small cracks* are ones in which the crack length is on the same order as individual microstructure features; microstructurally *short cracks* are characterised by cracks with length on the order of several repeating microstructure features. This hypothesis is tested by comparing CPFE-simulated microstructurally short paths, in combination with XFEM, controlled by (i) the maximum slip criterion, (ii) maximum energy release rate and (iii) a new maximum normal energy criterion, directly with experiments. Crack paths for (ii) and (iii) are constrained by considering active crystallographic slip planes only. The hypothesis is developed on the basis that dislocation slip contributes to damage and hence weakening of the plane, but that some other factor, e.g., stored energy is responsible for opening the crack on the damaged plane.

2. Methodology

2.1. Crystal plasticity finite element modelling

A dislocation based CPFE formulation is implemented to capture grain-scale slip activity in hexagonal close packed (HCP) Zircaloy-4. The mechanistic, rate-sensitive slip rule is given by Eq. (1).

Table 1
Crystal level elasto-plastic material properties used in CPFE modelling.

Parameter	Symbol	Value	Units
Elastic modulus in $\langle a \rangle$ direction	$E_{\langle a \rangle}$	98,308	MPa
Elastic modulus in $\langle c \rangle$ direction	$E_{\langle c \rangle}$	132,208	MPa
Shear modulus in $\langle c-a \rangle$ plane	$G_{\langle c-a \rangle}$	32,010	MPa
Poisson's ratio in $\langle a-a \rangle$ plane	$\nu_{\langle a-a \rangle}$	0.4006	–
Poisson's ratio in $\langle c-a \rangle$ plane	$\nu_{\langle c-a \rangle}$	0.2375	–
Density of mobile dislocations	ρ_m	0.01	μm^{-2}
Frequency of attempts	ν	1.0×10^{11}	s^{-1}
Burgers vector magnitude	b	3.2×10^{-4}	μm
Activation energy	ΔF	0.32	eV
Activation volume	ΔV	20.93	b^3

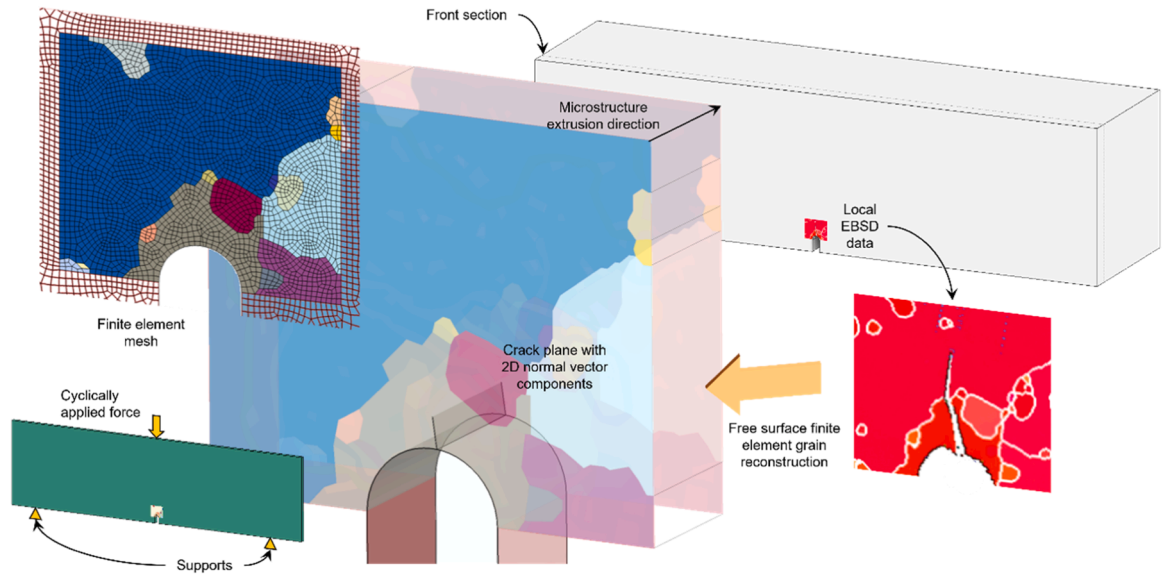


Fig. 2. CPFE modelling configuration. Post-mortem free surface EBSD data is used to reconstruct the 2D microstructure. A 3D model is constructed, which is just 150 μm thick to accurately represent the free surface stress state. Free surface microstructure is simply extruded due to absence of 3D data. As shown, crack planes are also represented as extrusions of their traces. Vertical boundary conditions are used to represent support pins in 3-point bend configuration. A distributed cyclic load is applied to a region at the top surface of the sample, which is representative of the loading pin from experiment.

$$\dot{\gamma}^i = \rho_m \nu b^i \exp\left(\frac{\Delta F}{k_B T}\right) \sinh\left(\frac{(\tau^i - \tau_c^i) \Delta V}{k_B T}\right) \quad (1)$$

where $\dot{\gamma}^i$ is rate of shear strain for slip system i , ρ_m is density of mobile dislocations, ν is a term describing the frequency of attempts for dislocations to overcome thermal energy barriers, b^i is Burgers vector magnitude for slip system i , ΔF is activation energy and represents the energy required to initiate glide of pinned dislocations (Reed-Hill, 1973). $\tau^i - \tau_c^i$ represents the difference between the applied and the critical resolved shear stress (CRSS) for slip system i , and ΔV is activation volume. Relevant Zircaloy-4 property values were reported previously (Long et al., 2022), and are summarised in Table 1. Room temperature CRSS values for various slip systems were measured experimentally by Gong et al. (2015) using micro cantilever testing. Strain-rate sensitive parameters including activation energy and activation volume, were calibrated using crystal plasticity modelling (Liu et al., 2021) against creep data from in-situ digital image correlation (DIC). Moreover, experimentally measured crystal-level anisotropic elastic properties are incorporated (Gong et al., 2015).

The microstructure-sensitive stored energy density (SED) is used as the fracture criterion (for propagation only) for each crack path selection method. SED is a measure of the recoverable energy stored in dislocation structure which accumulates during plastic deformation. Its numerical implementation in CPFE code is given by,

$$G = \xi \int \frac{\boldsymbol{\sigma} : d\boldsymbol{\varepsilon}^p}{\sqrt{\rho_{\text{SSD}} + \rho_{\text{GND}}}} \quad (2)$$

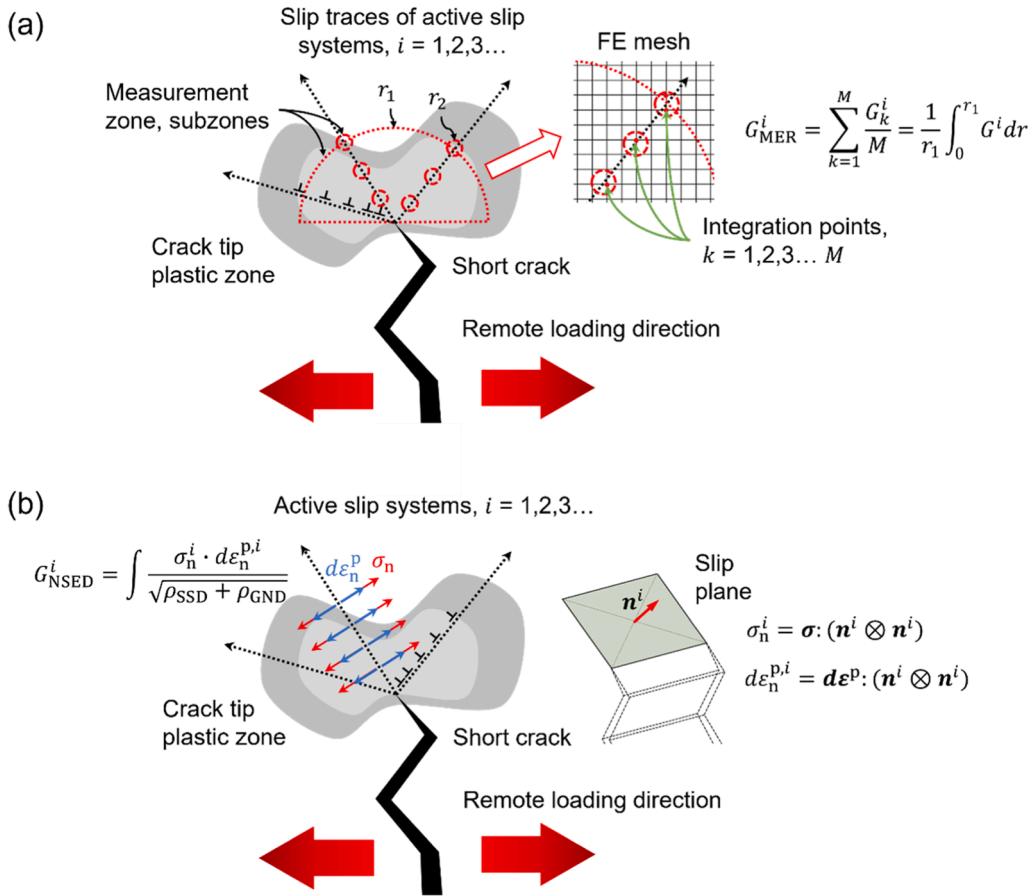


Fig. 3. (a) 2D illustration of implementation of maximum energy release rate criterion using a finite element mesh. The measurement zone refers to the semi-circular region centred at the crack tip. The measurement sub-zones are the circular regions spanning the individual slip traces and are used to encompass integration points from the finite element mesh. (b) Illustration describing normal stored energy density criterion for crack path. Red and blue arrows represent component of stress and plastic strain tensors, which act normal to the crack plane, respectively. The normal components are calculated by considering the crack plane orientations in 3D, given by their unit normal vectors, $\mathbf{n}^i$.

where σ is the stress tensor, $d\epsilon^p$ is plastic strain increment (corresponding to step increment in finite element modelling), and ρ_{SSD} and ρ_{GND} represent the density of statistically stored dislocations (SSD) and geometrically necessary dislocations (GND), respectively. For very short cracks ($< 10 \mu\text{m}$), GND density is thought to be the dominant source of crack tip dislocation structure due to highly localised lattice curvature (Gammer and An, 2022). ξ is the recoverable fraction of plastic strain energy, which is stored elastically in dislocation structure; its value is not known precisely, but is assumed here to equal 5%, and to be independent of loading conditions etc. (Cebbron and Kosel, 2014). Crack propagation is simulated using XFEM and is enabled when the value for SED ahead of the crack tip exceeds a critical value, G_c , which is a material constant. Since the focus of the current work is on crack path, and not rate of growth, the critical SED may be arbitrarily selected, such that it is high enough to capture sufficient crack path resolution, but low enough to enable practical simulation run times. In each case where a real microstructure is simulated, the critical SED is set to a value which permits crack growth within several hundred cycles. Hence, it is assumed that with large numbers of cycles that the various driving forces for crack path stabilise, and that crack path is unaffected by the chosen critical SED.

In this paper, free surface crack propagation is considered, and hence, crack plane normal vectors are parallel with the free surface plane. Crack paths and microstructure are represented within a 3D CPFE modelling space, but without subsurface information, i.e., free surface information is extruded in the out of plane direction. Two fatigue crack growth experiments in blocky alpha Zircaloy-4 samples are used as case studies in this paper. Grain growth was achieved by heat treating as-received material with rolled, i.e., strong textures and equiaxed grains at 800°C (below solvus) for 336 h. Beam samples measuring $3 \times 3 \times 12 \text{ mm}$ were notched and loaded in 3-point bending with $R = 0$ force-controlled loading, generating notch and crack tip stress intensity factors in the range $10 - 20 \text{ MPa}\sqrt{\text{m}}$. Notches measuring 0.3 mm were machined prior to testing. After testing, electron backscatter diffraction (EBSD) was used to characterise the microstructure and crystallography in the vicinity of each crack. As shown in Fig. 2, samples are not modelled entirely in the through-thickness direction to minimise computational expense but are thick enough to minimise boundary effects.

Eight node brick elements (C3D8) are used for the models, while enriched elements have an additional eight phantom nodes to

enable crack propagation via XFEM. In each case, the crack initiation site is specified prior to simulation by manual insertion of an edge crack based on experimental observations. In the first instance, the initial crack length is minimised by limiting it to a single finite element. However, as will be discussed in subsequent sections, different initial crack lengths are also considered. The crystal plasticity code is implemented via a user material (UMAT) subroutine in commercial finite element modelling software, Abaqus. For application of the SED fracture criterion in XFEM, the user-defined damage initiation (UDMGINI) subroutine is employed; when the value for SED at the centroid of the element ahead of the crack tip exceeds the predefined critical value, the element will fracture. The crack growth direction is controlled by the slip plane (based on one of the three criteria specified in this paper) free surface normal direction, with the out-of-plane component set to zero.

2.2. Maximum slip criterion for crack path

Using Eq. (1), the total accumulated slip is calculated for each HCP slip system i , by the following equation,

$$\gamma^i = \int \dot{\gamma}^i dt \quad (3)$$

where dt is time increment. Hence, according to the maximum slip criterion, the crack will extend along the slip plane of the system with maximum slip magnitude ahead of the crack tip, the orientation of which is given by its unit normal vector $\mathbf{n}$ (which depends upon grain orientation). The mechanistic basis for this is that planes with greatest damage, i.e., slip are most susceptible to cracking.

2.3. Maximum energy release rate criterion for crack path

In this section, a new method to predict short fatigue crack path based on the maximum energy release rate criterion is presented. The method involves utilisation of the crack tip SED field to select a crack path enabling maximal release of energy, i.e., SED. However, the key factor which differentiates this method from others is that it accounts for the crystallographic nature of short cracks by only considering paths controlled by crystallographic slip planes. An additional constraint, which ties with the current hypothesis, is that only active (damaged) slip systems are considered. The non-local methodology is described in greater detail in Fig. 3 (a).

As shown in Fig. 3 (a), a semi-circular measurement zone is defined ahead of the crack tip, throughout which SED measurements are recorded. It is assumed that for some measurement zone radius, r_1 , the crack path of maximal energy release is given by the path which traverses the greatest total SED. For simulation of 2D cracks, each slip system is compared by considering the release of energy given by the free surface slip plane trace of each active slip system. However, since the current CPFE approach involves SED calculation at discrete integration points, k , the total SED release along a given slip trace is unknown. Hence, circular measurement subzones, given by r_2 , are uniformly spaced along each active slip system trace to encompass local SED measurements, enabling an approximation of the energy release. Since the total number of encompassed integration points M may vary, the release of energy for slip system is normalised as, $G_{\text{MER}}^i = \sum_{k=1}^M \frac{G_k^i}{M}$. The mesh-independent unique solution is given by Eq. (4).

$$G_{\text{MER}}^i = \frac{1}{r_1} \int_0^{r_1} G^i dr \quad (4)$$

Hence, the short crack path which gives maximum energy release rate is given by the maximum value for G_{MER}^i from the set of i active slip systems. Criteria for r_1 and r_2 selection are presented in the results section.

2.4. Maximum normal stored energy density criterion for crack path

Thirdly, a new criterion for crack path is presented in this section, which also follows from the hypothesis that short crack paths are partially controlled by slip activation, but that another factor drives crack formation on active slip planes. Hence, as with the maximum energy release rate implementation, only active slip systems are considered using this method, but with maximum stored energy density normal to the slip plane controlling crack path. This criterion bears a resemblance to the maximum principal stress criterion, but an important difference (aside from considering only active slip planes) is that cyclic plasticity effects are accounted for, which are expected to be significant for short crack growth. As shown in Fig. 3 (b), the slip plane normal stress and normal plastic strain increment are first calculated, considering full 3D plane orientation and stress tensor etc. For a given slip plane orientation i , the normal stress is given by $\sigma_n^i = \boldsymbol{\sigma} : (\mathbf{n}^i \otimes \mathbf{n}^i)$, and the normal plastic strain increment $de_n^{p,i} = d\mathbf{e}^p : (\mathbf{n}^i \otimes \mathbf{n}^i)$, where $\mathbf{n}^i$ is the slip system unit normal vector, and $\otimes$ is the Kronecker product of the normal terms.

Hence, numerical integration enables calculation of each slip system normal stored energy density as,

$$G_{\text{NSEd}}^i = \int \frac{\sigma_n^i \cdot de_n^{p,i}}{\sqrt{\rho_{\text{SSD}} + \rho_{\text{GND}}}} \quad (5)$$

As before, crack path is controlled by the i^{th} slip plane corresponding to the maximum energy value. However, implementation of this method is local to the crack tip, i.e., energy terms calculated within the element directly ahead of the crack tip control crack path.

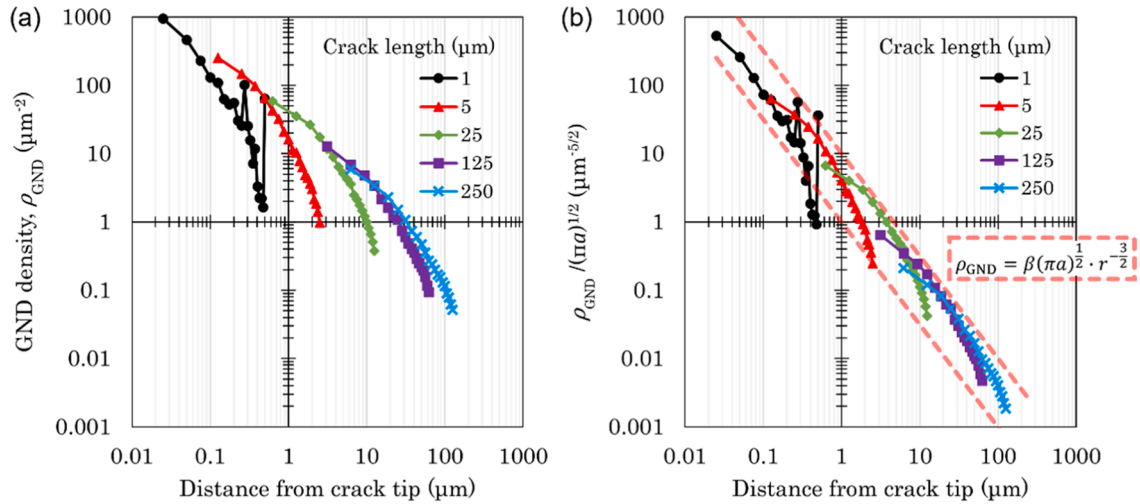


Fig. 4. CPFE modelling of GND density at crack tips. (a) Predicted distribution of GND density ahead of cracks of varying lengths. The remote applied stress is constant for each case. (b) Accounting for variations in crack length to establish a general relationship between crack tip GND density and distance from the crack tip. The red dashed lines follow the power law trend with exponent $-3/2$.

3. Results

3.1. Non-local measurement radius r_1 for maximum energy release rate

As discussed in Section 2.1, the mechanistic basis for the SED driving force for crack growth is that elastically recoverable energy, which is stored in crack tip dislocation structure (specifically GND), is released when it exceeds a critical value. Hence, for the maximum energy release rate criterion for crack path, the non-local distance over which measurements are taken is linked with the distribution of crack tip GNDs. Several single crystal CPFE simulations were carried out in which a remote stress of 200 MPa was applied to edge-cracked material with crack lengths ranging from 1 to 250 μm (crack lengths within the physically and micro-structurally short crack growth range). Fig. 4 (a) shows the spatial distributions of GND density ahead of each crack. It should be noted that due to the current limitations of XFEM, linear brick elements are used in these analyses. Hence, since GND density is related to the second order spatial derivative of displacement, it is not easily calculated using conventional linear elements. The sub-element method (Dunne et al., 2007) for calculating spatial gradients of plastic deformation and GND density is used here; details are provided in Appendix A.

As described by Xu et al. (2021), a one-dimensional analytical solution for crack tip GND density can be derived via the radial plastic strain gradient (Ashby, 1970), $\rho_{\text{GND}} = \frac{1}{b} \frac{\partial \gamma^p}{\partial r}$, where b is Burgers vector magnitude, γ^p is plastic shear strain, and r is a measurement of distance (in this instance, radial distance from the crack tip). Assuming a blocked slip system, where GNDs are contained between the crack tip dislocation free zone (DFZ) and the plastic-elastic boundary, the equation (Xu et al., 2021) is given by,

$$\rho_{\text{GND}} = \frac{K_\theta}{2b\mu(2\pi)^{1/2}} r^{-3/2} \quad (6)$$

where K_θ is an orientation-specific shear stress intensity factor term (which is directly proportional to the global crack tip stress intensity factor) and μ is shear modulus. Hence, Fig. 4 (b) shows the radial distributions of GNDs, normalised for each crack length by crack tip stress intensity factor, i.e., $\frac{\rho_{\text{GND}}}{\sqrt{\pi a}}$, since $K_\theta \propto \sqrt{\pi a}$.

Fig. 4 (b) shows that by normalising results against stress intensity factor, an approximate convergence for each crack length is achieved, which is demonstrated to conform to the power law relation as, where $\beta = \frac{1}{2b\mu(2\pi)^{1/2}}$. Therefore, using this analytical relationship, an estimate is obtained for the distance from the crack tip in which the majority of GNDs are contained. It is estimated that 99% of GNDs are contained within 18.97 μm from the crack tip. Hence, a non-local radius, $r_1 = 20 \mu\text{m}$ is selected for SED measurement using the maximum energy release rate criterion. As radius, r_2 has no physical meaning, it is chosen on the basis of mesh size alone, such that at least three integration points are accounted for with each measurement. Here, the measurement radius is set to equal the mean element size, which for the microstructure simulations presented is 3 μm .

3.2. Simulated crack paths in HCP single crystals

The maximum slip criterion for crack path has been shown in several studies to capture short crack phenomena such as tortuosity (Zhang et al., 2020; Zhang et al., 2021), which is a key feature of short crack growth in HCP materials. This is most commonly observed

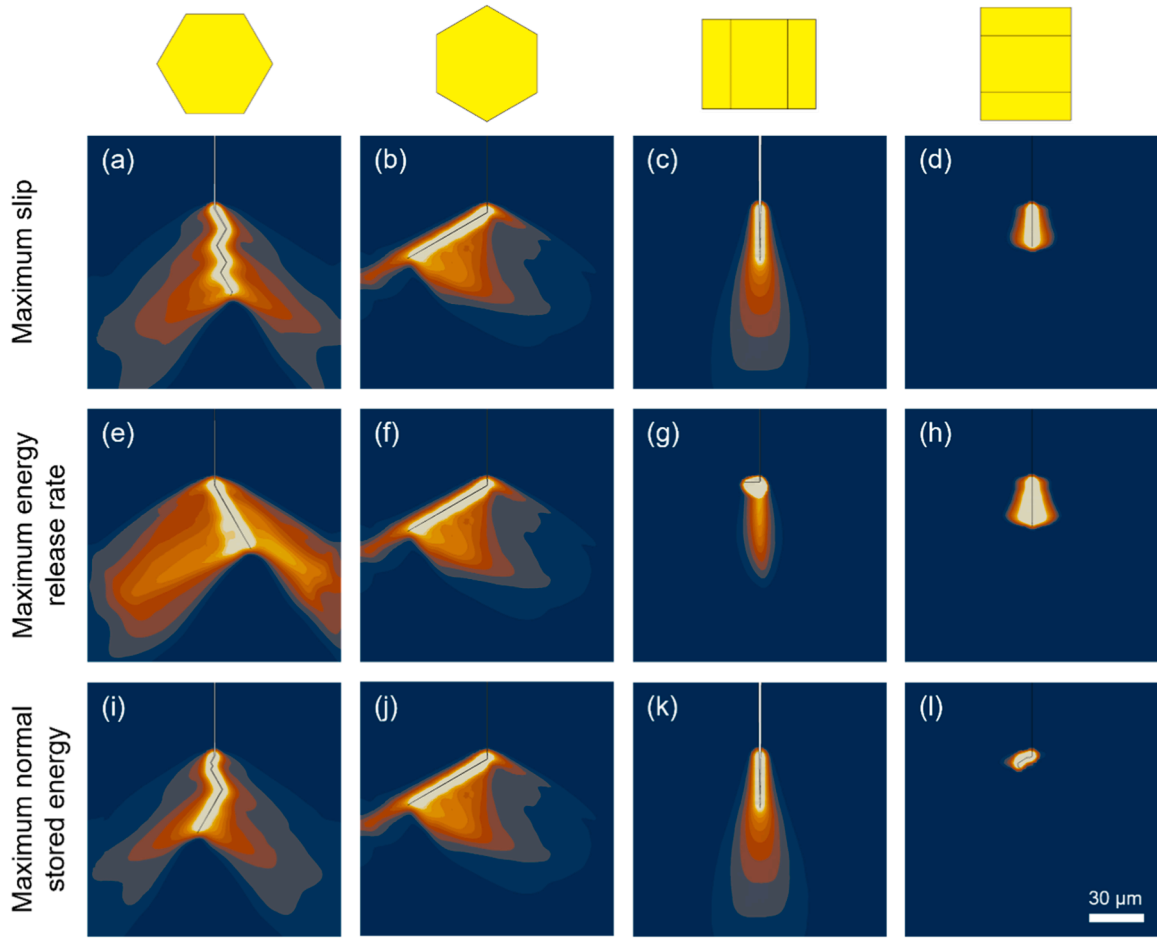


Fig. 5. Comparison of single crystal crack path predictions using the maximum slip (a – d), maximum energy release rate (e – h), and maximum normal stored energy (i – l) criteria. The corresponding SED fields (with arbitrary units) are also shown for illustration, which are particularly important for the maximum energy release rate criterion.

in HCP grains which are orientated such that the prismatic plane Burgers vector directions lie in the plane of crack growth and are inclined slightly relative to the mean crack growth direction (Long et al., 2022). In Fig. 5, which presents results from the current single crystal studies, the first orientation (from left to right) meets this description. Note that crystal orientation is represented by yellow HCP unit cell orientations, corresponding to the orientation observed from the sample free surface.

The predicted crack paths for the first single crystal orientation are shown in Fig. 5 (a), (e), and (i). Similar results using the maximum slip criterion have been presented by Wilson and Dunne, (2019) in previous studies. Hence, as anticipated, a tortuous crack path which oscillates between symmetric prismatic planes (parallel with their Burgers vector directions) is predicted in Fig. 5 (a). Another key feature of this crack path is that the frequency of oscillations tends to increase with increasing crack length; an explanation for this was given in previous work by the current authors (Long et al., 2022). Interestingly, the maximum energy release rate criterion (Fig. 5 (e)) predicts crack growth along a single prismatic plane direction (the selection of which is arbitrary due to symmetry) and does not predict tortuosity. The SED field around the crack shows that the highest levels are not ahead of the crack tip but are to the left of the inclined crack. However, the predicted crack path is based on energy ahead of the crack tip (i.e., energy which can affect crack path) only, which directs the crack path linearly. This suggests that if crack nucleation were included within the current model, crack bifurcation may be predicted, for which there is ample experimental evidence (Waddell et al., 2020; Doquet and Bertolino, 2008; Sabnis et al., 2016; Suzuki et al., 2022). The maximum normal stored energy criterion does predict a tortuous path for the first orientation, which differs slightly from the maximum slip result in that the segment length between oscillations increases, and therefore the frequency of oscillations decreases with increasing crack length. For the second orientation, each of the three methods produced the same result, which is a straight crack path along a prismatic slip plane. Due to symmetry, each model could have equally predicted growth along the prismatic plane which slopes downward and to the right. Due to near inactivity of the third (vertical) prismatic slip system, crack growth is not predicted along it using any method. However, if the slip activity constraint were not applied when using the maximum normal energy criterion, it is foreseeable that a vertical crack path along this plane may have been initially predicted. For the third crystal orientation considered, a vertical crack path following prismatic planes (perpendicular to their Burgers

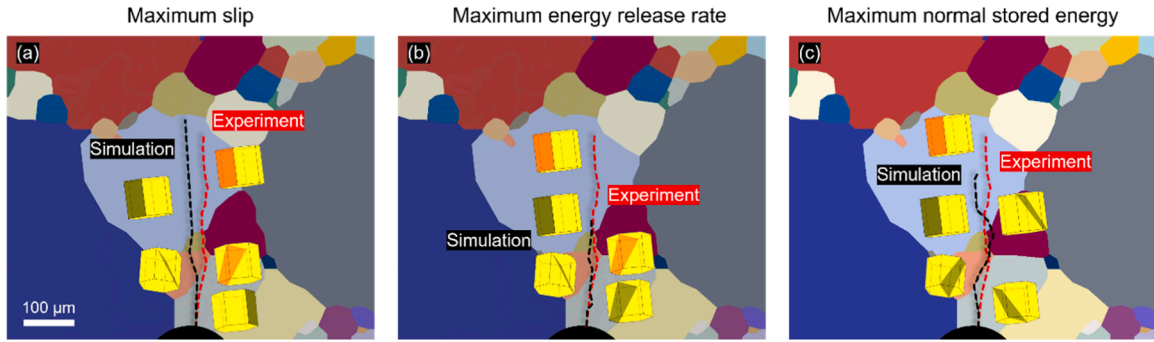


Fig. 6. Comparison of three short crack prediction methods with experimental crack path in sample A. Apparent experimental crack planes are shown with red shading, model-predicted crack planes are shown with black shading. (a) Simulated crack path using maximum slip criterion. (b) Simulated crack path using the crystallographic maximum energy release rate criterion. The simulation terminated prematurely due to local convergence issues. (c) Simulated crack path using the crystallographic maximum normal stored energy density criterion.

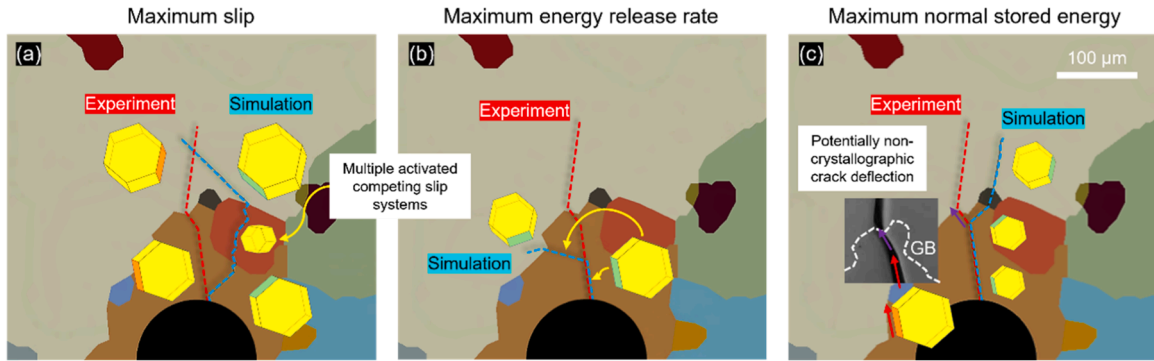


Fig. 7. Comparison of three short crack prediction methods with experimental crack path in sample B. Apparent experimental crack planes are shown with red shading, model-predicted crack planes are shown with cyan shading. (a) Simulated crack path using maximum slip criterion. The initial crack direction is such that it propagates into a grain for which there is no experimental data for comparison. (b) Simulated crack path using the crystallographic maximum energy release rate criterion. (c) Simulated crack path using the crystallographic maximum normal stored energy density criterion. Experimental crack path deflection near the grain boundary is shown in detail with a SEM image.

vector directions) is predicted using both the maximum slip and normal stored energy criteria. However, the maximum energy release rate method predicts basal cracking (Fig. 5 (g)), resulting in a crack path which is parallel with the remote loading direction. Lastly, maximum slip and maximum energy release rate agree for the final orientation, predicting basal cracking, while a tortuous path along basal, prismatic, and pyramidal planes is predicted using the maximum normal stored energy criterion.

3.3. Simulation of crack paths in polycrystalline Zircaloy-4

In this section, the three criteria for short crack path are compared directly with two sets of experimental data. Both samples used for comparison have very large grain (blocky alpha) microstructures, which enable clear single crystal crack path resolution; both also have strong texture. The samples will be referred to as sample A and sample B hereafter. Sample A is characterised by a strong texture in which the HCP c-axes lie predominantly parallel with the free surface and orthogonal to the remote loading direction. Sample B's texture is dominated by out-of-plane c-axes, i.e., basal planes are parallel with the free surface. The microstructures are presented in Figs. 6 and 7. The experimental crack path from sample A is compared against the theoretical criteria in Fig. 6. Fig. 6 (a) shows reasonable agreement between the maximum slip model and experimental results; the key difference here is that the simulated path deviates leftward initially due to crack growth along a prismatic plane, rather than an apparent rightward crack path along a pyramidal plane. General crack path trends are captured within individual grains after this point, particularly in the final grain, where prismatic cracking is dominant.

Fig. 6 (b) shows strong agreement between the model using the maximum energy release rate criterion and experiment (up to the point at which the simulation terminates). Specifically, in the first grain, the predicted crack path first oscillates and is then propagated along a pyramidal plane, which corresponds closely with the apparent experimental crack plane. Moreover, in the second and third grains, a combination of pyramidal and prismatic cracking, respectively, is predicted. This is in accord with the maximum slip model. Little maximum energy release rate data is available for cracking in the last grain; however, the predicted crack segment agrees with the maximum slip model and the (majority of the) experimental path. The maximum normal stored energy criterion is compared with

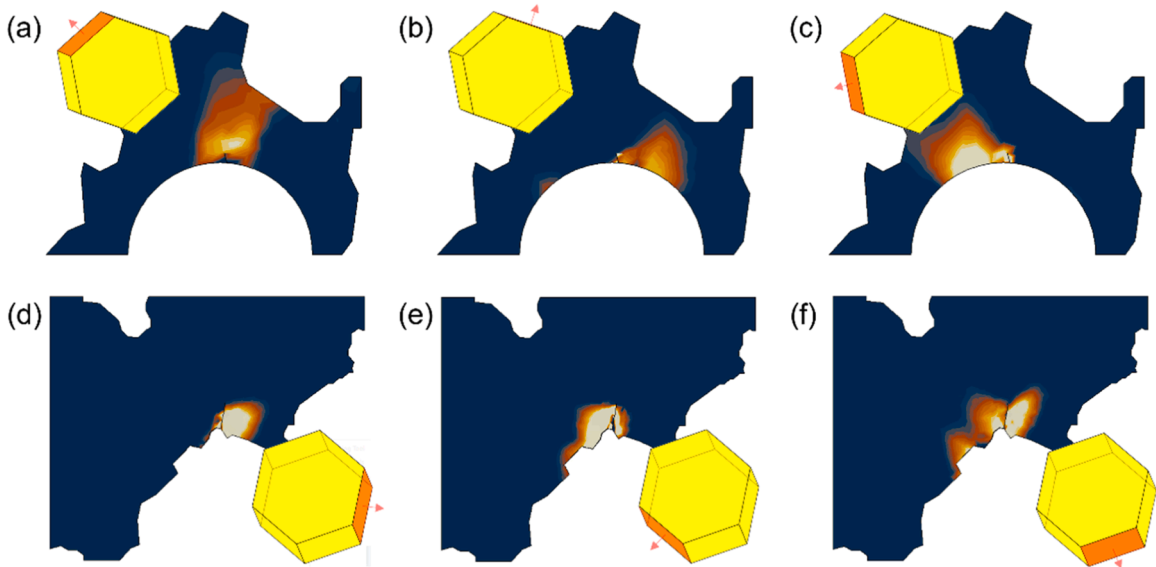


Fig. 8. Differences in prismatic slip activity at two stages of crack growth in sample B (using the maximum normal stored energy criterion). (a) – (c) predicted prismatic slip fields in the first grain after 10 fatigue cycles. (d) – (f) predicted prismatic slip fields in the second grain (with reference to the experimental crack path) after several hundred fatigue cycles.

the experiment in Fig. 6 (c). While the overall crack path trend is reasonably captured here, most individual crack segments disagree. In the first grain, the crack path is pyramidal, but deviates leftward, rather than rightward. Contrarily, like the experiment, the simulated path in the second grain is also pyramidal, but deviates rightward rather than leftward, as shown in the experiment. In the final grain, crack tortuosity is predicted, which is followed by prismatic cracking, which is in conformity with the experiment and the other theoretical criteria considered.

The experimental crack path from sample B is compared against the theoretical criteria in Fig. 7. The maximum slip criterion, which is most widely used, is shown in Fig. 7 (a) to fail dramatically at capturing the experimental path. Hence, this result formed part of the motivation for this work, and sample B is discussed in greater detail than sample A.

The experimental crack path in sample A is dominated by a single prismatic slip plane direction in both grains through which it propagates. As the crack first approaches the grain boundary, it deviates slightly leftward, seemingly along a pyramidal plane. Fig. 7 (a) shows that in both grains, the maximum slip criterion also predicts prismatic-dominated paths, but which differ significantly from the experiment. Naturally, the model predicts maximum shear strain (slip) on planes which are inclined closest to 45° relative to the remote loading direction (in 3-point bending, this is the horizontal direction, though in reality, the stress-state is multiaxial due to the notch and microstructure). A simple Schmid factor analysis, based on uniaxial loading in the horizontal direction reveals that the prismatic slip systems controlling the experimental crack path have the lowest Schmid factors amongst all prismatic systems (0.18 and 0.16 for the first and second grains, respectively). By contrast, the Schmid factors for the maximum slip criterion predicted cracks were highest, at 0.48 and 0.42, respectively. The maximum energy release rate criterion predicts an entirely different result, shown in Fig. 7 (b). In the first grain, there is initially concurrence with the experiment (crack growth along low Schmid factor prismatic plane), until there is a leftward deflection along the third (intermediate Schmid factor) prismatic plane, before crossing into the second grain. At this point, a downward deflection is predicted, resulting in artefactual self-termination of crack growth; this is discussed later in greater detail (see Fig. 9). Fig. 7 (c) shows the maximum normal stored energy criterion predicts a markedly improved crack path compared the other methods. The initial crack direction matches the experiment closely until it approaches the grain boundary; just as in the experiment, there is a deflection close to this grain boundary, but in a different direction to the experiment. Note that most of the crack growth in the first grain is controlled by the prismatic system shown in Fig. 7 (c), but cracking is also predicted on pyramidal planes, which effectively produce the same crack path at the free surface. In the final grain, maximum normal stored energy predicts the experimental prismatic crack path precisely. Hence, the experimental crack path for sample B is captured using this new method is reasonably captured, including the microstructure-driven crack deflection prior to the grain boundary.

A fuller presentation of the prismatic slip system Schmid factor analysis is given in Fig. 8 for the first (a) – (c) and second (d) – (f) grains in sample B (grain numbering is according to the experimental crack path).

Based on the maximum slip simulation of sample B, shown in Fig. 7 (a), subfigures (a) and (c) of Fig. 8 are of most interest, since the predicted crack propagates along the plane shown in Fig. 8 (a), while the experimental path appears to propagate along plane shown in Fig. 8 (c). The slip fields indicate clearly that the prismatic system with maximum slip ahead of the specified crack initiation location (which is according to the experiment) is that which is presented in Fig. 8 (a). However, it should be noted that due to the notch geometry, the overall maximum slip magnitude within the first grain (at this stage of crack growth) occurs on the slip system shown in Fig. 8 (c), but in a different region to the crack initiation site. Meanwhile, lowest prismatic slip is predicted to occur on the slip system

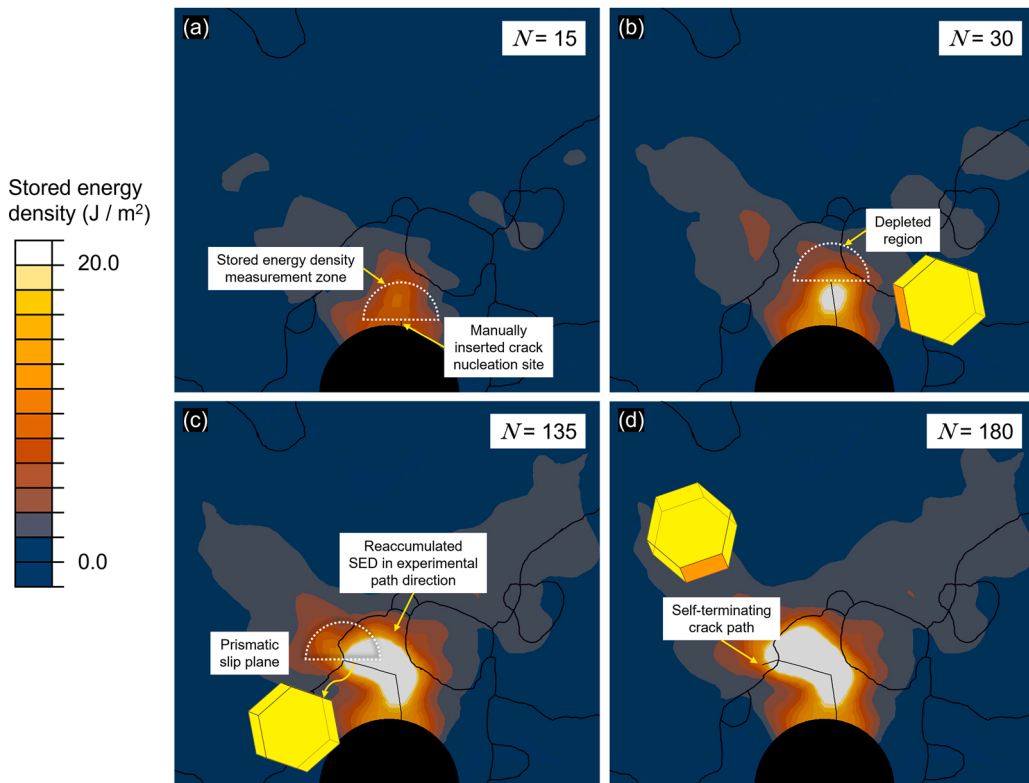


Fig. 9. SED fields in microstructure B at key four key stages of crack growth using maximum energy release rate criterion. (a) SED field at 15th fatigue cycle ($N = 15$), prior to crack propagation. Energy measurement semi-circle is shown ahead of the manually inserted edge crack. Direction corresponding to maximum energy release agrees with the experiment. (b) Energy field at first point of crack deflection. Within the semi-circular measurement zone, there is a region which is depleted of energy in the original crack growth direction. (c) Energy field at $N = 135$, where the crack first interacts with a grain boundary. The crack is clearly growing away from the region of highest SED, as there is reaccumulated energy in the experimental crack growth direction. (d) Final crack path, as crack artefactually propagates in a self-terminating direction due to cross-over of measurement zone between grains.

shown in Fig. 8 (b). Hence, it could be speculated that notch geometry or inaccurate crack initiation site definition may adversely affect the final crack path using the maximum slip model; to address this, four equally spaced crack initiation sites spanning $100\ \mu\text{m}$ of the notch are considered. In some cases, particularly those where the crack initiation site is towards the left side of the notch, there is up to $30\ \mu\text{m}$ of crack growth in a direction which agrees with the experiment. However, each case ultimately results in cracking along the plane shown in Fig. 8 (a), and hence the final crack path is effectively independent of initiation site and notch geometry. Fig. 8 (d) – (f) shows prismatic slip activity in the second grain; using the maximum slip criterion, crack growth is predicted to occur on the plane shown in (e), whereas the experimental path, and that predicted using the maximum normal stored energy criterion is controlled by the prismatic plane shown in (d).

Results at different stages of crack growth in sample B using the maximum energy release rate criterion are presented in Fig. 9. Fig. 9 (a) shows that after several fatigue cycles, the region of highest stored energy within the measurement zone is slightly to the left of the specified crack initiation site, which results in the prismatic crack path shown in Fig. 9 (b). Up to this point, the model is consistent with the experiment. Due to depletion of stored energy ahead of the crack (i.e., by maximum rate of release), the crack is propagated leftward along an alternative prismatic plane, as shown in Fig. 9 (c). This crack path results in the accumulation of energy ahead of the initial crack path, rather than the crack tip; however, since the measurement zone using this method is kept ahead of the crack tip, this is unaccounted for. This is considered in greater detail in the discussion section for prediction of short crack bifurcation phenomena. Lastly, as the crack traverses the grain boundary (see Fig. 9 (d)), it is propagated in a downward facing direction, resulting in crack arrest.

In terms of sample B, the maximum normal stored energy density criterion is shown to best capture the experimental crack path; the main difference is that before traversing the grain boundary, the crack is deflected towards the right, rather than the left, as it does in the experiment. To understand the combined influence of microstructure features and the crack tip on the predicted crack path using this method, Fig. 10 shows the cyclic evolution of predicted crack plane at two points in the first grain.

At point P in Fig. 10, it is shown that for over 100 cycles before the crack reaches this point, the plane with maximum normal stored energy density is the one on which maximum slip is predicted, i.e., agrees with the maximum slip model. However, as the crack length increases, and the crack tip stress fields begin to take greater effect, the predicted crack plane switches to pyramidal (which is one of

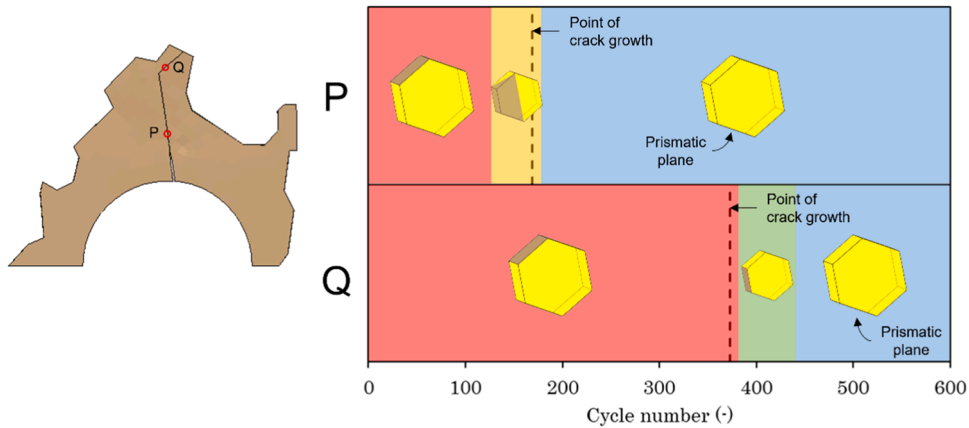


Fig. 10. The evolution of predicted crack path planes during crack growth for the first 600 cycles in sample B using the maximum normal stored energy density criterion. Two points (P and Q) in the first grain of sample B are selected for analysis. The cycle number at which crack growth occurs for each location is indicated using a vertical dashed line, i.e., the ‘point of crack growth’.

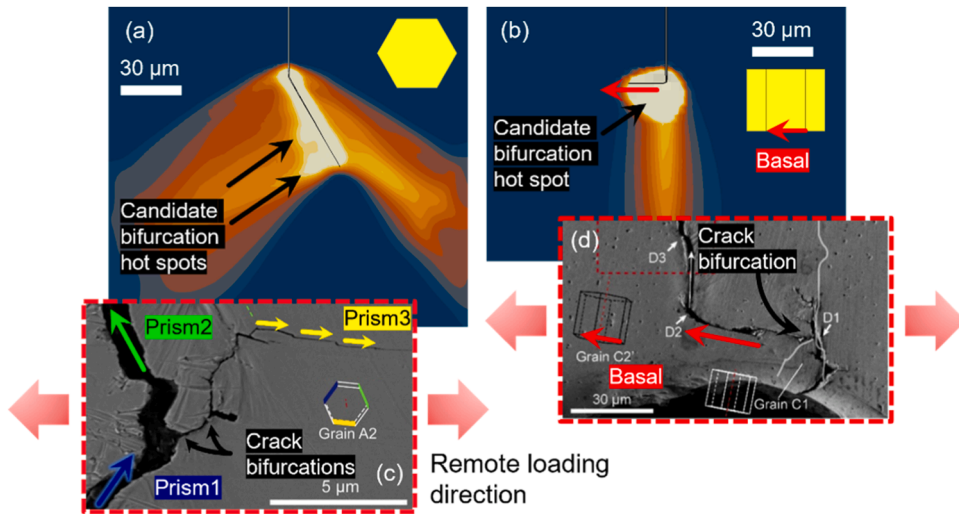


Fig. 11. Single crystal observations using the maximum energy release rate criterion in the context of the literature. (a) Single prismatic crystal crack path highlighting two potential locations for crack bifurcation to occur based on stored energy field. (b) Single crystal basal crack path, where the crack growth direction is parallel with the remote applied loading direction. The stored energy density field indicates crack bifurcation may be favourable. (c) Several examples of prismatic crack bifurcation in Zircaloy-4 (Wan, 2020). (d) Example of crack bifurcation and crack growth along a basal plane which is approximately parallel to the remote loading direction (Wan, 2020).

the predicted crack planes which agrees with the experiment) for approximately 50 cycles before the crack passes through point P. As expected after cracking, there are large redistributions of stress, and hence, a different prismatic crack plane is predicted at point P thereafter. The evolution of predicted crack plane at point Q is more interesting. As with point P, the initial predicted crack plane at point Q agrees with the maximum slip criterion. However, due to its adjacency to the grain boundary, cyclic accumulation of stored energy density due to grain-grain interactions results in the path at this point being less affected by the crack tip than at point P. Hence, this is a highly microstructure-sensitive method.

4. Discussion

Simulated crack paths in single crystals with various orientations show both examples of agreement and contradiction between the maximum slip, maximum energy release rate, and maximum normal stored energy density criteria. The HCP crack path tortuosity phenomenon (Wan, 2020) is captured using both the maximum slip and normal stored energy density criteria, and not maximum energy release rate. However, it is interesting to note that while the maximum energy release rate criterion predicts a straight prismatic crack path (Fig. 5 (e)), there are regions with significant localisation of stored energy density which are not ahead of the crack tip. Fig. 11 (a) shows this crack path again, with arrows indicating regions with localised stored energy density; the idea of crack path

bifurcation is alluded to here, where these so-called ‘hot spots’ could act as potential sites for crack bifurcation, and hence crack growth in another direction. In a grain with similar orientation, Fig. 11 (c) shows several prismatic crack bifurcations (Wan, 2020), which could potentially be explained using the maximum energy release rate criterion. Bifurcation could also enable the tortuous crack path phenomenon to be captured. However, since XFEM is used in the current studies, it is not possible to simulate bifurcated cracks explicitly. More advanced methods such as combined XFEM and cohesive zones modelling (Nikolakopoulos et al., 2020) could potentially enable this in the future. Another interesting example of single crystal cracking using maximum energy release rate is given in Fig. 11 (b). Here, unlike the other methods where prismatic cracking is predicted, there is basal cracking parallel to the remote loading direction. This prediction reflects experimental observations shown in Fig. 11 (d). As discussed with the prismatic cracking case, if crack bifurcation were enabled using some critical stored energy density for initiation of new cracks, it is likely that an alternative crack path would be predicted using maximum energy release rate, where bifurcation from the basal crack would lead to vertical prismatic crack growth.

Advancing to the polycrystal studies, each of the three criteria predicted the experimental crack path in sample A reasonably well. Despite the simulation ending prematurely, it could be argued that the maximum energy release rate criterion demonstrates the greatest overall agreement with experiment. Interestingly however, the maximum normal stored energy criterion predicts pyramidal cracking (which appears to occur in the experiment also) in both the first and second grains, but in wrong directions. As a consequence, the predicted crack path using the maximum normal stored energy density is most tortuous. The crack growth simulations of sample B reveal that the maximum normal stored energy density criterion is unequivocally superior to the other methods. It captures the straight prismatic (and pyramidal) cracks in the first and second grains, as well as the microstructure-driven crack deflection (in the wrong direction) prior to crossing the grain boundary. Though the crack deflection is predicted in a direction which differs from the experiment, it is significant that a deflection is predicted using this microstructure-sensitive method; the free surface extrusion approximation could potentially play a role here, since there are substructural effects which may have guided the experimental path. It is also shown that while the crack tip stress and strain states have a strong impact on the subsequent crack path, cyclic interactions between neighbouring grains can have a strong effect. It is interesting to highlight that within the first grain of sample B, without the crack tip present, the predicted crack plane agrees with the maximum slip method. Hence, for microstructurally *small* cracks, i.e., for crack initiation, it is anticipated that maximum slip and maximum normal stored energy density criteria would yield similar results. Therefore, it is conceivable that the maximum normal stored energy density model could act as a reliable crack path predictor across microstructurally and physically *small* and *short* fatigue cracks. Nonetheless, the new maximum energy release rate criterion initially gives promising results in sample B also. As discussed previously, regarding Fig. 9, with the introduction of some crack bifurcation capability, this criterion is likely to predict results with greater agreement with experiments.

5. Conclusion

To determine the mechanistic driving force for short fatigue crack path is non-trivial. Based on the hypothesis that dislocation slip activity plays a key role but is not the dominant factor in controlling short fatigue crack paths, two new energy-based criteria are developed. This paper has compared these new modelling methods and the conventional maximum slip criterion with experimental results in polycrystalline Zircaloy-4. In overall terms, the novel maximum normal stored energy density criterion is demonstrated as the most reliable and robust method (considered in this work) for prediction of crack paths in real microstructures. Further, it is shown to be capable of capturing the crack path tortuosity phenomenon in HCP single crystals. The maximum energy release rate criterion predictions are also shown to compare well against experimental crack paths but would likely require crack bifurcation capabilities to reach full potential. In summary, it is demonstrated that there is a requirement for alternative crystallographic crack path prediction methods for microstructurally short fatigue cracks, which are not based on dislocation slip activity alone.

CRedit authorship contribution statement

Daniel J. Long: Conceptualization, Methodology, Software, Validation, Formal analysis, Writing – original draft. **Fionn P.E. Dunne:** Conceptualization, Resources, Writing – review & editing, Supervision, Project administration, Funding acquisition.

Declaration of Competing Interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests:

Daniel J Long reports financial support was provided by Engineering and Physical Sciences Research Council. Daniel J Long reports financial support was provided by Rolls-Royce plc. Daniel J Long reports a relationship with Rolls-Royce plc that includes: non-financial support.

Data availability

Data will be made available on request.

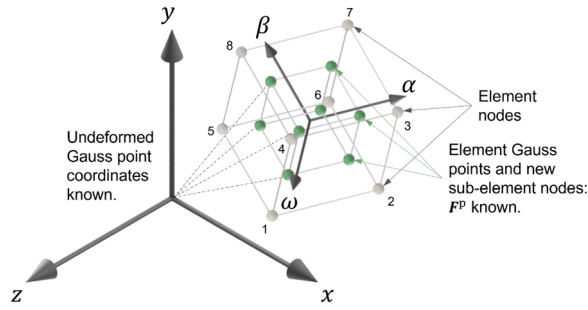


Fig. A1. Schematic showing sub-element method used to calculate spatial gradients of plastic deformation in 3D eight-node linear brick elements (C3D8). The figure shows that the nodes of the internal (sub) element are defined at the Gauss points of the original elements.

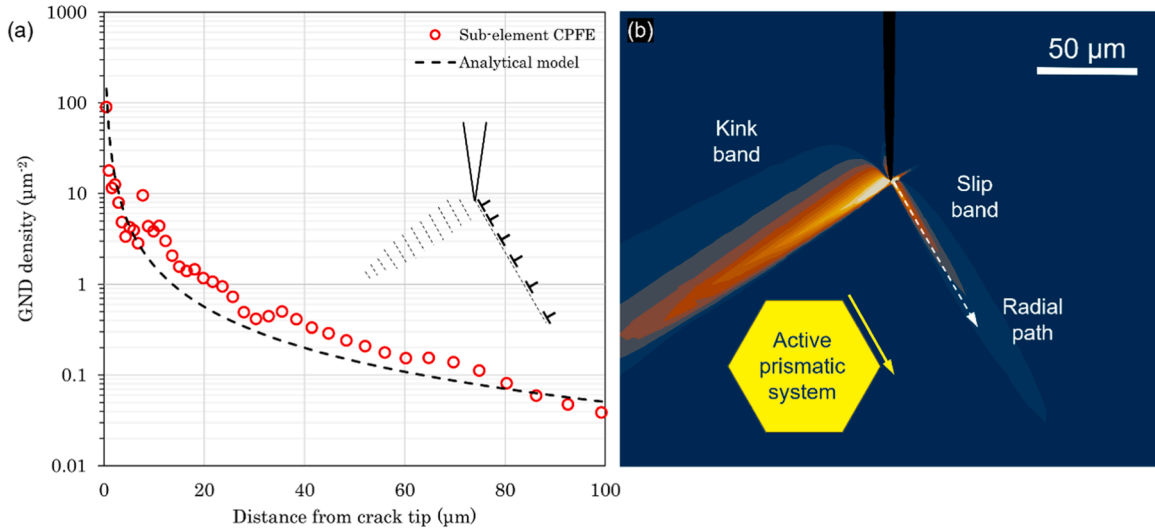


Fig. A2. (a) Comparison of CPFE-predicted radial distribution of GND density along a single prismatic slip system ahead of a crack tip with 1D analytical solution. The CPFE simulation was constrained to allow slip on this slip system only. (b) Figure showing crystal orientation and corresponding CPFE crack tip slip field. The radial path used to plot GND density is shown using a white dashed line and is parallel with the slip band. The CPFE model also predicts the formation of a kink band which projects orthogonally to the slip band from the crack tip.

Appendix A. The sub-element method for calculating GND density with linear elements

As outlined in the main body of this paper, it is necessary to calculate GND density for estimation of crack tip stored energy density and both new energy-based criteria for crack path. Eq. (6), which was derived from Ashby's 1D expression (Ashby, 1970) for GND density allows for estimation of the radial distribution of GND density along a single slip line ahead of a crack tip. Within an implicit finite element integration scheme, the full GND density increment is given by Eq. (A1) (Dunne et al., 2007), which was derived from Busso et al. (2000).

$$\Delta \rho_{\text{GND}}^i = \frac{\Delta \gamma^i}{b} \nabla \times [n^i F^p] \quad (\text{A1})$$

where F^p is the plastic deformation gradient. However, simulation of crack propagation using XFEM is limited to the use of linear elements only; eight-node linear brick elements with full integration ($2 \times 2 \times 2$) are used in this paper. Hence, this presents a problem, as it is not possible to calculate second order spatial derivatives using linear shape functions alone. Dunne et al. first presented the sub-element method (Dunne et al., 2007) for eight-node reduced integration 2D elements. As illustrated in Fig. A1 (for 3D elements), the method involves defining a sub-element internally within each finite element with eight new nodes at each Gauss point, where the plastic deformation gradient, F^p is known.

There is then a spatial distribution of plastic deformation between nodes of the sub element, which can be described simply using linear shape functions, r , within the local, α , coordinate system. The derivatives of plastic deformation within the global coordinate system, x , are then related to the local coordinate system as follows (Dunne et al., 2007),

$$\frac{\partial \mathbf{F}^p}{\partial \mathbf{x}} = \frac{\partial}{\partial \mathbf{x}} (\mathbf{r} \mathbf{F}_j^p) = \frac{\partial \mathbf{r}}{\partial \boldsymbol{\alpha}} \mathbf{F}_j^p = \frac{\partial \mathbf{r}}{\partial \boldsymbol{\alpha}} \mathbf{J}^{-1} \mathbf{F}_j^p \quad (\text{A2})$$

where $\mathbf{F}_j^p$ is the plastic deformation gradient at Gauss point, j . $\mathbf{J}$ is the Jacobian matrix, which maps from the external to the internal elements and is given by $\mathbf{J} = \mathbf{G}^x \frac{\partial \mathbf{x}}{\partial \boldsymbol{\alpha}}$, where $\mathbf{G}^x$ is a 3×8 matrix containing the global Gauss point coordinates for each element.

For validation of the sub-element method for GND calculation in combination with XFEM, a static crack finite element simulation is carried out, in which plastic slip is constrained to occur on a single prismatic slip system; this enables a comparison of the CPFE-predicted crack tip GND density distribution with the analytical solution given by Eq. (6). The results of this comparison are shown in Fig. A2. The crack length and applied stress are 300 μm and 280 MPa, respectively, resulting in a crack tip stress intensity factor of 11.8 MPa $\sqrt{\text{m}}$. It should be noted that for applied stresses greater than 280 MPa, agreement between CPFE and analytical predictions for GND density was observed to decline. Moreover, at lower levels of stress, the overall trends predicted using CPFE agreed with the analytical model, despite an increase in random variations, presumably due to mesh sensitivity, since there is considerable room for error with second order differentiation.

Overall, there is strong agreement between the sub-element method and the analytical solution for GND density, particularly in the 0–10 μm range ahead of the crack; discrepancies are likely due to mesh sensitivity in the CPFE model. A schematic illustration of the crack tip slip field is shown in Fig. A2 (a). Deformation to the left of the crack tip is accommodated for by the only active slip system (by constraint), resulting in the formation of a kink band. However, since the analytical solution only considers single slip on the right-hand side of the crack, this phenomenon could account for differences between the numerical results, particularly as the applied stress is increased.

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