



3D CP-XFEM modelling of short crack propagation interacting with twist/tilt nickel grain boundaries

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ABSTRACT

Short fatigue crack growth across grain boundaries of differing tilt and twist combinations has been investigated in three dimensions using coupled crystal plasticity and extended finite element methods. Crack path selection and growth rate are mechanistically determined by considering crystallographic planes containing the highest shear strain and the achievement of a critical stored energy density respectively. Tilt angle is found to have weak influence on crack growth rates approaching the grain boundary but increasing twist angle was shown to lead to higher growth rate retardation, as observed in experiments. Large twist angle was also shown to lead to multi-slip system activation as the crack tip traversed the grain boundary, potentially giving rise to multiple crack planes and hence faceted cracks. Elastic stored energy density was shown to capture observed sensitivity of crack growth rates and retardations to grain boundary tilt and twist, and in combination, thereby offering an improved metric over residual Burgers vector and geometric compatibility.

1. Introduction

In fatigue failure of metal alloys, short crack propagation (SCP) is a key stage which links fatigue crack nucleation and long crack propagation (Jiang et al., 2020). Understanding the mechanisms of SCP is important for improved design of advanced engineering components, particularly those which are safety-critical. Fatigue cracks nucleate from key microstructural features (e.g. pores, some types of grain boundaries, non-metallic inclusions), and undergo short crack growth which is microstructurally sensitive in which grain boundaries often show an interesting effect on propagation rate and crack path deflection (Jiang et al., 2020). SCP rate can be described by a function of the distance from crack-tip to grain boundary (Navarro and de los Rios, 1988). This distance plays an important role and it has been observed that rate retardation commences before the crack tip reaches the grain boundary, suggesting the effect of the grain boundary is associated with the stress field ahead of the crack-tip and its interaction with the grain boundary (Marx et al., 2010). Moreover, grain boundaries may affect the transition from short crack to long crack, and this depends on the blocking of the plastic zone in front of the crack-tip (Scharnweber et al., 2012). As a result of this distance effect from crack-tip to grain boundary, grain size is recognized as a key factor which affects fatigue crack initiation and the propagation rate. Generally, small grains with low Schmid factor show stronger resistance in short crack propagation (Jiang et al., 2015; Liu et al., 2020). However, the grain size effect may also reflect the number of twin boundaries contained within local region, since twins act as obstacles to dislocation motion, such that higher resolved shear stresses are required to generate slip transfer (Schneider et al., 2020).

In addition to grain size, the crystallographic parameters of an individual grain boundary are also important, particularly for cracks at short distances from grain boundaries. Differing crystal orientations can drive elastic-plastic incompatibility which affects the local stress state at grain boundaries (Barat et al., 2022). This incompatibility is a result of the crystal anisotropy, particularly in the metal alloys with high elastic anisotropy such as nickel (Zhang et al., 2021; Gonzalez et al., 2014). In polycrystal nickel, the elastic mismatch

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leads to stress concentration at the grain boundary, and the difference of Burgers vector contributes to slip blocking and potentially to crack arrest (Barat et al., 2022). Both mismatch of elasticity and plasticity can be quantitatively correlated with the crystallography of the grains on either side of a grain boundary (eg. the twist/tilt angle of favoured slip planes). Previous X-ray microtomography observation found that grain boundaries with high twist angle may inhibit the crack transmission through a grain boundary (Ludwig et al., 2003). Based on the crystallographic angles at a grain boundary, a model has been suggested in which twist and tilt angle are considered as the potential factors in rate retardation and it was found that grain boundary twist angle shows a stronger effect than tilt angle in inhibiting crack propagation (Zhai et al., 2000). The role of twist angle in resistance to crack propagation was also observed in Fang et al. (2016), Wen et al. (2016). Moreover, a new criterion has been developed which considers the residual Burgers vector (Lee et al., 1990) and geometric compatibility parameter (Luster and Morris, 1995; Livingston and Chalmers, 1957; Shen et al., 1988) and achieved good agreement with experiments in determining the ability of crack transmission through a grain boundary (Jiménez et al., 2019). Another statistical study addressing the above two parameters was recently reported in Fu et al. (2021) and found that a lower geometric compatibility parameter and higher residual Burgers vector led to easy crack nucleation at a grain boundary followed by short crack propagation. At the sub-grain level, dislocation channels reflecting slip interact with grain boundaries, resulting in slip transfer or blocking and this behavior shows crystallographic sensitivity (discontinuous dislocation channels are easy to form in the adjacent grains with low Schmid factor) in experimental observations (McMurtrey et al., 2014). Microstructure sensitive cracking is of course related to the plastic field ahead of the crack-tip, but when a crack-tip approaches a grain boundary, the crack tip stress field interacts with the grain boundary which may ultimately lead to slip transmission (Sangid et al., 2011), which has also been demonstrated as an important factor in crack growth across grain boundaries (Rovinelli et al., 2018; Sangid et al., 2020). The above experimental studies predominantly focus on the crystallography local to crack-tip and grain boundary, and have clearly demonstrated the strong crystallographic dependence of SCP in the region of a grain boundary. This local crystallographic effect demonstrates that the remote stress is not appropriate to quantify the behaviour of SCP near to grain boundaries (Singh et al., 2020). Instead, the local stress state may be a much better descriptor to be considered, not least because slip localization is common near both crack tip and grain boundary (Wilkinson et al., 1998).

Based on this understanding of local stress state and importantly dislocation density, a new criterion based on critical stored energy density has been developed (Wan et al., 2016; Wilson and Dunne, 2019; Wilson et al., 2018). This quantity has been used in crystal plasticity extended finite element method (CP-XFEM) modelling work to predict crack paths in polycrystals showing good agreement with experiments (Wilson et al., 2019). In addition, stored energy density as a mechanistic driver of crack growth has the considerable advantage over other quantities (such as crack tip stress, plastic strain, or dissipated energy) in that it is non-singular and defined at crack tips (Xu et al., 2021).

This paper aims to investigate the relationship between grain boundary twist/tilt angles (as a key part of microstructure features but not the whole story) and SCP rate in microstructurally-sensitive three-dimensional crack growth. Focused studies on bicrystals are employed in order to remove potential heterogeneous effects of surrounding grains in a polycrystal analysis (Potirniche and Daniewicz, 2003; Yang et al., 2022), for example, so as to simplify and quantify grain boundary crystallographic effects on rate of propagation alone. A systematic study of the mechanistic link between the SCP behaviour and grain-boundary crystallography is carried out, which utilises a series of grain boundary crystal orientation combinations which are implemented within a 3D CP-XFEM bicrystal crack growth model. The results of crack propagation rate and local stress state corresponding to differing twist/tilt combinations are extracted for 3D cracks and discussed in the following sections. The results are also assessed qualitatively in the context of experimental observations in the literature.

2. Methodology

2.1. Crystal plasticity and XFEM

A dislocation-based crystal plasticity model coupled with elastic anisotropy is utilized to investigate microstructurally-sensitive crack propagation in polycrystal nickel alloy. The plastic velocity gradient L_p is calculated in terms of slip, and slip system directions and normals by

$$L_p = \sum_{i=1}^{12} \dot{\gamma}^i s^i \otimes n^i \quad (5)$$

where s^i and n^i are the slip direction and plane normal of the i^{th} slip system respectively. $\dot{\gamma}^i$ is slip rate, which is based on both thermal activated dislocation escape and glide, and on athermal slip system hardening processes resulting from both sessile statistically stored (SSD) and geometrically necessary (GND) dislocations (Dunne et al., 2007, 2012). The slip rule is given by

$$\dot{\gamma}^i = \rho_{SSD}^m b^2 \nu \exp\left(-\frac{\Delta F}{kT}\right) \sinh\left(\frac{|\tau^i - \tau_c^i| \Delta V}{kT}\right) \quad (6)$$

where ρ_{SSD}^m is the density of mobile dislocations, b the Burgers vector magnitude, ν the attempt frequency of dislocations to jump the energy barrier, ΔF the activation energy associated with dislocation escape and ΔV is the volume associated with the activation. k is the Boltzmann constant and T the environment temperature. τ^i is the resolved shear stress on the i^{th} slip system, and τ_c^i is the slip system strength, which evolves with slip accumulation following dislocation hardening given by

$$\tau_c = \tau_0 + \alpha G b \sqrt{\rho_{SSD}^s + \rho_{GND}} \quad (7)$$

where τ_0 is the initial intrinsic slip strength, G the shear modulus, α the coefficient of Taylor hardening, and ρ_{SSD}^s and ρ_{GND} the densities of SSDs and GNDs respectively. ρ_{SSD}^s is assumed to evolve according to an isotropic strain hardening law

$$\dot{\rho}_{SSD}^s = \lambda \dot{p} \quad (8)$$

where λ is a hardening coefficient, and p is the effective plastic strain, which is defined as

$$p = \left(\frac{2}{3} \mathbf{e}^p : \mathbf{e}^p \right)^{\frac{1}{2}} = \left[\frac{2}{3} \left((\epsilon_{xx}^p)^2 + (\epsilon_{yy}^p)^2 + (\epsilon_{zz}^p)^2 + 2(\epsilon_{xy}^p)^2 + 2(\epsilon_{yz}^p)^2 + 2(\epsilon_{xz}^p)^2 \right) \right]^{\frac{1}{2}} \quad (9)$$

ρ_{GND} which accommodates the lattice curvature is calculated from Nye's dislocation tensor $\mathbf{A}$ (Cheng and Ghosh, 2015) given by

$$\mathbf{A} = \text{curl}(\mathbf{F}_p) = \sum_{i=1}^{12} \rho_{Gs}^i \mathbf{b}^i \otimes \mathbf{s}^i + \rho_{Gen}^i \mathbf{b}^i \otimes \mathbf{n}^i + \rho_{Get}^i \mathbf{b}^i \otimes \mathbf{t}^i \quad (11)$$

where $\mathbf{s}^i$, $\mathbf{n}^i$ and $\mathbf{t}^i$ are the three orthogonal unit vectors, ρ_{Gs}^i the density of screw dislocations parallel to $\mathbf{s}^i$, ρ_{Gen}^i the density of edge dislocations parallel to $\mathbf{n}^i$, and ρ_{Get}^i the density of edge dislocation parallel to $\mathbf{t}^i$. Because FCC nickel crystals have 12 slip systems, the GND tensor comprises 36 independent variables (12 edge branches, 12 screw branches along $\mathbf{n}^i$, 12 edge branches along $\mathbf{t}^i$), which need to be solved from nine equations. These can be re-written in matrix form

$$\hat{\mathbf{A}} = \mathbf{A} \boldsymbol{\rho}_{GND} \quad (12)$$

where $\hat{\mathbf{A}}$ is a 9×1 column vector of Nye's dislocation tensor, and $\mathbf{A}$ a 9×36 matrix containing the basis tensors $\mathbf{b}^i \otimes \mathbf{s}^i$, $\mathbf{b}^i \otimes \mathbf{n}^i$, $\mathbf{b}^i \otimes \mathbf{t}^i$. $\boldsymbol{\rho}_{GND}$ is a 36×1 column vector of GND components. However, the 36 independent GND components may generate a non-uniqueness problem with the above nine equations, hence an L_2 norm of GND density minimization is used to determine the local GND density (Arsenlis and Parks, 1999) and an overall density determined as

$$\rho_{GND} = \sqrt{\sum_{i=1}^{12} (\rho_{Gs}^i)^2 + (\rho_{Gen}^i)^2 + (\rho_{Get}^i)^2} \quad (13)$$

In this study, elastic stored energy density is investigated as the primary driving force for fatigue crack growth, which has been reported for several alloys and shows good agreement with experimental observations (Wan et al., 2014; Chen et al., 2017, 2018). The evolution of elastic stored energy density can be calculated from

$$G = \int \dot{G} dN \quad (14)$$

where $\dot{G}$ is the rate of elastic stored energy density per cycle, which can be obtained from

$$\dot{G} = \int \frac{\xi \boldsymbol{\sigma} : d\mathbf{e}^p}{\sqrt{\rho_{SSD}^s + \rho_{GND}}} \quad (15)$$

where ξ is the coefficient which specifies the fraction of dissipated energy which is stored in the material as dislocation structure. Here ξ is chosen to be 0.05 (Wan et al., 2014). The stored energy density is a crystal plasticity approximation to the dislocation configurational energy density which is the recoverable (elastic) energy stored by dislocation interactions and structures (Zheng et al., 2019) resulting from slip. The crystal plasticity approximation was argued in Wan et al. (2014) where choosing the fraction of plastic work stored as ~ 0.05 was shown to give reasonable estimates of the dislocation configurational energy density, and also shown to capture experimentally observed crack locations.

To minimize the effect of mesh-sensitivity, a non-local averaging method is introduced based on Nguyen et al. (2015), in which integration point quantities are calculated from a discrete sum over the surrounding integration points within a defined radius, l .

$$G = \sum_{i=1}^n G_i g(r) \quad (16)$$

$$g(r) = e^{-\frac{r^2}{l^2}} \quad (17)$$

where n is the number of surrounding integration points, G_i is the local stored energy at the integration point i and r is the distance to the integration point. l reflects the length scale over which the dislocation structures (dominated by GND density) affect the SCP, which is here chosen to follow previous work and to be three times the element size selected (Wilson and Dunne, 2019).

XFEM is utilized to introduce and propagate cracks. This method has been implemented in Abaqus software with an additional user defined damage subroutine. XFEM enables the modelling of discontinuities such as a moving crack in solid parts, and alleviate the

Table 1
Material properties for Rene88DT.

C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	τ_{c0} (MPa)	$b(\mu\text{m})$
273.6	170.7	125.8	420	2.54×10^{-4}
$\lambda(\mu\text{m}^{-2})$	$\nu(\text{s}^{-1})$	$\Delta F(\text{J/atom})$	$\rho_{\text{ssdm}}(\mu\text{m}^{-2})$	$\Delta V(\mu\text{m}^3)$
12	1.0×10^{11}	8.2×10^{-20}	0.02	$22b^3$

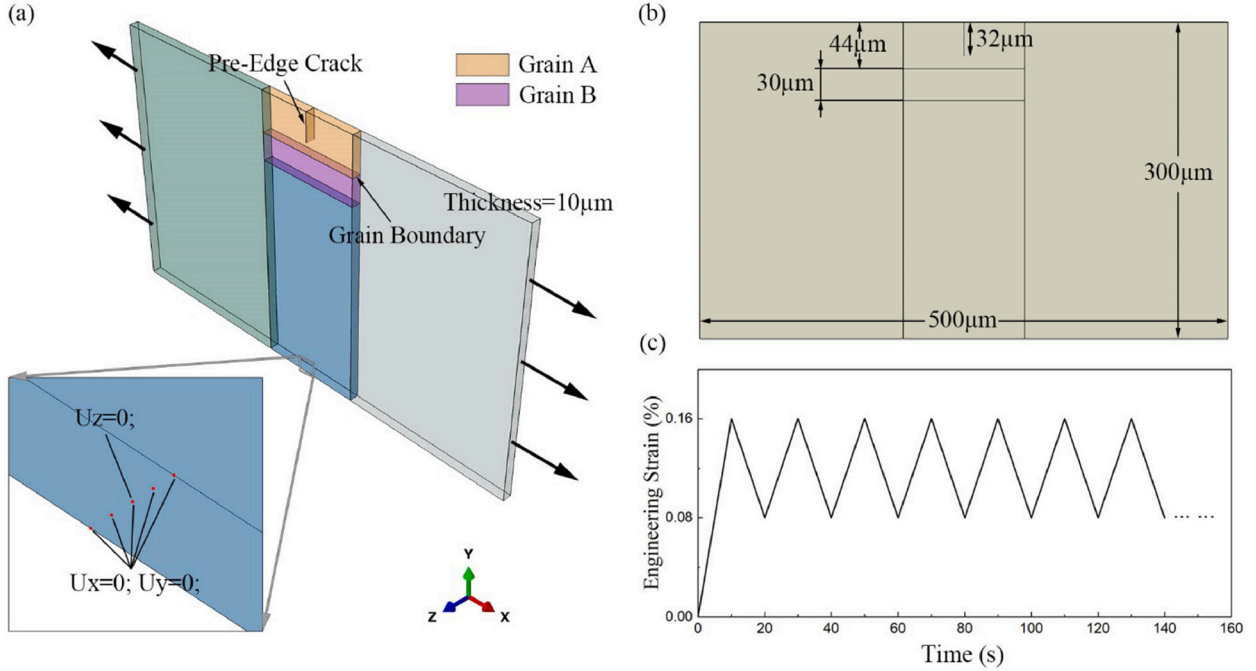


Fig. 1. (a) Loading and boundary conditions of the edge-cracked bicrystal model, (b) dimensions and (c) strain-controlled loading history.

requirement of remeshing at crack tips. In this method, the element to contain the crack is bisected by introducing phantom nodes when the element's damage criterion is achieved specified by a critical value. The bisection plane is the fracture plane which can be set in the user defined damage subroutine. In this study, the bisection/fracture plane is set as the slip plane (plane nomenclature given in Appendix A) which contains the highest slip, and the damage criterion chosen for crack advance at its tip is the non-local stored energy density (Eq. (15)) once a critical energy value is reached. The CP-XFEM introduced in this section has been used in previous work with differing materials, and more details about algorithm and convergence studies can be found in [Wilson and Dunne \(2019\)](#), [Schaefer and Marx \(2012\)](#), [Scharnweber et al. \(2012\)](#), [Yang et al. \(2022\)](#).

2.2. Material properties, and edge-cracked model set up

Rene88DT is a polycrystal nickel-based superalloy which is widely used for aero-engine turbine discs, with an average grain size $\sim 26 \mu\text{m}$ and fatigue behaviour strongly associated with grain boundaries ([Echlin et al., 2016](#)). Its single crystal anisotropic elastic and slip properties have been calibrated previously ([Zhang et al., 2021](#)) and are shown in Table 1.

A fully three-dimensional bicrystal finite element model has been designed as shown in Fig. 1(a) and (b) with dimensions reflecting the polycrystal average grain size. This bicrystal model includes two grains of interest (Grain A coloured orange, Grain B coloured violet). The thickness of the plate is chosen to be $10 \mu\text{m}$ to minimize the variation along the fracture plane in the z -direction. A $32 \mu\text{m}$ pre-edge crack is inserted in Grain A, which has a plane aligned with the global YZ plane and goes through the whole thickness ($10 \mu\text{m}$). The model is meshed using 18848 C3D8 Abaqus elements following a mesh sensitivity study, reported in Appendix B. The orientations of grains A and B are chosen to give a systematic range of tilt and twist angles. The grains to the left and right of grains A and B are chosen to be purely elastic (since plasticity is confined locally to the crack tip) and facilitate the far-field applied loading. Cyclic strain-controlled loading is applied on the sides of the plate, and simulation is terminated when the crack grows to a length (projected length $\sim 24 \mu\text{m}$, 62 $\sim$ 140 cycles) sufficient to extract growth rates as a grain boundary is traversed, and dimensions and loading boundary conditions can be found in Fig. 1(b) and (c).

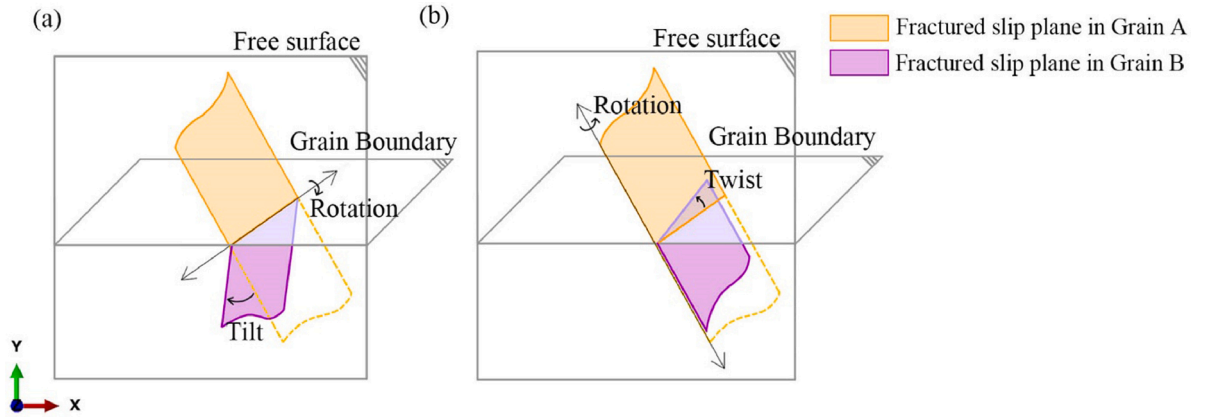


Fig. 2. Schematic diagram of (a) tilt rotation and (b) twist rotation to give desired tilt/twist combinations.

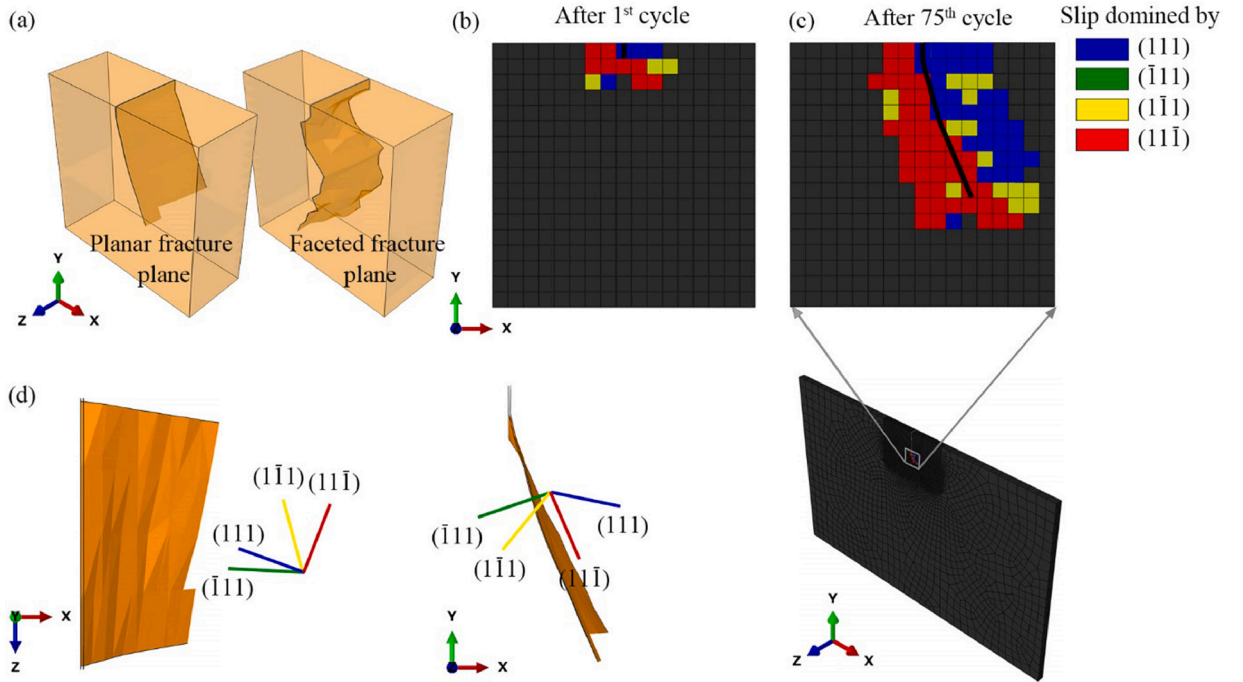


Fig. 3. (a) A morphological comparison between a single fracture plane and faceted fracture planes. Slip activations at the crack tip after (b) 1st cycle and (c) 75th cycle, where colour is used to differentiate the four crystal plane types, and (d) the morphology of fracture plane of Grain A in two views shown

2.3. Selection and quantification of tilt/twist grain boundary combinations

Grains A and B and their common grain boundary form the region of interest (ROI) in this analysis. A systematic study of tilt and twist angles on progressive growth rates as the crack grows through a series of crystal orientation combinations is carried out based on these two grains and the model described in Fig. 1. Here the tilt and twist angles used in this paper refer to the geometric relationship between the two fracture planes on either side of the grain boundary, rather than the lattice misorientation (Zhai et al., 2000). Because the fracture plane is determined as the slip plane which contains the slip system with the highest plastic slip, the definition of tilt and twist can be schematically shown by fractured slip planes in Fig. 2. Of course, a priori, that slip system with the highest slip is not yet known so the crack planes developing from the initial crack similarly remain unknown until a given analysis is completed.

To generate such fracture planes with particular tilt/twist combinations (Fig. 2), we assume to begin that the two fracture planes on either side of the grain boundary have the same Miller indices, that is, we take the slip systems with highest plastic slip in Grain A and B to be in identical slip systems. A crystal rotation scheme shown in Fig. 2 is then used to create a series of slip planes which have certain tilt/twist combinations.

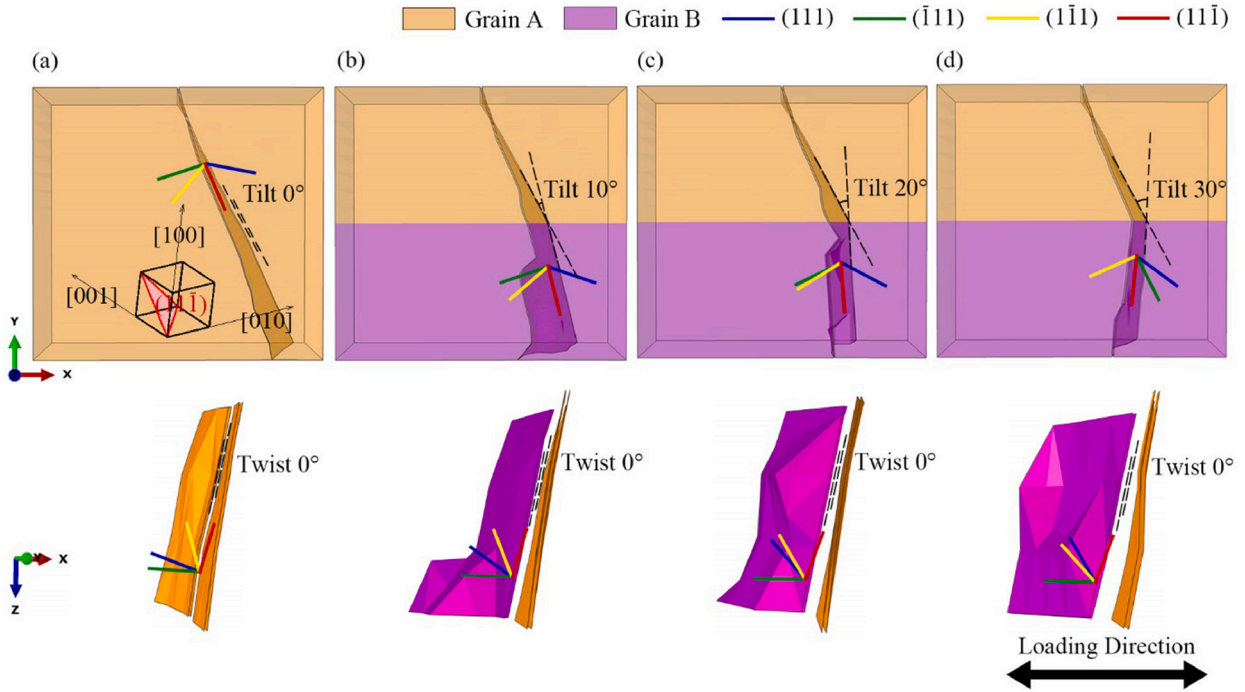


Fig. 4. Morphologies of the fracture planes for four differing tilt angles of (a) 0°/Single crystal; (b) 10°; (c) 20°; and (d) 30°, all for a twist angle of 0°. The crystal lattice overlapping on (a) shows the reference crystal orientation (Grain A).

Fig. 2 schematically shows possible tilt/twist angles which can be obtained by rotating Grain A about an axis which is determined either by the intersection between Grain A's slip plane and the grain boundary to give a tilt angle, or by the intersection of Grain A's slip plane and the free surface, to give the twist angle. However, there are four equivalent $\{111\}$ slip planes in FCC crystals such that the crack planes selected depends upon which plane is activated for slip to the highest extent. A whole range of combinations of slip system orientation combinations are therefore modelled and the resulting crack plane activations near the grain boundary which occur under cyclic loading are determined. With knowledge of the planes on either side of the grain boundary which have been found to crack, the true tilt and twist angles for each analysis are then extracted.

The applied cyclic loading (Fig. 1) leads to slip activation at the crack-front, resulting in local accumulation of stored energy density. Every uncracked element located along the crack front has its non-local stored energy density calculated, and once this quantity achieves the defined critical value, this element is bisected with the extended crack along that slip plane containing the highest slip, in turn leading to incremental crack propagation and the redistribution of all local crack tip quantities (slip, stress, etc). Because the model plate is meshed such that the out of plane Z-direction contains four elements through thickness, the stored energy density is nonuniform along the thickness. A consequence is that the crack front need not remain straight, and for example, the free surface (corresponding to plane stress state) crack growth may occur at a different rate to that sub-surface (approximately approaching a plane strain state for thick plates). In addition, non-planar cracks may grow, made up of multiple 'facets' on differing planes during the propagation process, and an example of this is shown in Fig. 3(a), resulting from differing slip systems activated containing the highest slip along the crack front, for example resulting from changing stress state. Although a fracture plane consisting of multiple facets is more representative of actuality and observation in polycrystal alloys in experiment, it adds complexity of fracture morphology for a quantitative study of short crack propagation in terms of the difficulty of quantifying growth rates near grain boundaries. On the contrary, ideal scenarios of two non-faceted fracture planes on either side of a grain boundary are preferred for which definitive twist and tilt geometric relationships between the two fracture planes can be quantified, removing the potential effects of minor deviations of fracture planarity arising from the facets.

In this study, a very large number of crystal orientation combinations were studied to seek a sufficient number of 'special' crystal orientation which led to predominantly single slip in Grain A so that planar fracture planes either side of the grain boundary were developed for a distance suitably removed from the grain boundary to allow quantification of crack propagation rates with uniformly planar cracks. An example for a particular selected edge-cracked (single) crystal orientation is selected to show the slip activations ahead of a crack tip in Fig. 3(b) and (c). Four differing colours are used to show the strongest activated slip system ahead of a crack tip where, for example, red means the element's strongest activated slip system belongs to the slip plane $(11\bar{1})$, and the other three colours correspond to the slip planes shown. In this case, it can be seen that the field ahead of the crack-tip is dominated by red indicating that the slip activation at the crack front is dominated by $(11\bar{1})$. Fig. 3(d) shows the morphology of the fracture plane in two perspectives (X-Z and X-Y views), and the corresponding four lines are plotted by the intersections between the slip planes and the corresponding view planes. In both of the two views, the observed fracture plane can be seen to be aligned with the $(11\bar{1})$ plane (red line in Fig. 3(d)). Based

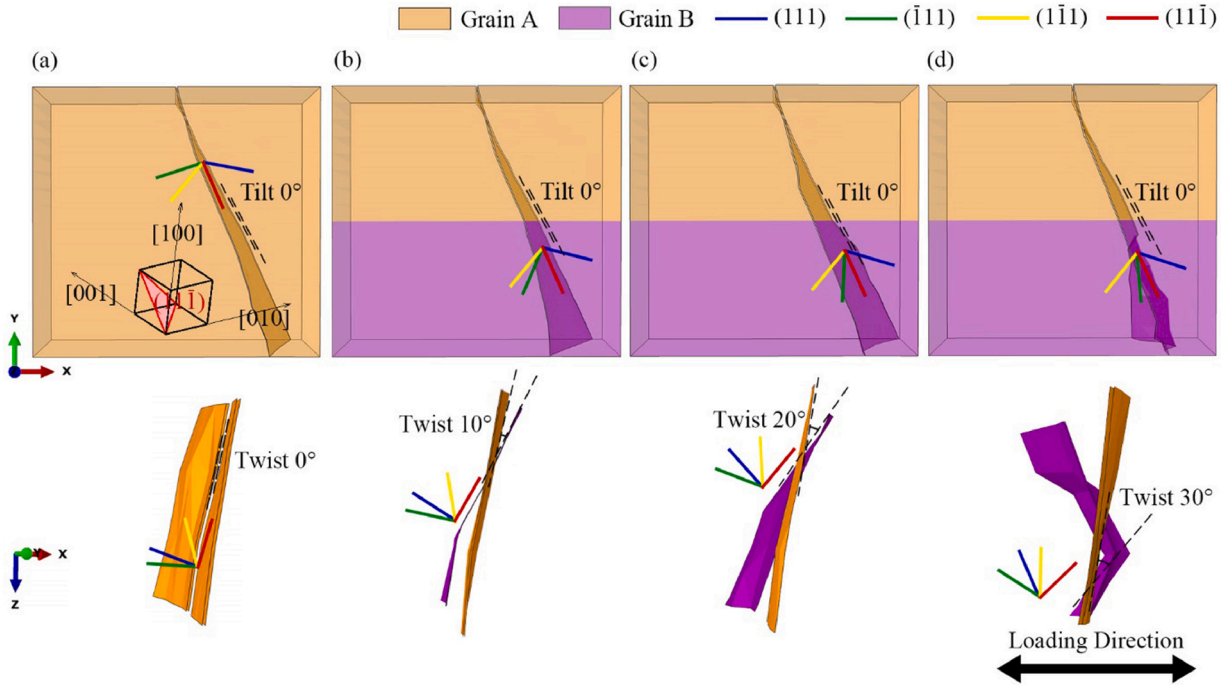


Fig. 5. Morphologies of the fracture planes for differing twist angles of (a) 0°/Single crystal; (b) 10°; (c) 20°; and (d) 30°, all for a tilt angle of 0°. The crystal lattice overlapping on (a) shows the reference crystal orientation (Grain A).

on the above analysis, the resulting single fracture plane which develops and is shown in (d) can be identified to be on slip plane $(11\bar{1})$.

The crystal orientation selected and shown in Fig. 3 therefore satisfies the requirement for a single fracture plane (Fig. 3(a)) because its crack front is dominated by $(11\bar{1})$ in the single crystal case (Fig. 3(b)(c) and (d)) with a planar fracture fashion. Hence, this special crystal orientation with respect to the pre-crack and loading direction (termed the reference crystal orientation subsequently) is used for modelling Grain A and in the determination of Grain B orientations selected in order to obtain the desired tilt/twist grain boundary misorientation combinations of interest, as discussed in Section 2.2 (Fig. 2). However, it's noted at this stage that the fracture plane that develops in Grain B after loading cannot be determined a priori for a given crystal orientation combination, so the crack tilt/twist orientation which actually results needs to be confirmed for each model analysis post-analysis.

3. Results – assessment of short crack propagation for selected tilt and twist grain boundaries

The crack paths selected and the corresponding propagation rates of short cracks with differing tilt/twist angles are analysed in this section. In the latter, the focus is placed on the growth rate variations local to the grain boundary and a quantitative study for this is addressed in Section 3.2, in which the roles of tilt and twist angles are independently assessed against experimental data. In addition, combined grain boundary tilt and twist are also assessed.

3.1. Crack paths

In order to investigate the role of tilt and twist angle on crack propagation paths, we assess 3D crack growth through a grain boundary under cyclic fatigue loading with varying tilt angles while keeping the twist angle in these cases to be zero. The crystal orientations of grains A and B have been selected on the basis of the discussion just presented in order to achieve a range of tilt-twist combinations.

Fig. 4 shows the four bicrystal orientation combinations selected (where the first is simply a single crystal with grain B taking the same orientation as grain A). The orientation of grain A is selected as discussed above and is assigned the reference orientation. Grain B orientations are selected in order to achieve as close as possible to the desired resulting tilt angles of 10, 20, and 30° respectively. Fig. 4 (a) shows the crystal configuration in which both of grains A and B are assigned with reference crystal orientation (the single crystal case). This case shows a near-smooth fracture plane crossing the whole ROI, and this fracture plane is identified as $(11\bar{1})$ through a crystallographic analysis and corresponds to a tilt angle of zero (and with a twist angle of zero). Fig. 4(b), (c) and (d) show three resulting bicrystal fatigue cracks with tilt angles of 10°, 20° and 30° respectively. In these crystal configurations, each grain B orientation is generated by rotating from the crystal orientation of grain A (the reference crystal orientation) by an appropriate angle (see Fig. 2(a)), where the latter angles are determined post-analysis once the crack growth paths are known. The results of the 3D fatigue crack growth analyses are shown in Fig. 4(b)(c) and (d) respectively. A few deflections of the fracture planes developing in

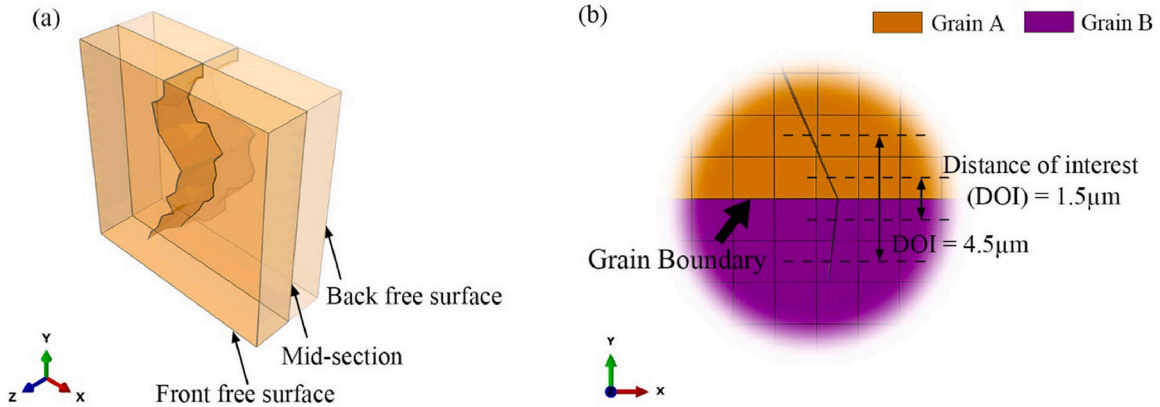


Fig. 6. (a) Three key sections used for collecting the crack propagation rates near the grain boundary, and (b) the two distances of interest from the grain boundary for which data are extracted.

grain B occur because sometimes the strongest activated slip system may change to another slip plane, but the deflections are small and the fracture planes can still clearly be identified as $(11\bar{1})$ through a crystallographic analysis (see the red lines parallel to the fracture plane). In all these crystal configurations, $(11\bar{1})$ is always the slip plane with strongest plastic shear strain. In addition, the three desired tilt angles are achieved by the deflected fracture plane in grain B without twist (see the dashed lines). The results demonstrate that the selected reference crystal orientation of grain A and the (rotated) crystal orientation of grain B can correctly generate a series of fracture planes which have the required (varying tilt and zero twist) geometric relationships.

A similar systematic study of grain boundary twist angle effects on crack path has been carried out for a tilt angle of zero where grain crystal orientation combinations have been determined to give the desired crack twist angles. The fracture planes for twist angles between 0 and 30° are shown in Fig. 5(a), (b), (c), and (d). Fig. 5(a) is the 0° twist case, which is therefore the same single crystal analysis as that in Fig. 4(a). In Fig. 5(b) and (c), the fracture planes are $(11\bar{1})$ and show twist angles of 10° and 20° without tilt, in agreement with expectations. However, in Fig. 5(d), the predicted fracture plane in grain B was found to comprises two main slip planes, namely (111) and $(11\bar{1})$, where the latter $(11\bar{1})$ is the expected fracture plane that shows a 30° twist relationship with respect to the fracture plane in grain A. Fig. 5(d) shows a case of multiple fracture planes as described in Fig. 3(d). This complex fracture arises because of the multiple slip activations within the ROI associated with the high twist angle. Fig. 4 and Fig. 5 show that anticipated crack plane tilt/twist angles have been obtained in the predicted CP-XFEM modelling except for the case of a twist angle of 30° which gives more complex crack morphology. In the next sections, the crack growth rates are investigated as the cracks grow through the grain boundaries of differing types such that the role of tilt and twist angles on propagation rates may be analysed.

3.2. Crack propagation rates

Stored energy density is a recently developed fatigue criterion which considers the local stress state and dislocation density at crack tips. The mechanistic details and validation for this criterion can be found in Wilson et al. (2019), Xu et al. (2021), and it is employed here, as outlined in Methods, as the criterion to control crack advance implemented by finite element bisection within XFEM, as outlined above. A critical stored energy density of 0.65J/m² is selected pragmatically simply to ensure that sufficient 3D crack growth occurs over reasonable numbers of fatigue cycles to facilitate crack growth rate measurements local to the grain boundary of interest, within tractable CPU times. An examination of the selection of the critical value chosen and its ramifications can be found in Appendix C, which demonstrates that increasing critical energy decreases crack advance rate, and vice versa but that the qualitative effects of grain boundaries on crack advance are not changed with selection of the critical stored energy density.

In CP-XFEM, the finite element is the minimum unit of crack advance, which is calculated for every element at the crack front independently utilising the non-local method outlined in Methods. Hence differing crack advance rates at the crack front are anticipated because of varying local stress state (macroscopically from free to sub-surface, but also generated by the crack tip in an elastically anisotropic crystal). In order to consider the crack propagation rates in fully 3D growth near grain boundaries, three key planes within the model ROI are selected at which crack propagation rates at defined projected crack lengths a_i are collected for subsequent analysis, namely the bicrystal front free surface, the mid-section, and the back free surface, corresponding to three depths along the Z-direction shown in Fig. 6(a). With these data, average projected crack growth rate in the Y-direction is then calculated as

$$\frac{da_i}{dN_{averaged}} = \frac{d[element\ size \times n]}{d[(N1 + N2 + N3)/3]} \quad (18)$$

where n is the number of bisected elements projected onto plane YZ, $N1$, $N2$ and $N3$ are the cycle numbers required for the crack to grow to a_i on the front free surface, mid-section and back free surface respectively. An analysis of interest and importance is to assess the potential resistance (or enhancement) provided by the grain boundary to crack propagation. Based on the element size (1.5μm)

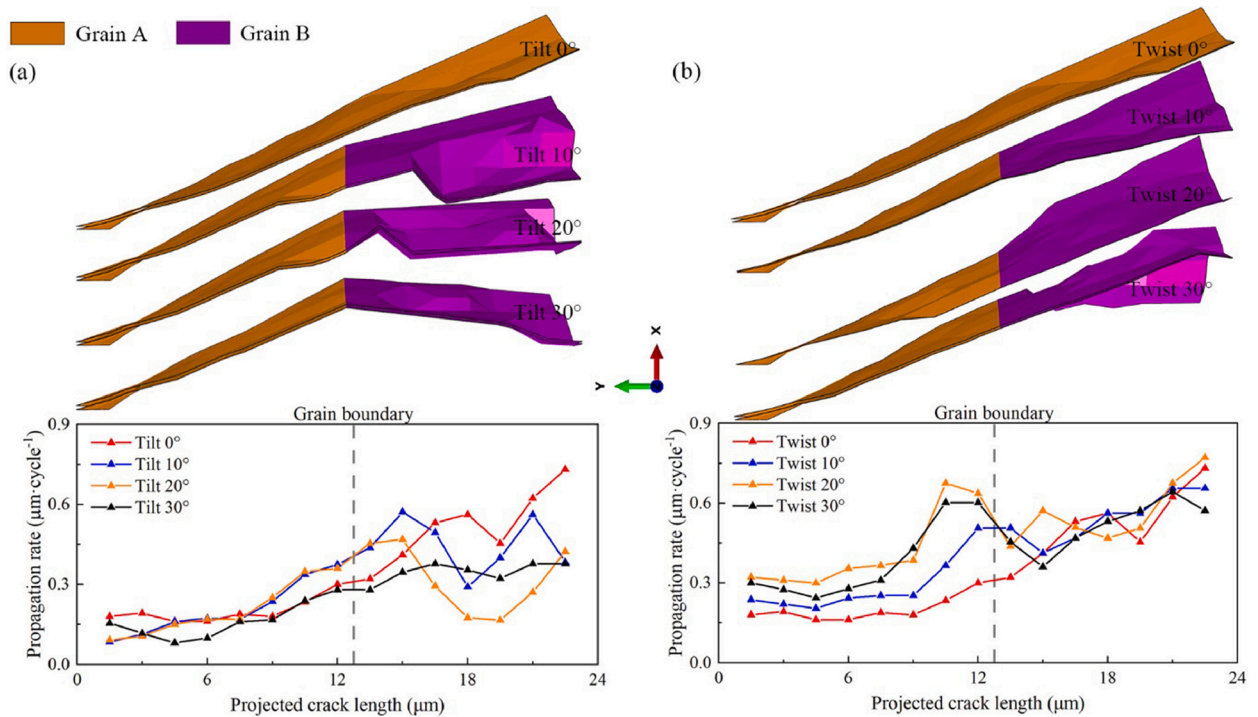


Fig. 7. Crack propagation rate versus projected crack length for fatigue crack growth across a grain boundary for (a) tilt 0° to 30° (zero twist) and (b) twist 0° to 30° (zero tilt).

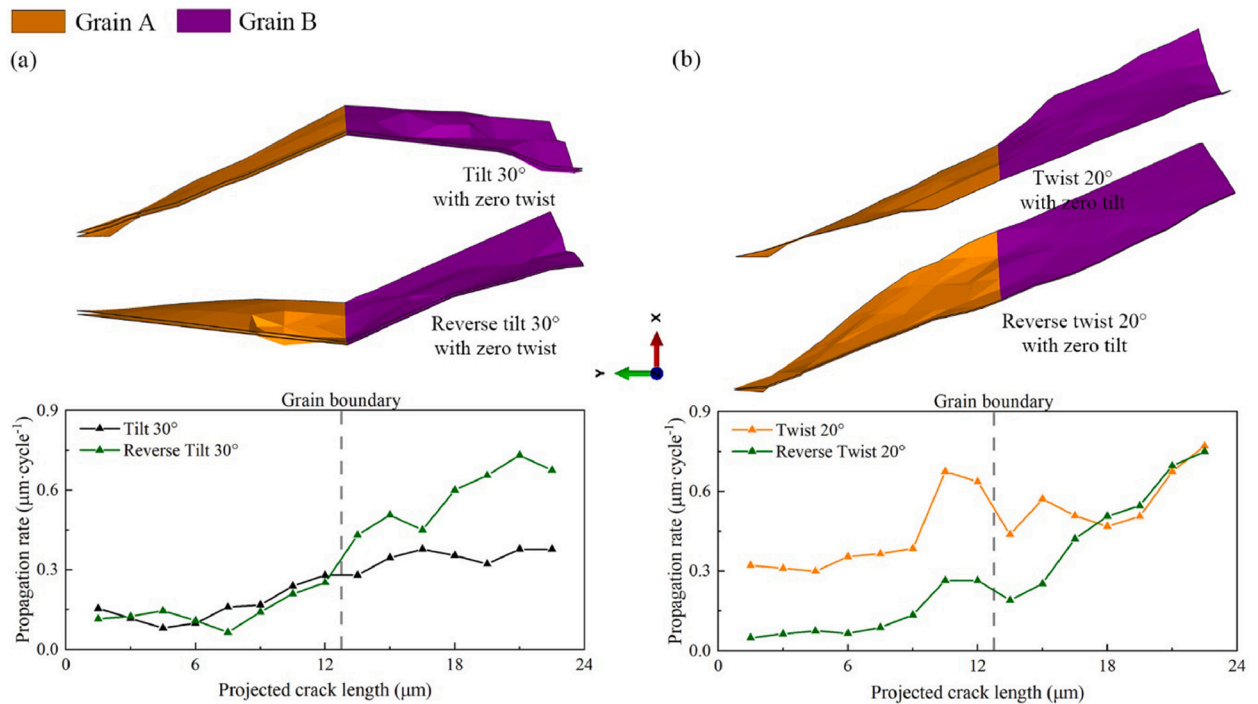


Fig. 8. Crack propagation rate versus projected crack length for (a) tilt of 30° and (b) twist of 20° showing specific results from Fig. 7 together with those obtained by exchanging the orientations of grains A and B.

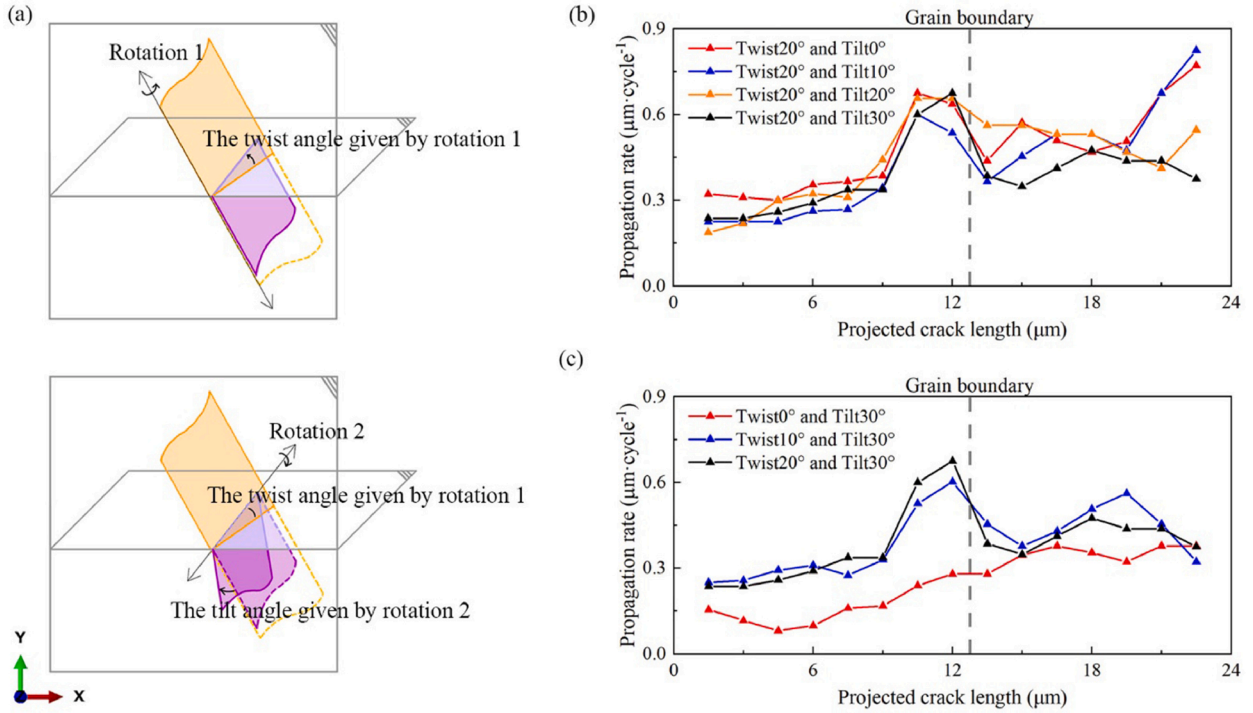


Fig. 9. (a) Schematic diagram showing combined grain boundary twist and tilt; (b) Crack propagation rates versus projected crack length in crystal configurations with fixed twist 20° and tilt angles between 0 and 30°; (c) Crack propagation rate in crystal configurations with fixed tilt of 30° and twist angles between 0 and 20°.

utilised, two specific distances of interest (DOI) from the grain boundary are defined to be 1.5μm and 4.5μm, at which quantitative analysis of growth rate and hence rate of retardation/enhancement is carried out, as shown schematically in Fig. 6(b). The rate retardation/enhancement is calculated from the difference of the propagation rates determined at the two positions located at both ends of the black arrows in Fig. 6(b)).

The crack propagation rates obtained for the differing grain boundary and crystal configurations to give the systematic variation of tilt and twist are plotted in Fig. 7. These rates are plotted against the projected crack length. For any particular crack length, the crack may well be static for multiple cycles before advancing again. In addition, the corresponding final fracture surfaces (in the XY plane) are extracted and given above the rate plots for each case considered.

Fig. 7(a) and (b) show the results for varying grain boundary tilt and twist respectively, in which the positions of grain boundaries are marked by grey dashed lines (as in later figures also). Fig. 7(a) shows that cracks propagate at similar rates in grain A, which then diverge having traversed the grain boundary. No clear rate retardation was observed as the cracks grew to approach the grain boundaries for tilt angles of 0° to 20°. A weak reduction in growth rate resulting from the grain boundary interaction can be seen for only a tilt angle of 30°. Interesting rate retardations can be seen post-GB for tilt 10° and 20°, which may be caused by the local deviations of fracture surfaces as shown in the fracture planes above the rate plots (Fig. 7). These 3D tortuous fracture planes may result in a change of stress/plastic strain field away from the GB in turn leading to a rate variation. In Fig. 7(b), higher twist angles (20°, 30°) are found to lead more clearly to faster propagation rates in grain A, and these two crystal orientation combinations result in strong retardations when the corresponding cracks approach the grain boundary. Though smaller, some retardation is also observed for the twist of 10° relative to the single crystal case (twist of zero).

The rate retardations observed in Fig. 7(b) seem to be intrinsically caused by the twist grain boundaries. However, some effect may additionally come from an unfavourably orientated crystal slip system inhibiting growth rate because lower slip favourability results in weaker plastic strain in turn leading to lower stored energy and hence crack propagation rate. To examine the effect of this possibility, two comparison studies are conducted using the previous crystal configurations of a tilt of 30° and twist of 20°. A twist of 30° has not been chosen in this and later studies due to the more complex fracture trends which may obscure the roles of twist and slip favourability. The previous results are compared in Fig. 8 with those obtained with a reversal of the orientation configurations, meaning the exchange of the crystal orientations of grains A and B. That is, the twist relationships remain as before (if fracture planes remain as (111)) but the slip favourability is reversed between Grains A and B as the loading remains unchanged.

In Fig. 8(a), the reverse tilt 30° (green line) shows a faster crack propagation rate than for tilt 30° (black line) in grain B, and no retardation can be observed around the grain boundary. Hence, the slight retardation in tilt 30° is a result of unfavourably orientated crystal slip systems. Fig. 8(a) demonstrates the geometric relationship of the tilt 30° grain boundary does not provide the resistance to crack propagation; however, a retardation can be expected if the adjacent grain B is unfavourably orientated for slip. In Fig. 8(b), the

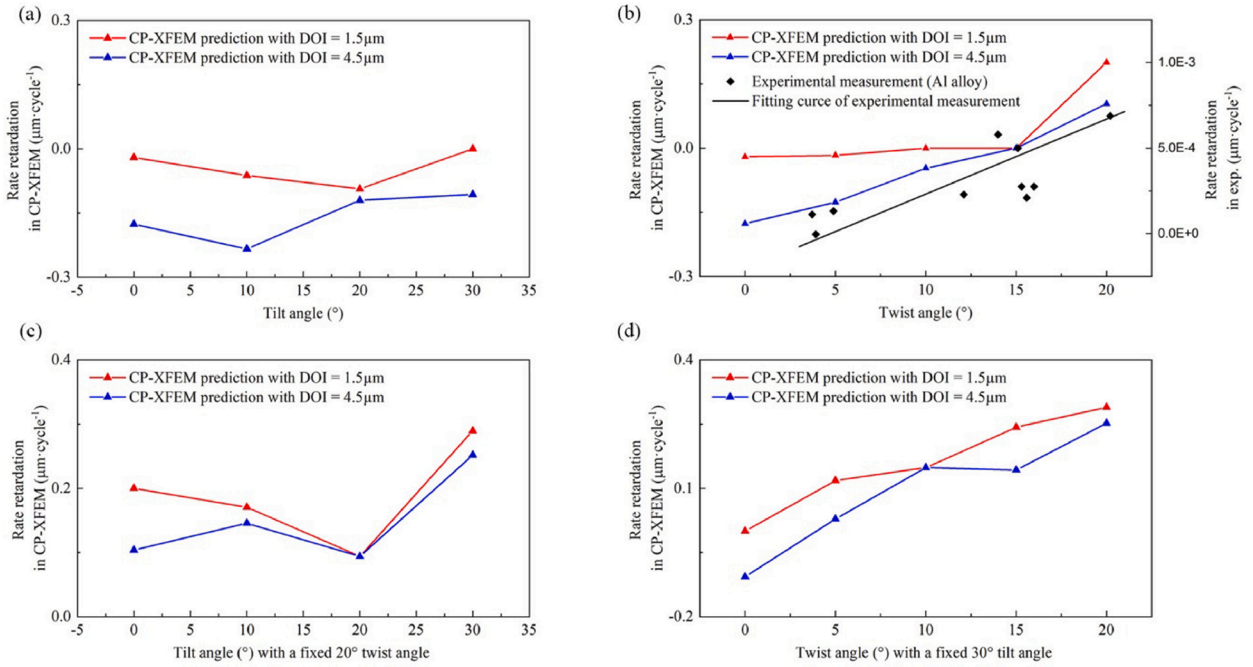


Fig. 10. Rate retardation caused by grain boundaries against (a) tilt angle between 0 and 30° (zero twist) and (b) twist angle between 0 and 20° (zero tilt) with inclusion of experimental data for Al-alloy (Wen et al., 2016); (c) tilt between 0 and 30° for twist of 20°; (d) twist between 0 and 20° for fixed 30° tilt.

twist 20° case shows a faster propagation rate in grain A than the reverse case, which means the slip favourability of the reference case is stronger than for twist of 20°. However, in the reverse twist 20° configuration (green line), the crack propagation rate experiences a retardation before it approaches the grain boundary, which indicates the grain boundary provides resistance to the crack propagation even though grain B has a higher slip favourability. The twist 20° case (orange line) shows stronger retardation than the reverse configuration near the grain boundary. These results suggest that the stronger retardation is provided by both the twist 20° grain boundary and the crystal unfavourably orientated for slip.

Figs. 7 and 8 have considered only crystal configurations which are purely tilt or twist, thus separating out the individual effects of tilt and twist angles. Some grain boundary misorientations, such as $\Sigma 3$ grain boundary (twist 60° in FCC), play significant roles in short crack propagation. However, most grain boundary misorientations are arbitrary and distributed randomly, thereby comprising combinations of tilt and twist. It is therefore useful to study example grain boundaries which have both a tilt and twist coupled crystal configuration, as shown schematically in Fig. 9(a). Tilt and twist angles of 30° and 20° respectively are chosen as the reference orientations (from the study above) and are compared then with other orientation combinations. The resulting predicted crack propagation rates through the bicrystal models are shown in Fig. 9(b) and (c).

Fig. 9(b) shows the propagation rates for crystal configurations of tilt angle between 0 and 30° with fixed twist angle of 20° and it is clear that all these grain boundary configurations show rate retardations near the grain boundaries. The twist angle (20°) contributes the resistance observed to the crack propagation near grain boundary, largely irrespective of the tilt angle. Rate retardations are also observed in the two curves of Fig. 9(c) for the crystal configurations of twist between 10° and 20° for fixed tilt angle of 30°. These two retardations (blue and black lines) are quite clear compared with the tilt angle of 30° without twist (red line), which agrees with expectation because the resistance of twist angle has been removed. In addition, in all curves which show rate retardation, the positions where the rate starts to decrease are located just prior to the grain boundaries, as opposed to at grain boundaries. This shift (decrease ahead of grain boundary) is in agreement with previous experimental observations (Marx et al., 2010; Wen et al., 2016; Schaefer and Marx, 2012), which may be associated with the far field stress generated by Grain B (the grain behind grain boundary) which is discussed in more detail in Section 4.

Because our CP-XFEM selects the crystal plane with highest slip as the fracture plane, hence the fracture twist/tilt is synonymous with grain boundary twist/tilt in this study. An overall summary from the analyses carried out strongly suggests that fracture plane twist (given from grain boundary twist) generates a stronger retardation of fatigue crack propagation rate near grain boundaries over that from tilt. This is explored further in a qualitative sense against some of the (rather limited) experimental data available.

3.3. Crack growth rate retardation associated with grain boundaries

Retardation of crack propagation rate was observed in all cases where grain boundary twist was considered in the previous analyses. It's useful to investigate whether a quantitative relationship exists between either or both of twist and tilt angle on grain

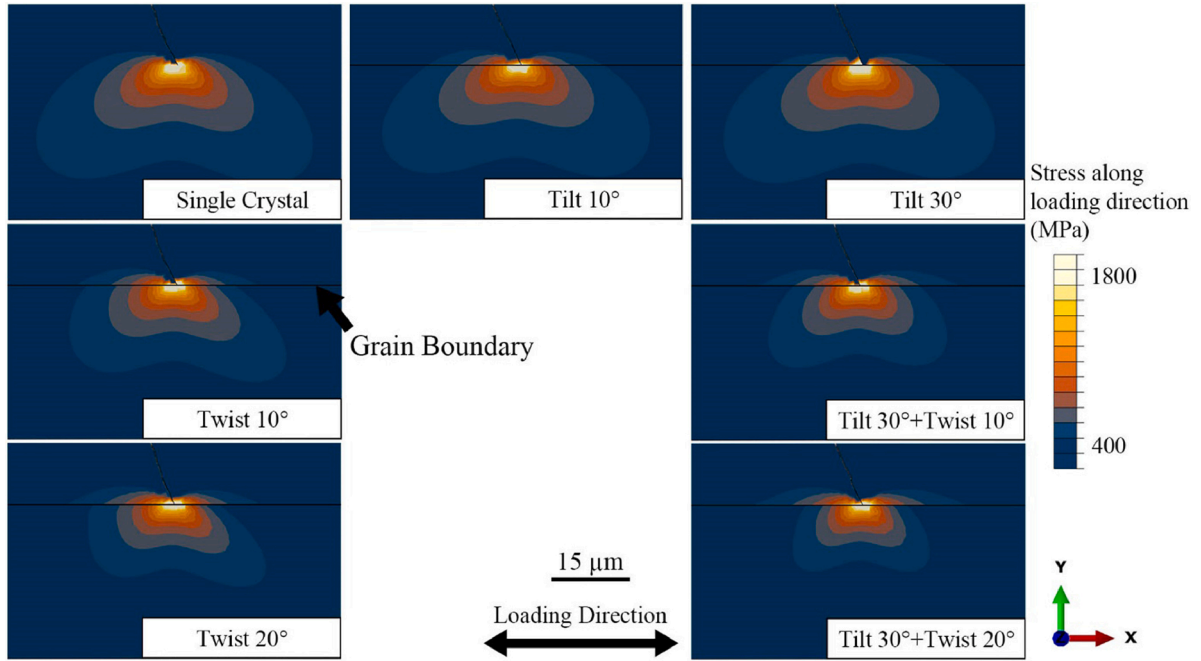


Fig. 11. The stress along loading direction (peaking loading step) in differing crystal configurations.

boundary retardation effect on crack growth rate. The method to calculate the rate retardation has been introduced in Fig. 6(b). The results of rate retardation versus tilt and twist angle are shown in Fig. 10 together with limited experimental data from Wen et al. (2016), but for a different (aluminium) alloy. Twist is expected to provide stronger resistance to short crack propagation, and to provide better resolution, additional results for twist angles of 5° and 15° were obtained and included in the graphs in Fig. 10.

In Fig. 10(a) and (c), as tilt angle is increased, there's some indication of an increase in retardation rate but it's by no means clear cut, for either distance from grain boundary used for calculating the rate. However, in Fig. 10(b) and (d), larger twist angle does seem to be more clearly related to higher rate of retardation, as determined at both DOIs from the grain boundary. This quantitative result demonstrates that higher twist angle indeed generates stronger resistance to short crack propagation when the crack-tip approaches and penetrates the grain boundary. In Fig. 10(b) for pure twist variation, independent experiments on Al-alloy (with the similarity of having FCC lattice as for Nickel considered here) show good qualitative agreement with the crack growth model predictions based on stored energy density. Although the rate magnitudes of experimental and CP-XFEM are different because of the need for relatively small numbers of fatigue cycles in modelling, the sensitivity of rate to twist angle is captured correctly, which demonstrates the twist angle can generate resistance in short crack propagation. Additionally, in Fig. 10(b) and (d), the retardation collected from DOI of 1.5μm is higher than the retardation of 4.5μm, which means this retardation behavior is enhanced as the crack tip is approaching the grain boundary.

4. Discussion

Crack propagation rate retardations due to twist are always found to occur when crack tips approach grain boundaries, which has been observed in previous experiments (Marx et al., 2010; Schaef and Marx, 2012; Wen et al., 2016) and verified through CP-XFEM (Figs. 7, 8, and 9). The heterogeneous stress field generated by a grain boundary was recognized as a key factor affecting this advanced retardation (Scharnweber et al., 2012). To investigate the potential crystallographic link associated with this resistance, the stress fields at crack-tips are extracted at the peak loading step when the cracks approach the grain boundaries and are shown in Fig. 11 captured from the mid-section (Fig. 6(a)) for key crystal configurations. It can be seen that the variation of tilt angle does not generate any significant change to crack tip stress field. However, a clear difference of the stress field can be seen for twist variation, and this mismatch is enhanced when the twist variation is hybridized with a 30° tilt angle. Hence, Fig. 11 demonstrates that a higher incompatibility stress can be developed due to the mismatch of twist-crystallography, and this incompatibility can be enhanced if the adjacent Grain (B) is hybridized with a tilt rotation.

With regards to microstructural parameters, Burgers vector and slip normal are key factors thought to play a significant role in

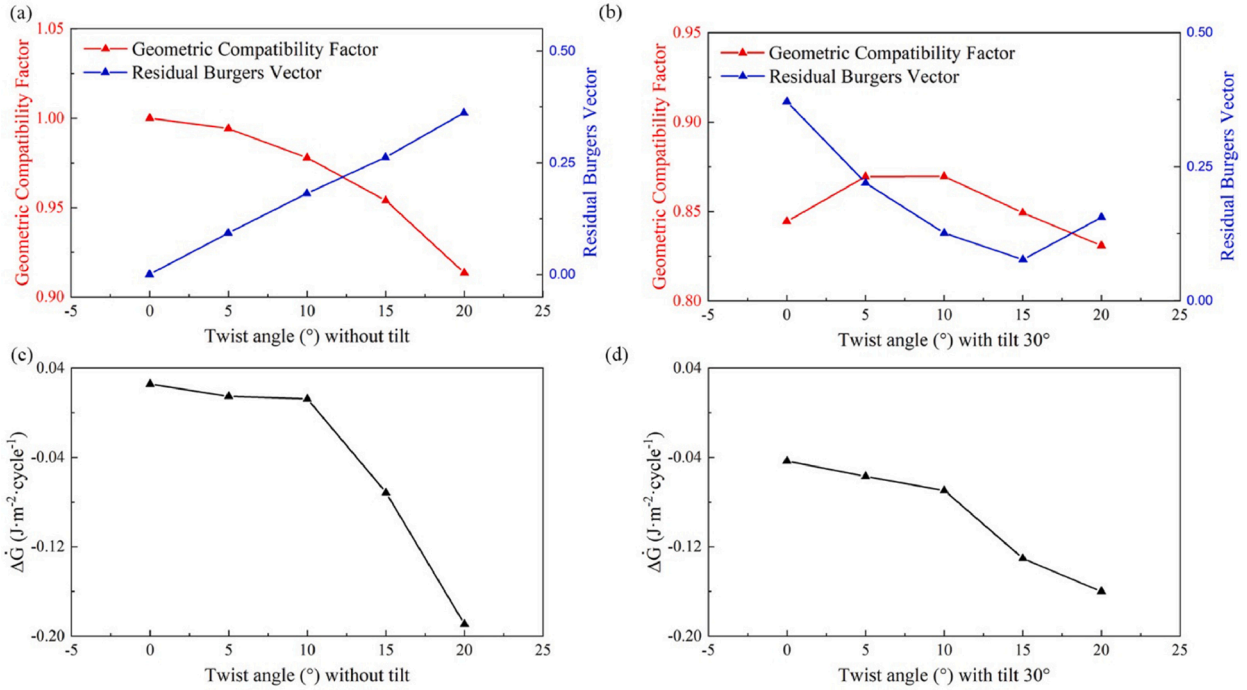


Fig. 12. Geometric compatibility factor and residual Burgers vector for (a) Twist 0°~20°; (b) Twist 0°~20° + tilt 30°. Evolution of stored energy density rate across grain boundary for (c) Twist 0°~20°; (d) Twist 0°~20° + tilt 30°.

crack penetration of grain boundaries (Fang et al., 2016; Jiménez et al., 2019). The residual burgers vector b_r has been raised by Lee et al. (1990).

$$b_r = |\mathbf{b}_{in} - \mathbf{b}_{out}| \quad (19)$$

where $\mathbf{b}_{in}$ is the Burgers vector of the fractured slip plane in Grain A, which is calculated by the slip system which contains the highest slip, and $\mathbf{b}_{out}$ that for the Burgers vector in Grain B calculated in the same way. Moreover, the relationship given by the geometric compatibility factor (Luster and Morris, 1995) between the two fractured slip planes has also been considered a criterion which is

$$m = \cos\theta \cdot \cos\varphi \quad (20)$$

where θ is the angle between the slip directions of the fracture planes in Grains A and B, and φ is the angle between the corresponding normal directions.

Residual Burgers vector and geometric compatibility factor quantify the crystallographic relationship between the two adjacent fracture planes, and their roles have been supported through some statistical experiments in terms of affecting crack transmission through the grain boundaries (Jiménez et al., 2019; Luster and Morris, 1995). However, the experiments considered are conducted generally in polycrystals which necessarily give rise to highly heterogeneous intragranular stress fields. In addition, the grain morphologies and tilt/twist angles obtained from experimental polycrystals are arbitrary and inhibit a systematic analysis of more idealised crystal configurations as employed in the present study. Hence, it is useful to comparatively assess three key criteria (namely, geometric compatibility factor, residual Burgers vector and stored energy density) for the model grain boundary tilt/twist combinations considered in this study in the context of fatigue crack growth. This assessment employs bicrystal model which can reduce the effect from neighboring grains thus highlighting the sole role of the grain boundary. Fig. 12 summarises the three measures which potentially control crack propagation across a grain boundary.

Residual Burgers vector and geometric compatibility factor are calculated as Eq. (21) and Eq. (22) respectively for the various grain boundary crystallographies considered. Only twist associated crystal configurations is considered because the tilt angle effect has been demonstrated to be quite weak in previous sections. In Fig. 12(a), higher twist angle corresponds to a higher residual Burgers vector and a lower geometric compatibility factor, which correlate in turn with previously observed stronger resistance to crack propagation (Fig. 10(b)). However, in Fig. 12(b), neither the residual Burgers vector nor geometric compatibility factor show a consistent increase nor decrease as the twist angle increases. Generally, it would be anticipated that higher residual Burgers vector and lower geometric compatibility factor would result in stronger resistance to short crack propagation, which is reflected in Fig. 12(a) for twist but not Fig. 12(b) for tilt and twist. In other words, the metrics of residual Burgers vector and geometric compatibility factor are indicative for

pure twist configuration effects but not suitable for more complex crystal orientations like the twist $0^\circ \sim 20^\circ$ + tilt 30° of Fig. 12(b).

Stored energy density has been investigated in other studies as a mechanistic driver of both fatigue crack nucleation (Wan et al., 2014; Wilson et al., 2019) and short crack propagation (Karamitros et al., 2022). Hence the stored energy density rate ($\dot{G}$) ahead and behind the grain boundary at the crack-tip has been extracted from the model simulations when the crack tip locates at $1.5\mu\text{m}$ (one element size) prior to ($\dot{G}_A$) and subsequent to ($\dot{G}_B$) the grain boundary. The change of stored energy density rate $\Delta\dot{G}$ is calculated by $\Delta\dot{G} = \dot{G}_B - \dot{G}_A$. The results are plotted in Fig. 12(c) and (d) for increasing twist angle both without and with a fixed tilt (30°). High $\dot{G}$ means that the cyclic evolution of crack tip stored energy is high giving a smaller number of cycles to achieve the critical energy, G_c , required for crack propagation. In Fig. 12(c), a twist of $0^\circ \sim 10^\circ$ is found to give positive $\Delta\dot{G}$ such that the propagation rate after traversing the grain boundary has increased, thus reflecting the negative rate of retardation (ie rate acceleration) shown in Fig. 10(b) for the same twist angles. Larger twist between 15° and 20° gives negative $\Delta\dot{G}$ which means the propagation rate is decreasing, thereby reflecting the positive rates of retardation shown in Fig. 10(b). So, the $\Delta\dot{G}$ decrease from positive to negative values as the twist angle increases from 0° to 20° , leads to the appropriate experimentally observed sensitivity of rate of retardation to twist angle for the case of pure twist. For the case of increasing twist but with a fixed tilt of 20° , Fig. 12(d) shows a similar trend to that in Fig. 12(c), however, all data point values are negative meaning that the twist + tilt cases all generate rate retardations, reflecting both Fig. 10(d) and the positive rate retardation values and the enhanced incompatibility stress shown in Fig. 11. Hence, Fig. 12(c) demonstrates the trend of rate retardation with increasing twist angle from an initial acceleration (for the case of twist 0°). Hence the stored energy density provides the mechanistic explanation for the effect of twist with and without tilt, in fatigue crack propagation traversing a grain boundary.

5. Conclusion

A series of model three-dimensional grain boundaries formed from defined crystal orientation combinations have been created, reflecting a range of tilt and twist angles, with which to analyse crack propagation paths and rates of growth as the grain boundaries are traversed. The mechanistic hypothesis is that grain boundary crack advance is controlled by elastic stored energy density and that crack path is crystallographic, and influenced by slip transmission at the grain boundary, and the key conclusions are:

1. Grain boundaries with increasing twist angle provide increasing resistance to short crack propagation. However, the pure tilt angle effect is found to be weak unless the second grain's crystal orientation is unfavourable for slip. Higher twist angle has also been shown to facilitate more local grain boundary slip system activations at the crack tip, thereby generating multiple potential fracture planes, and potentially faceted crack growth away from the grain boundary.
2. Retardation of crack propagation rate is predicted to occur prior to the crack tip reaching a grain boundary, in agreement with experimental observations, which is associated with the heterogeneous stress field generated by the grain boundary elastic mismatch, and the former's interaction with the crack tip stress field.
3. For complex grain boundary combinations comprising both tilt + twist, the residual Burgers vector and geometric compatibility measures for quantifying grain boundary resistance to crack propagation are ambiguous, but the stored energy density rate captures this sensitivity. The latter has also been shown to properly reflect crack growth retardation near grain boundaries reflecting sensitivity to twist and tilt.

CRedit authorship contribution statement

Xiaoxian Zhang: Conceptualization, Methodology, Software, Formal analysis, Writing – original draft, Visualization. **Fionn P.E. Dunne:** Conceptualization, Methodology, Writing – review & editing, Supervision.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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Appendix. A

Fig. A

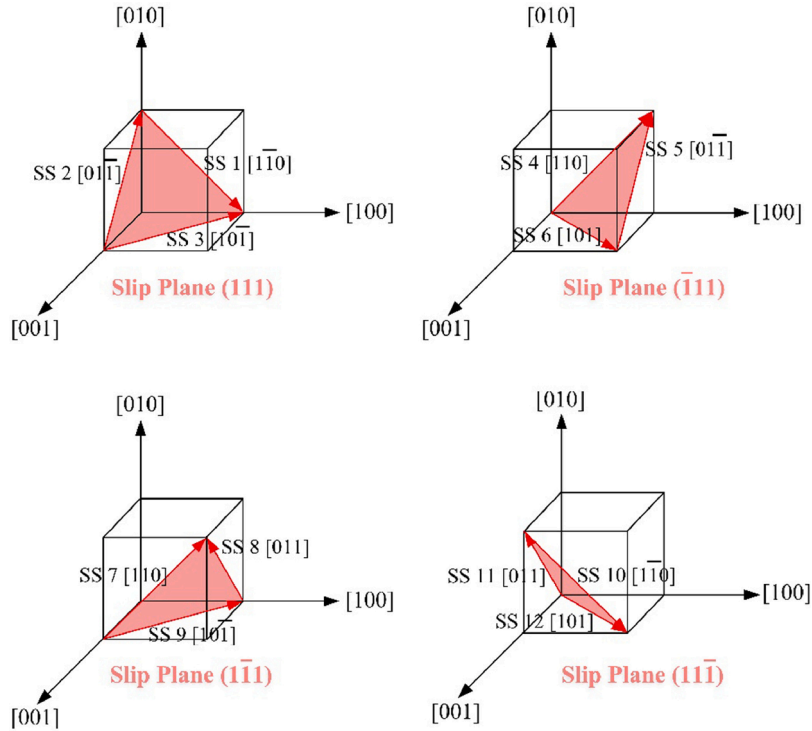


Fig. A. Identification of 12 slip systems in FCC nickel.

Appendix. B

A mesh sensitivity study is conducted to ensure the element size is sufficient for the CP-XFEM models to obtain reliable micro-mechanical results. The study employs monotonic loading of an edge-cracked single crystal with six differing mesh refinements (specified in terms of numbers of elements, namely 6696 (element size $3.0\mu\text{m} \times 3.0\mu\text{m} \times 3.3\mu\text{m}$), 9888 ($2.0\mu\text{m} \times 2.0\mu\text{m} \times 3.3\mu\text{m}$),

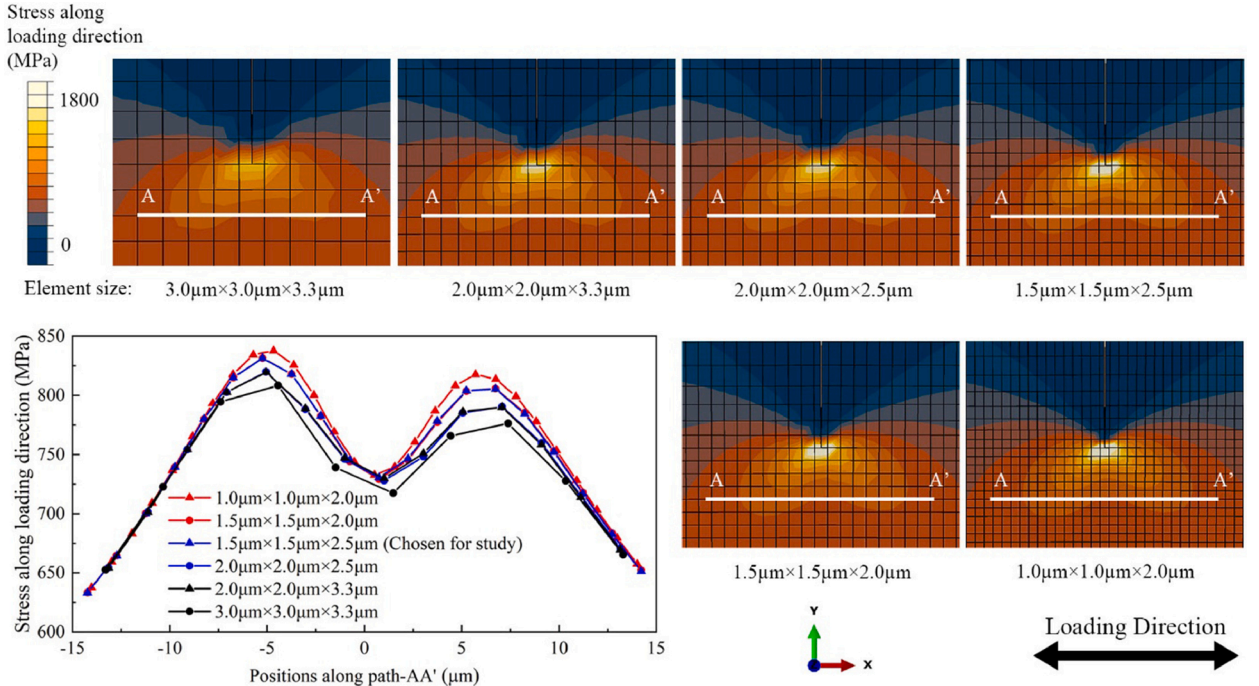


Fig. B. Results of mesh sensitivity study under six different mesh sizes.

13184 ($2.0\mu\text{m} \times 2.0\mu\text{m} \times 2.5\mu\text{m}$), 18848 ($1.5\mu\text{m} \times 1.5\mu\text{m} \times 2.5\mu\text{m}$), 23610 ($1.5\mu\text{m} \times 1.5\mu\text{m} \times 2.0\mu\text{m}$) and 43240 ($1.0\mu\text{m} \times 1.0\mu\text{m} \times 2.0\mu\text{m}$). The stress field at the crack-tip and along the path-AA' for the six meshing schemes are shown in Fig. B. It can be seen that finer meshes ($1.5\mu\text{m} \times 1.5\mu\text{m} \times 2.5\mu\text{m}$, $1.5\mu\text{m} \times 1.5\mu\text{m} \times 2.0\mu\text{m}$, $1.0\mu\text{m} \times 1.0\mu\text{m} \times 2.0\mu\text{m}$) show similar results in respect of the stress contour fields and their path plots. As a consequence, the mesh scheme ($1.5\mu\text{m} \times 1.5\mu\text{m} \times 2.5\mu\text{m}$ with 18848 elements totally, and 4 elements normal to free surface) is selected for crack propagation studies.

Appendix. C

To optimise computational time and disk space, a low critical stored energy density (0.65J/m^2) is used as the selected fatigue criterion. To examine the potential ramification of this critical value, a series of tests were conducted using differing critical stored energy densities (0.65J/m^2 , 0.70J/m^2 , 0.80J/m^2) but with the same microstructure (twist 20°). The results are shown in Fig. C, which demonstrate that higher critical stored energy density leads to lower crack propagation rate but the trends with respect to grain boundary crack rate of advance are not changed. Therefore, it's appropriate to use the selected critical value to investigate the effect of twist/tilt on crack propagation near a grain boundary.

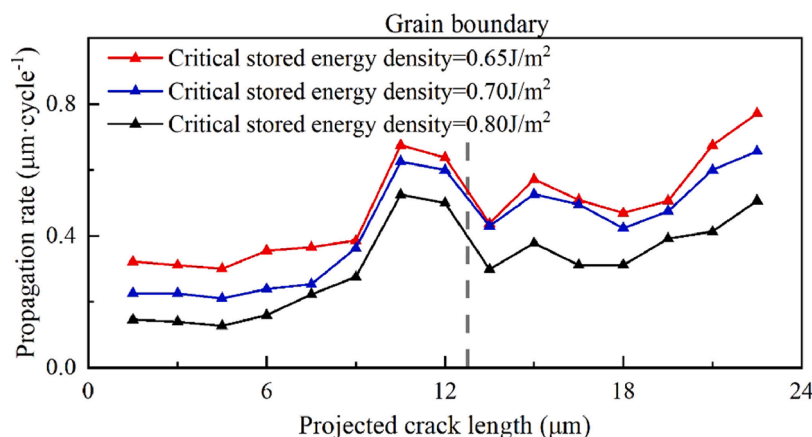


Fig. C. Results of critical stored energy density study with same twist angle 20° .

References

- Arsenlis, A., Parks, D.M., 1999. Crystallographic aspects of geometrically-necessary and statistically-stored dislocation density. *Acta Mater.* 47 (5), 1597–1611. [https://doi.org/10.1016/S1359-6454\(99\)00020-8](https://doi.org/10.1016/S1359-6454(99)00020-8).
- Barat, K., Ghosh, A., Doharey, A., Mukherjee, S., Karmakar, A., 2022. Crystallographic evaluation of low cycle fatigue crack growth in a polycrystalline Ni based superalloy. *Int. J. Plast.* 149 (September 2021), 103174 <https://doi.org/10.1016/j.ijplas.2021.103174>.
- Chen, B., Jiang, J., Dunne, F.P.E., 2017. Microstructurally-sensitive fatigue crack nucleation in Ni-based single and oligo crystals. *J. Mech. Phys. Solids* 106, 15–33. <https://doi.org/10.1016/j.jmps.2017.05.012>.
- Chen, B., Jiang, J., Dunne, F.P.E., 2018. Is stored energy density the primary meso-scale mechanistic driver for fatigue crack nucleation? *Int. J. Plast.* 101 (December 2017), 213–229. <https://doi.org/10.1016/j.ijplas.2017.11.005>.
- Cheng, J., Ghosh, S., 2015. A crystal plasticity FE model for deformation with twin nucleation in magnesium alloys. *Int. J. Plast.* 67, 148–170. <https://doi.org/10.1016/j.ijplas.2014.10.005>.
- Dunne, F.P.E., Kiwanuka, R., Wilkinson, A.J., 2012. Crystal plasticity analysis of micro-deformation, lattice rotation and geometrically necessary dislocation density. *Proc. R. Soc. A Math. Phys. Eng. Sci.* 468 (2145), 2509–2531. <https://doi.org/10.1098/rspa.2012.0050>.
- Dunne, F.P.E., Rugg, D., Walker, A., 2007. Lengthscale-dependent, elastically anisotropic, physically-based hcp crystal plasticity: application to cold-dwell fatigue in Ti alloys. *Int. J. Plast.* 23 (6), 1061–1083. <https://doi.org/10.1016/j.ijplas.2006.10.013>.
- Echlin, J.C.S.M.P., Bridier, D.T.F., & Pollock, P.B.T.M. (2016). sub-grain scale digital image correlation by electron microscopy for polycrystalline materials during elastic. 197–216. [10.1007/s11340-015-0083-4](https://doi.org/10.1007/s11340-015-0083-4).
- Fang, W., Xie, H., Yin, F., Li, J., Khan, D.F., Fang, Q., 2016. Molecular dynamics simulation of grain boundary geometry on crack propagation of bi-crystal aluminum. *Mater. Sci. Eng. A* 666, 314–319. <https://doi.org/10.1016/j.msea.2016.04.077>.
- Fu, H., Chen, X., Wang, W., Pia, G., Zhang, J., Li, J., 2021. Statistical study on the effects of heterogeneous deformation and grain boundary character on hydrogen-induced crack initiation and propagation in twinning-induced plasticity steels. *Corros. Sci.* 192 (September), 109796 <https://doi.org/10.1016/j.corsci.2021.109796>.
- Gonzalez, D., Simonovski, I., Withers, P.J., Quinta Da Fonseca, J., 2014. Modelling the effect of elastic and plastic anisotropies on stresses at grain boundaries. *Int. J. Plast.* 61, 49–63. <https://doi.org/10.1016/j.ijplas.2014.03.012>.
- Jiang, R., Karapatis, N., Gao, N., Reed, P.A.S., 2015. Effects of microstructures on fatigue crack initiation and short crack propagation at room temperature in an advanced disc superalloy. *Mater. Sci. Eng. A* 641, 148–159. <https://doi.org/10.1016/j.msea.2015.05.065>.
- Jiang, R., Song, Y.D., Reed, P.A., 2020. Fatigue crack growth mechanisms in powder metallurgy Ni-based superalloys—a review. *Int. J. Fatigue* 141 (May), 105887. <https://doi.org/10.1016/j.ijfatigue.2020.105887>.
- Jiménez, M., Ludwig, W., Gonzalez, D., Molina-Aldareguia, J.M., 2019. The role of slip transfer at grain boundaries in the propagation of microstructurally short fatigue cracks in Ni-based superalloys. *Scr. Mater.* 162, 261–265. <https://doi.org/10.1016/j.scriptamat.2018.11.008>.
- Karamitros, V., MacLachlan, D.W., Dunne, F.P.E., 2022. Mechanistic fatigue in Ni-based superalloy single crystals: a study of crack paths and growth rates. *J. Mech. Phys. Solids* 158 (June 2021), 104663. <https://doi.org/10.1016/j.jmps.2021.104663>.

- Lee, T.C., Robertson, I.M., Birnbaum, H.K., 1990. An *In situ* transmission electron microscope deformation study of the slip transfer mechanisms in metals. *Metall. Trans. A* 21 (9), 2437–2447. <https://doi.org/10.1007/BF02646988>.
- Liu, G., Winwood, S., Rhodes, K., Biroscas, S., 2020. The effects of grain size, dendritic structure and crystallographic orientation on fatigue crack propagation in IN713C nickel-based superalloy. *Int. J. Plast.* 125 (May 2019), 150–168. <https://doi.org/10.1016/j.ijplas.2019.09.010>.
- Livingston, J.D., Chalmers, B., 1957. Multiple slip in bicrystal deformation. *Acta Metall.* 5 (6), 322–327. [https://doi.org/10.1016/0001-6160\(57\)90044-5](https://doi.org/10.1016/0001-6160(57)90044-5).
- Ludwig, W., Buffière, J.Y., Savelli, S., Cloetens, P., 2003. Study of the interaction of a short fatigue crack with grain boundaries in a cast Al alloy using X-ray microtomography. *Acta Mater.* 51 (3), 585–598. [https://doi.org/10.1016/S1359-6454\(02\)00320-8](https://doi.org/10.1016/S1359-6454(02)00320-8).
- Luster, J., Morris, M.A., 1995. Compatibility of deformation in two-phase Ti-Al alloys: dependence on microstructure and orientation relationships. *Metall. Mater. Trans. A* 26 (7), 1745–1756. <https://doi.org/10.1007/BF02670762>.
- Marx, M., Schaeff, W., Vehoff, H., 2010. Interaction of short cracks with the local microstructure. *Procedia Eng.* 2 (1), 163–171. <https://doi.org/10.1016/j.proeng.2010.03.018>.
- McMurtrey, M.D., Was, G.S., Cui, B., Robertson, I., Smith, L., Farkas, D., 2014. Strain localization at dislocation channel-grain boundary intersections in irradiated stainless steel. *Int. J. Plast.* 56, 219–231. <https://doi.org/10.1016/j.ijplas.2014.01.001>.
- Navarro, A., de los Rios, E.R., 1988. Short and long fatigue crack growth: a unified model. *Philos. Mag. A Phys. Condens. Matter Struct. Defects Mech. Prop.* 57 (1), 15–36. <https://doi.org/10.1080/01418618808204496>.
- Nguyen, G.D., Korsunsky, A.M., Belnoue, J.P.H., 2015. A nonlocal coupled damage-plasticity model for the analysis of ductile failure. *Int. J. Plast.* 64, 56–75. <https://doi.org/10.1016/j.ijplas.2014.08.001>.
- Potirniche, G.P., Daniewicz, S.R., 2003. Finite element modeling of microstructurally small cracks using single crystal plasticity. *Int. J. Fatigue* 25 (9–11), 877–884. [https://doi.org/10.1016/S0142-1123\(03\)00124-5](https://doi.org/10.1016/S0142-1123(03)00124-5).
- Rovinelli, A., Sangid, M.D., Proudhon, H., Guilhem, Y., Lebensohn, R.A., Ludwig, W., 2018. Predicting the 3D fatigue crack growth rate of small cracks using multimodal data via Bayesian networks: *in-situ* experiments and crystal plasticity simulations. *J. Mech. Phys. Solids* 115, 208–229. <https://doi.org/10.1016/j.jmps.2018.03.007>.
- Sangid, M.D., Ezaz, T., Sehitoglu, H., Robertson, I.M., 2011. Energy of slip transmission and nucleation at grain boundaries. *Acta Mater.* 59 (1), 283–296. <https://doi.org/10.1016/j.actamat.2010.09.032>.
- Sangid, M.D., Rotella, J., Naragani, D., Park, J.S., Kenesei, P., Shade, P.A., 2020. A complete grain-level assessment of the stress-strain evolution and associated deformation response in polycrystalline alloys. *Acta Mater.* 201, 36–54. <https://doi.org/10.1016/j.actamat.2020.09.051>.
- Schaeff, W., Marx, M., 2012. A numerical description of short fatigue cracks interacting with grain boundaries. *Acta Mater.* 60 (5), 2425–2436. <https://doi.org/10.1016/j.actamat.2012.01.013>.
- Scharnweber, M., Tirschler, W., Mikulich, V., Jacob, S., Oertel, C.G., Skrotzki, W., 2012. Influence of crack length and grain boundaries on the propagation rate of short cracks in austenitic stainless steel. *Scr. Mater.* 67 (7–8), 677–680. <https://doi.org/10.1016/j.scriptamat.2012.07.007>.
- Schneider, M., George, E.P., Manescau, T.J., Zálezák, T., Hunfeld, J., Dlouhý, A., Laplanche, G., 2020. Analysis of strengthening due to grain boundaries and annealing twin boundaries in the CrCoNi medium-entropy alloy. *Int. J. Plast.* 124 (August 2019), 155–169. <https://doi.org/10.1016/j.ijplas.2019.08.009>.
- Shen, Z., Wagoner, R.H., Clark, W.A.T., 1988. Dislocation and grain boundary interactions in metals. *Acta Metall.* 36 (12), 3231–3242. [https://doi.org/10.1016/0001-6160\(88\)90058-2](https://doi.org/10.1016/0001-6160(88)90058-2).
- Singh, R., Singh, A., Singh, P.K., Mahajan, D.K., 2020. Effect of microstructural features on short fatigue crack growth behaviour in SA508 grade 3 class I low alloy steel. *Int. J. Press. Vessels Pip.* 185 (May), 104136. <https://doi.org/10.1016/j.ijpvp.2020.104136>.
- Wan, V.V.C., MacLachlan, D.W., Dunne, F.P.E., 2014. A stored energy criterion for fatigue crack nucleation in polycrystals. *Int. J. Fatigue* 68, 90–102. <https://doi.org/10.1016/j.ijfatigue.2014.06.001>.
- Wan, V.V.C., MacLachlan, D.W., Dunne, F.P.E., 2016. Integrated experiment and modelling of microstructurally-sensitive crack growth. *Int. J. Fatigue* 91, 110–123. <https://doi.org/10.1016/j.ijfatigue.2016.05.027>.
- Wen, W., et al., 2016. An experimental methodology to quantify the resistance of grain boundaries to fatigue crack growth in an AA2024 T351 Al-Cu Alloy. *Mater. Sci. Eng. A* 666, 288–296. <https://doi.org/10.1016/j.msea.2016.04.071>.
- Wilkinson, A.J., Roberts, S.G., Hirsch, P.B., 1998. Modelling the threshold conditions for propagation of stage I fatigue cracks. *Acta Mater.* 46 (2), 379–390. [https://doi.org/10.1016/S1359-6454\(97\)00290-5](https://doi.org/10.1016/S1359-6454(97)00290-5).
- Wilson, D., Dunne, F.P.E., 2019. A mechanistic modelling methodology for microstructure-sensitive fatigue crack growth. *J. Mech. Phys. Solids* 124, 827–848. <https://doi.org/10.1016/j.jmps.2018.11.023>.
- Wilson, D., Wan, W., Dunne, F.P.E., 2019. Microstructurally-sensitive fatigue crack growth in HCP, BCC and FCC polycrystals. *J. Mech. Phys. Solids* 126, 204–225. <https://doi.org/10.1016/j.jmps.2019.02.012>.
- Wilson, D., Zheng, Z., Dunne, F.P.E., 2018. A microstructure-sensitive driving force for crack growth. *J. Mech. Phys. Solids* 121, 147–174. <https://doi.org/10.1016/j.jmps.2018.07.005>.
- Xu, Y., Wan, W., Dunne, F.P.E., 2021. Microstructural fracture mechanics: stored energy density at fatigue cracks. *J. Mech. Phys. Solids* 146 (August 2020), 104209. <https://doi.org/10.1016/j.jmps.2020.104209>.
- Yang, Q., Yang, X., Huang, W., Shi, Y., Shi, D., 2022. Small fatigue crack propagation rate and behaviours in a powder metallurgy superalloy: role of stress ratio and local microstructure. *Int. J. Fatigue* 160 (February), 106861. <https://doi.org/10.1016/j.ijfatigue.2022.106861>.
- Zhai, T., Wilkinson, A.J., Martin, J.W., 2000. Crystallographic mechanism for fatigue crack propagation through grain boundaries. *Acta Mater.* 48 (20), 4917–4927. [https://doi.org/10.1016/S1359-6454\(00\)00214-7](https://doi.org/10.1016/S1359-6454(00)00214-7).
- Zhang, X., Stinville, J.C., Pollock, T.M., Dunne, F.P.E., 2021. Crystallography and elastic anisotropy in fatigue crack nucleation at nickel alloy twin boundaries. *J. Mech. Phys. Solids* 155 (March), 104538. <https://doi.org/10.1016/j.jmps.2021.104538>.
- Zheng, Z., Prastiti, N.G., Balint, D.S., Dunne, F.P.E., 2019. The dislocation configurational energy density in discrete dislocation plasticity. *J. Mech. Phys. Solids* 129, 39–60. <https://doi.org/10.1016/j.jmps.2019.04.015>.