

Mechanisms of fatigue crack growth – a critical digest of theoretical developments

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ABSTRACT Recent advances in the processing technology are permitting the manufacture of novel metallic materials with superior fatigue properties via microstructure tailoring. In the light of these promising developments, there is a rising need for establishing a synergy between state-of-the-art experimental characterizations and physically based theoretical underpinnings. A revisit to the existing predictive literature is thus a timely requirement prior to furthering new design guidelines against cyclic damage. To that end, this paper recounts an overview of the key mechanistic and analytical theories on the fatigue crack growth mechanisms. Emphasis is placed on categorizing the proposed modelling endeavours based on their fundamental principles. In doing so, contributions and limitations thereof are carefully examined on the basis of most updated experimental revelations. The objective is to provide a perspective to the current generation of engineers and researchers alike. This concise yet critical narrative would essentially assist in formulating even more advanced microstructure–damage relationships in the modern context. A commentary is added at the end outlining the promising avenues for future research.

Keywords cyclic damage; damage models; dislocation; fracture mechanics; microstructure.

NOMENCLATURE

CTOD, FCG = crack tip opening displacement, fatigue crack growth
 MD, DFT = molecular dynamics, density functional theory
 RVE = representative volume element
 LEFM, EPFM = linear elastic and elastic plastic fracture mechanics
 E, H = Young's modulus, plastic modulus
 GB = grain boundary
 K_{\max} , K_{\min} , K_{open} , = maximum, minimum and opening stress-intensity factors
 K_c = fracture toughness under mode I loading
 $\Delta K_{\text{th}}^{\text{eff}}$, ΔK_{th} = (effective) threshold stress intensity factor range
 da/dN = fatigue crack growth rate per cycle (a is the crack length and N is the number of cycles)
 L_{deflect} , θ_{deflect} = length and angle of a deflected crack respectively
 θ = angle between slip and crack paths
 σ_{yield} , $\sigma_{\text{yield}}^{\text{cyclic}}$, σ_{fracture} = monotonic, cyclic yields strengths and static fracture strength
 σ'_f , ϵ'_f = strength and ductility coefficient in Coffin–Manson–Basquin rule: $\Delta \epsilon_{\text{plastic}} = 2\epsilon'_f (2N_f)^c$
 σ_{eff} , σ_{hydro} = effective and hydrostatic stress
 ρ^* = effective radius of a sharp crack
 ρ_{slip} , $\dot{\rho}_{\text{vacancy}}$, $\rho_{\text{interface}}$ = dislocation density, vacancy generation rate and interface density
 P_{H_2} , P_{O_2} = partial pressures of hydrogen and oxygen
 m , C = Paris exponent, Paris proportionality constant
 m_{Schmid} = Schmid factor
 τ_{friction} , $\tau_{\text{friction}}^{\text{forward}}$, $\tau_{\text{friction}}^{\text{reverse}}$ = friction (Peierls) stress for free (unobstructed), forward and reverse dislocation glide

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- $r_{plastic}, r_{plastic}^{cyclic}$ = monotonic and cyclic plastic zone sizes respectively
- $R = \frac{\sigma_{min}}{\sigma_{max}}$ (load ratio)
- T = temperature in absolute (Kelvin) scale
- U^* = critical hysteresis energy density
- V^* = activation volume
- $x_i^{forward}, x_i^{reverse}$ = positions of dislocations ($i = 1, 2, 3, \dots$) during forward and reverse loading
- $u_{forward}, u_{reverse}$ = forward and reverse cracktip displacements
- $\vec{F}_{Peach-Kohler}$ = Peach-Kohler force on continuum dislocations
- $f_{frequency}$ = frequency of applied loading
- \vec{g}_{hkl} = crystal orientation vector where h, k and l are the miller indices
- $\dot{\epsilon}$ = strain rate
- γ_{us} = unstable stacking fault energy (i.e. slip energy barrier)
- b_r = magnitude of residual dislocation Burgers vector, \vec{b}_r

MOTIVATION AND OBJECTIVE

The issue of metal fatigue persists in today’s world spanning a wide spectrum of industries such as structural, aeronautical, naval, automotive and locomotive^{1,2} (Fig. 1). The problem consistently plagues the service components therein (e.g. transmission gears, turbine blades) to catastrophic failure. The matter of alarm with fatigue is that the microscopic damaging processes are instigated far below the safe static load margin, which eventually leads to complete fracture. Thus, designing service components against cyclic damage remains a crucial engineering

challenge to date. Evidently, the more knowledge a modern engineer can be equipped with, the better design it would be possible to implement. However, the study of fatigue is not easily amenable to precise experimental evaluation as of today. Unlike monotonic properties, determination of cyclic attributes requires more rigorous tests, sophisticated measurements of local flow behaviour, crack lengths, etc. Moreover, the standardized experiments are very lengthy, expensive and by themselves do not absolutely address the inherent material response to the damage accurately.³ The persistent hurdle in establishing a uniform law is that the fatigue is a very strongly microstructure-

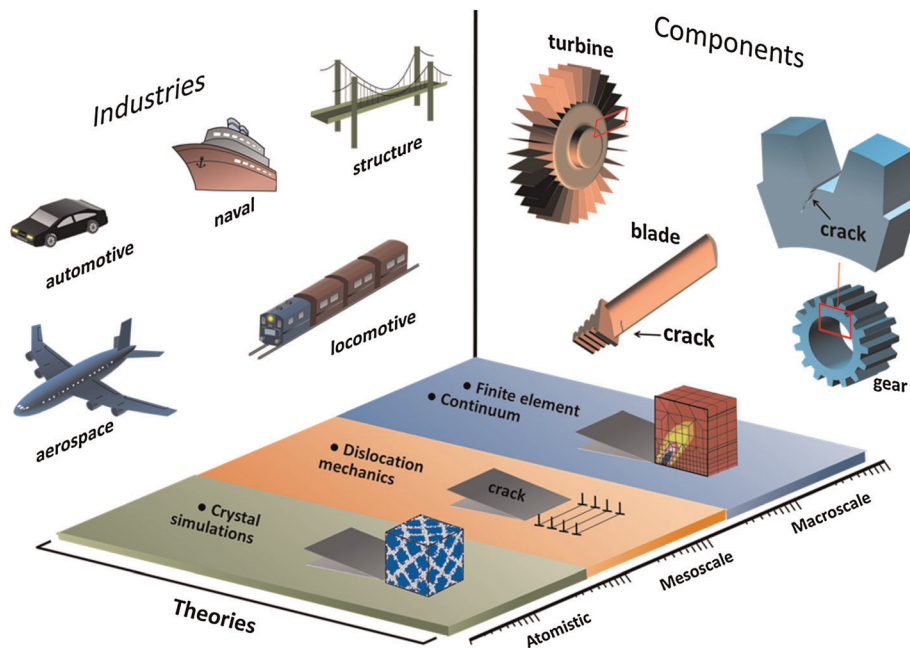


Fig. 1 Fatigue-induced component failures in modern industries and the current theoretical approaches at various length scales.

sensitive phenomenon. Therefore, the variability in the microstructure, as a result of processing and/or thermo-mechanical treatments, imparts considerable uncertainty in the measured damage trends even for the same material. With a view to elucidating the governing micromechanisms, a number of theories have been proffered addressing different aspects of sub-structural phenomena as well as global loading conditions.⁴ The current narrative provides a concise and critical review of these theories. We list the mechanistically based analytical models, which are capable of predicting quantifiable metrics as opposed to purely empirical equations. In this report, we focus on the fatigue crack growth (FCG) theories in polycrystalline metallic materials with predominantly ductile fracture mode. We note that mechanistic processes of damage propagation in non-metallic materials such as polymers, ceramics are drastically distinct and thus merit a separate treatment.

We particularly discuss the key theories, which have proved instrumental in advancing the modern perception of cyclic damage mechanisms. In doing so, a critical assessment of the model validity is also conducted considering the most recent experimental findings of special import. Given the great number of existing predictive literature, we propose a systematic classification thereof on the basis of their fundamental assumptions. Evidently, the vast extent of modelling efforts only serves to assert that the FCG mechanistic processes could easily subtend to a wide spectrum of scenarios. This certainly precludes the development of a single unified model to account for all the observed variabilities concerning the damage propagation. We adhere to classifying the models along with necessary critical commentary on each category. The explicit aim is to familiarize the readers with the theories of contributory importance, particularly from modern engineering standpoint. This digest would also enable one to quickly distinguish a model from another based on the central premise, applicability, limitations as well as future potential for extension. Eventually, the implicit motive is of course to build towards an understanding of a unifying fatigue damage theory in a synergistic effort of the scientific and engineering communities. As an endnote, we discuss the possible avenues of future treatments working towards a feasible unification of the diverse theories within a single modelling framework and the relevant developments in the making.

Prior to delving into the descriptions of the theories, we present a short account of what is experimentally known about the nature of the fatigue crack propagation mechanism(s). This would assist a reader to follow more closely how various models attempt to capture different aspects of the cyclic damage advancement. At the end of the paper, we conclude with a short note on possible avenues of future pursuits.

A BRIEF OVERVIEW OF EXPERIMENTAL FATIGUE CRACK GROWTH BEHAVIOURS

Physics of fatigue crack growth

It is well known today that repeated loading induces continuous accumulation of localized irreversible slip at the microscopic stress concentration sites^{5,6} (e.g. grain/twin boundaries inherent in a polycrystalline material), eventually triggering material separation, that is, crack formation at the microlevel.⁷ Following the nucleation, the cracks propagate incrementally through the microstructural obstacles. Essentially, the specific nature and the distribution of the interfacial defects would dictate the crack growth properties. The entire spectrum of the crack advancement in ductile polycrystals is understood as: (i) the microstructure-sensitive stage I and (ii) microstructure-independent stage II regimes as shown schematically in Fig. 2.

The length of a stage I crack is comparable with the host grain dimension. It advances by combined opening (mode I) and sliding (mode II and/or III) mechanisms. The crack grows along the slip system with maximum resolved shear stress, which differs from grain to grain, thus generating the path tortuosity. From modelling standpoint, it is imperative to examine the crack growth in a single crystal configuration to understand the near-tip slip characteristics in stage I. The driving force for stage I crack growth is influenced by the degree of obstruction and the irreversibility of the crack-emitted slip. The extent of slip activities at the very early stage of crack growth is confined to only very few grains. Prior to the crack intercepting the nearest interface en route, the tip-emitted dislocation slip would first interact therewith. Depending on the nature of the slip/interface reaction, the slip penetration strength and the irreversibility would

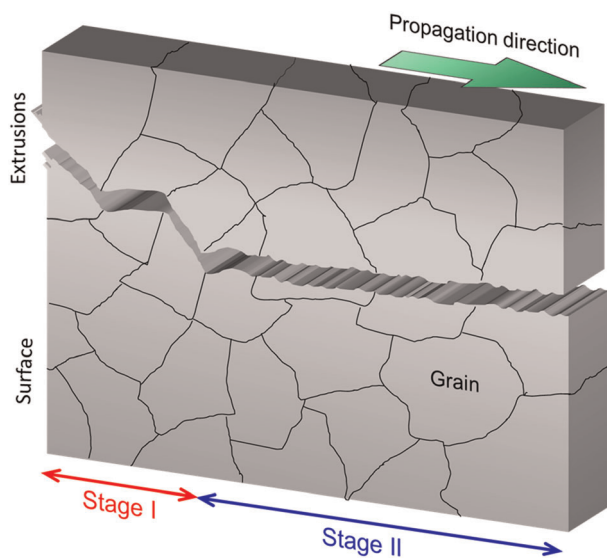


Fig. 2 Tortuous stage I (microstructure-sensitive) and straight stage II (microstructure-independent) fatigue crack growth.

vary substantially. For a stage I crack, the physical lengthscale of the per-cycle cracktip extension would be on the order of the several lattice spacings, originating from the aggregate Burgers vectors of the irreversible slip. Evidently, such behaviour can only be understood by considering the near-tip interfacial plasticity (Fig. 3).

It is experimentally observed that a stage I crack growth undergoes fluctuating, although gradually subsiding, rates due to its encounters with multiple boundaries.^{8–10} The diminishing role of the boundaries can be attributed to the history of irreversible slip accumulation, which constitutes an ever-building plastic zone ahead of the crack. Excessive near-tip slip creates such a high pile-up stress that the boundaries offer little resistance thereto as the crack becomes progressively longer.

Eventually, the crack growth reaches the stage II, where it is no longer affected by any interfaces, and continues until the final rupture. At this point, the plastic zone covers a multitude of grains (unlike only very few grains in stage I), which gives rise to the observed microstructure-insensitivity of crack propagation as shielded by the plastic envelope. In standard fatigue experimentations, a stage I crack (smaller than about 500 μm) is indiscernible by means of the commonly practiced non-destructive techniques (e.g. eddy current, ultrasonic or dye penetration). Therefore, the entire micro-crack growth period is treated as part of an incubation period prior to the appearance of a more detectable macro-crack. Intuitively, any tailored microstructure (say, with an increased distribution of interface), which would prolong the stage I period, would be highly desirable. On the macroscale, the effect would be demonstrated as an enhanced mechanical ΔK_{th} .

Thanks to the cutting-edge characterizations in the last few decades, we have a very clear picture of the mechanistic

processes underlying the fatigue damage. Such revelations have benefitted tremendously from electron backscatter diffraction,^{11,12} digital image correlation,¹³ electron microscopy,¹⁴ X-ray tomography^{15,16} and atomic force microscopy^{17,18} (Fig. 4).

Beginning with the very early analytical theories, experimental FCG characteristics (both at the microscopic and macroscopic levels) supplied critical foundation for specific assumptions. Therefore, we briefly narrate the notable mechanistic models (i.e. the ones elucidating the underlying mechanisms, rather than predicting any quantifiable metrics) as follows. Unravelling of these mechanisms paved the way for ensuing predictive analyses (to be discussed in the subsequent sections).

Forsyth and Schijve \rightarrow multiple stages of fatigue crack growth

Forsyth¹⁹ first gave an account of the dual-stage FCG noting the aluminium alloy behaviours. It was proposed that a stage I crack is driven by the maximum shear stress prior to becoming the striation-forming stage II crack aligned perpendicular to the maximum tensile direction (Fig. 5). With increasing applied ΔK , the stage II crack begins transitioning to a mixed mode one by developing shear lips (Fig. 6) as reported by Schijve.^{20,21} Before the final fracture (i.e. when the ΔK level nears the static fracture toughness, K_C), the mixed mode crack, part stage II, part inclined, was observed to fully transform into a 45° tilted crack.

Laird, McEvily and Boettner and Neumann \rightarrow stage II growth mechanisms

Laird^{22,23} envisioned the stage II crack propagation as a process of alternate ‘blunting’ followed by ‘re-sharpening’ of the

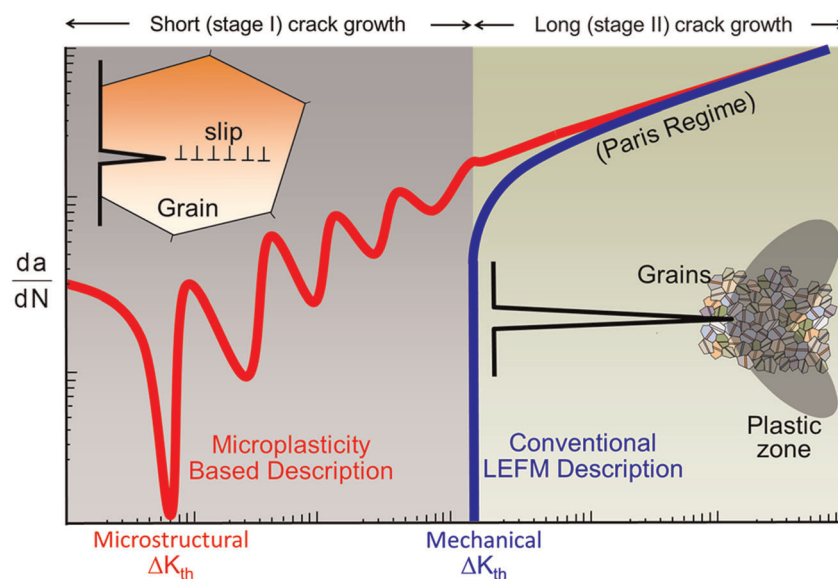


Fig. 3 Conventional linear elastic fracture mechanics (LEFM) versus microplasticity-based fatigue crack growth characterizations.

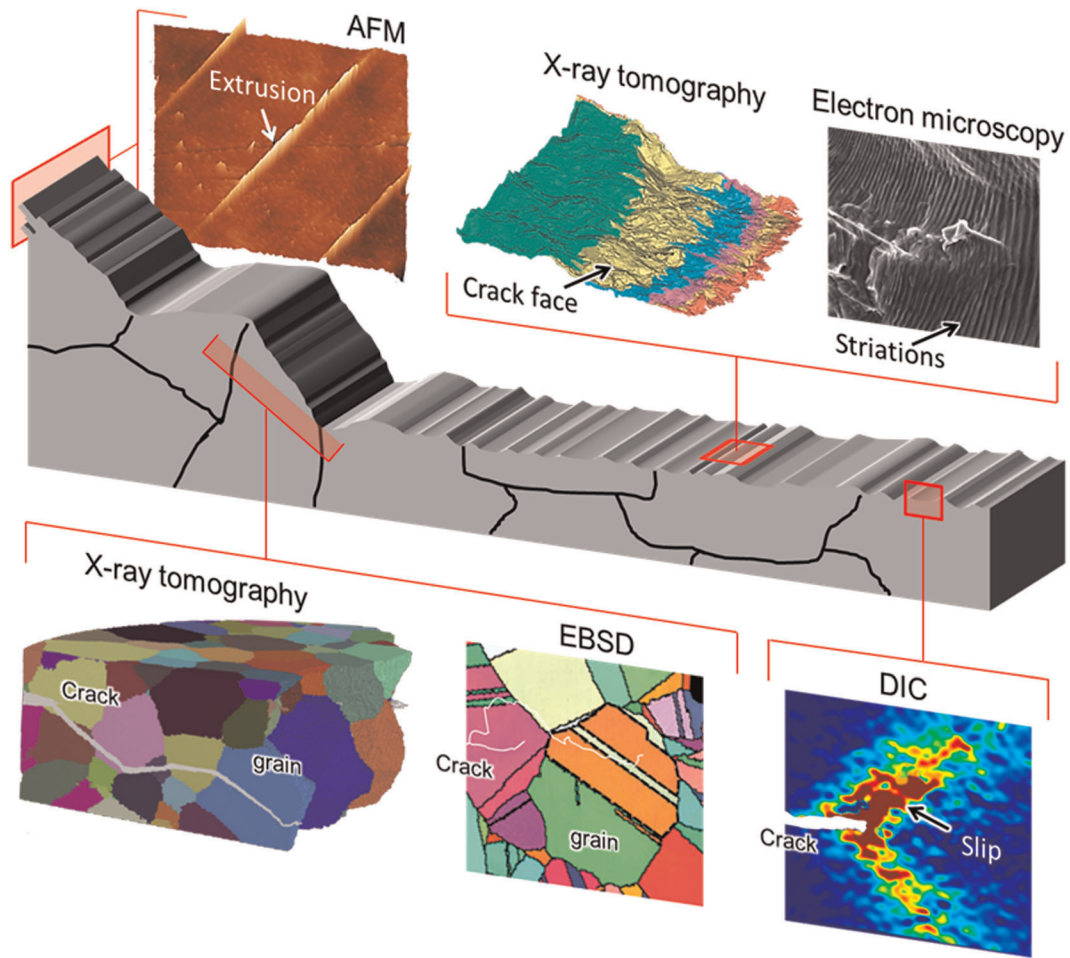


Fig. 4 Some modern experimental techniques [e.g. atomic force microscopy (AFM),^{13,14} X-ray tomography,^{15,16} digital image correlation (DIC),¹³ electron backscatter diffraction (EBSD)^{11,12} and electron microscopy¹⁴] for characterizing fatigue crack growth.

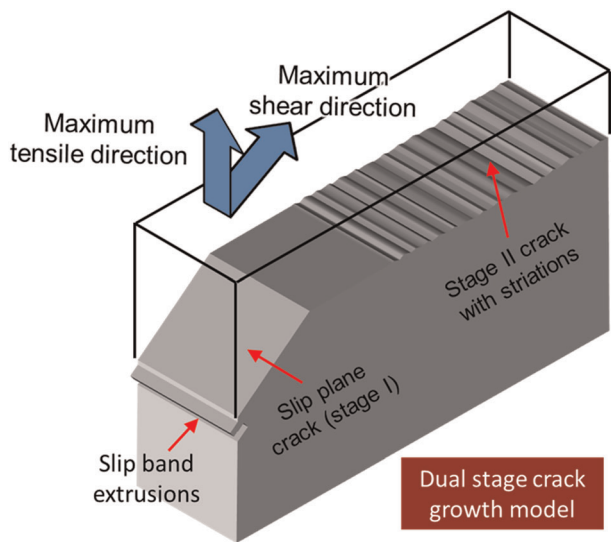


Fig. 5 Stage I and II crack growth regimes as perceived by Forsyth.¹⁹

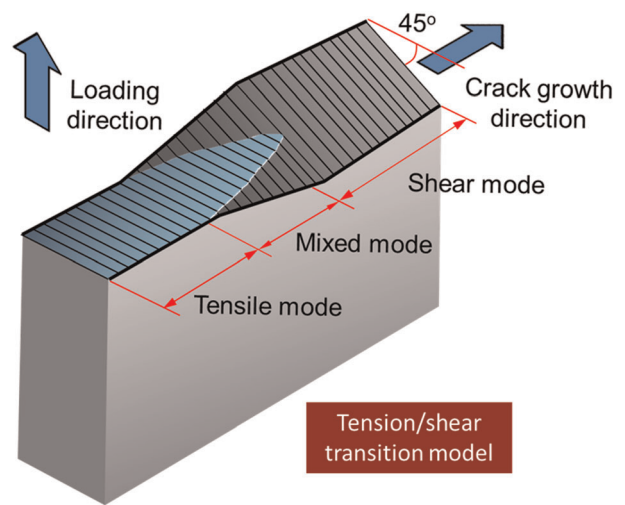


Fig. 6 Final growth stage at high ΔK with the development of 45° inclined shear planes (Schijve^{19,20}).

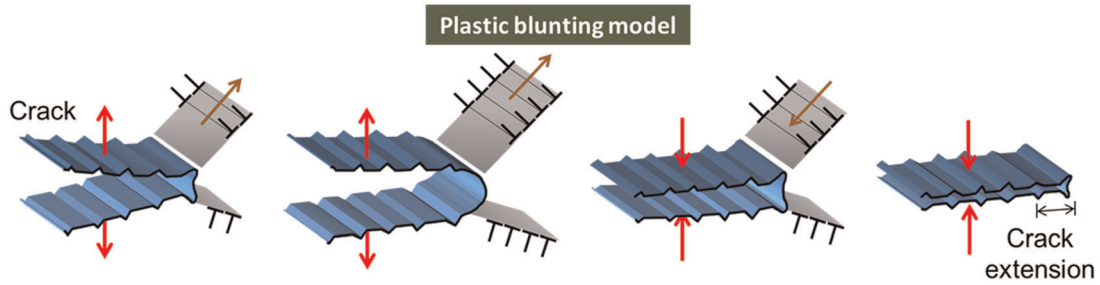


Fig. 7 Stage II fatigue crack growth due to blunting/re-sharpening via slip emission by Laird.^{38,39}

cracktip (Fig. 7). Blunting was surmised to occur under tension (i.e. during the crack opening portion of the cycle) due to significant slip emission causing material separation. On compression, the newly separated material at the cracktip simply shut close, ready to be open on next tensile half of the cycle. Such intermittent nature of slip emanations provided a physical rationale for the observed striation formation. Subsequently, Tvergaard²⁴ verified such mechanism using finite element simulations in a model material with non-hardening plasticity under plane strain condition. Tvergaard particularly employed a cracktip re-meshing technique, thus making possible studying several hundred cycles of crack growth. McEvily and Boettner^{25,26} postulated that

the slip is activated along two alternating systems on consecutive loading cycles (Fig. 8). They argued that the crack extension per cycle is directly related to the total slip step from the aggregate Burgers vectors. These researchers essentially perceived the mere process of slip emission as the principal reason for damage extension.

By contrast, Neumann^{27,28} emphasized the kinematic irreversibility of the emitted slip as the most crucial driving mechanism. It was suggested that if the emitted slip is completely reversible on compression, the net crack extension is zero. Thus, an alternating slip model (Fig. 9) was proposed. Under tension, slip emanates on a specific system, which undergoes work-hardening, therefore, activating another alternate slip

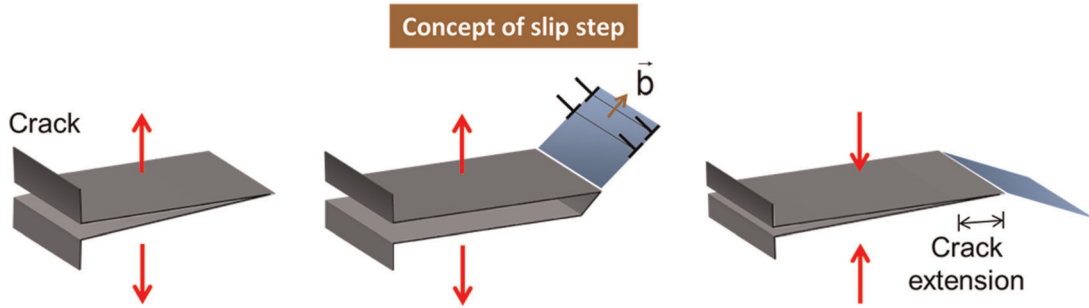


Fig. 8 McEvily and Boettner^{25,26} explained the crack tip extension as a result of the aggregate Burgers vectors.

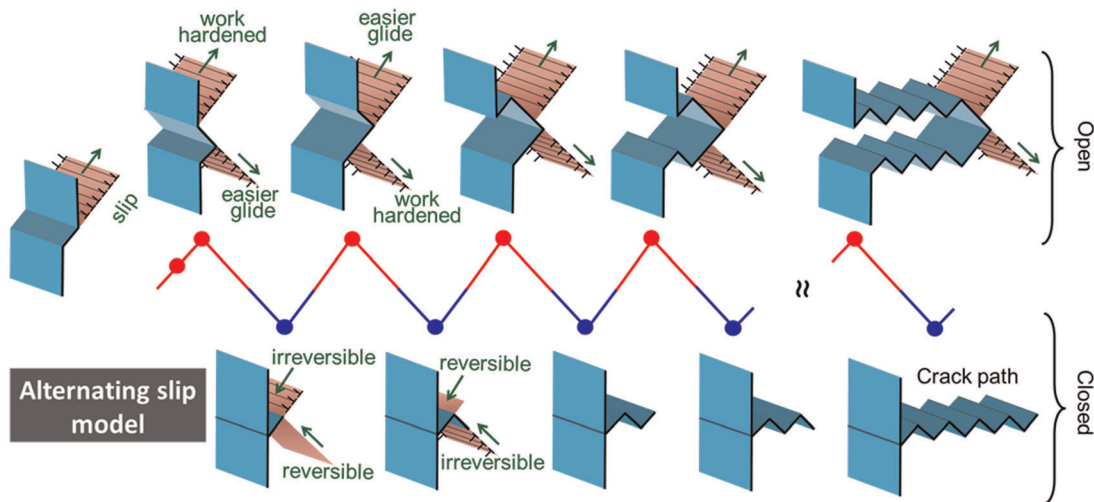


Fig. 9 Alternating slip model for stage II crack growth by Neumann.^{27,28}

system at the end of the half-cycle. On compression, the slip from the non-hardening system completely returns to the cracktip (i.e. reversibly), thereby nullifying the emission-generated collective slip steps. However, the dislocations from the work-hardened system remain as residual products (i.e. irreversibly), thus causing crack extension along that particular plane. Similar process is repeated on subsequent tensile halves of the cycles (crack being closed and non-propagating on the compression half). As a result, the stage II crack creates the striations marks while advancing. Using a similar concept of slip irreversibility, Pelloux²⁹ explained the observed accelerated crack growth in the air compared with the vacuum because the oxide layers formed in the gap between the crack flanks (in the air) promote irreversibility.

Inspired by the revelation of the foregoing mechanisms, predictive theories have been offered to capture useful damage metrics. On careful review, the analytical FCG models hitherto forwarded in the literature could be classified into two primary categories: (i) fracture mechanics-based and (ii) dislocation mechanics-based. Further ramifications of these two principal categories are presented in Fig. 10 and summarized in Tables 1 and 2.

FRACTURE MECHANICS-BASED FATIGUE CRACK GROWTH THEORIES

We identify three broad categories of fracture mechanics-based models, namely, (i) the linear elastic, (ii) the geometrical and (iii) the plastic accumulation models.

LINEAR ELASTIC MODELS

Linear elastic fracture mechanics (LEFM)-based models are conceived so as to capture the microstructure-insensitive stable propagation of a stage II crack. Even though there exists a significant degree of plastic activities at the cracktip, the primary assumption dictates the non-existence of plasticity (or a negligible one). The postulation of very small scale plasticity is because a stage II crack is typically so large that the ratio of the plastic zone size to the crack length (of several millimetres) is considerably small. Thus, the growth rate, da/dN , is considered to depend only on the continuum parameters such as the farfield stress range $\Delta\sigma$, the crack length a and load ratio R . Utilizing the elastic solutions of the near-tip stress fields within static fracture mechanics framework, the driving force for a stage II crack extension can best be represented by the stress intensity factor range, $\Delta K = K_{max} - K_{min} = (\sigma_{max} - \sigma_{min})\sqrt{\pi a}$.

Paris, Walker and Forman → empirical da/dN law

Noting the foregoing considerations, Paris and co-workers^{30,31} proposed the single most significant empirical crack growth rate law in the history of fatigue studies.

$$\frac{da}{dN} = C(\Delta K)^m \tag{1}$$

Paris and co-workers

where, C and m are constants. One should also note that the modifications accounting for the threshold stress-

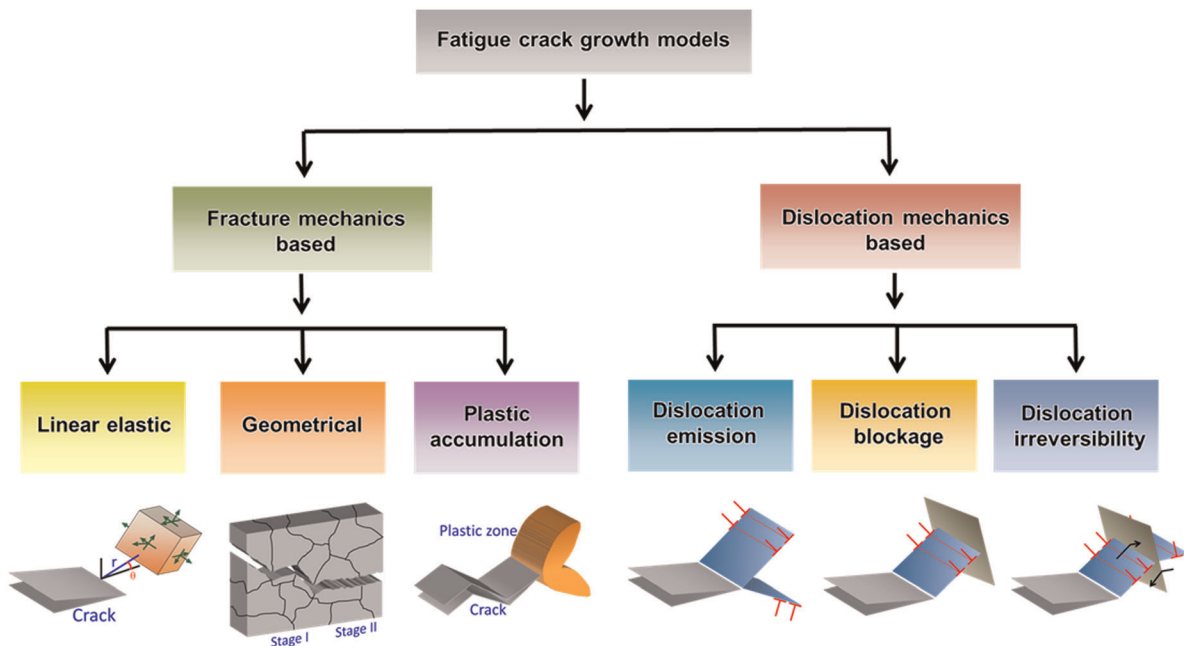
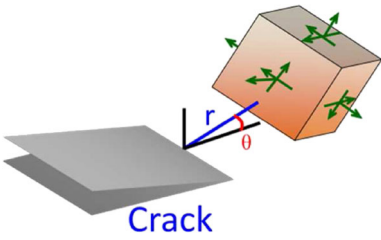
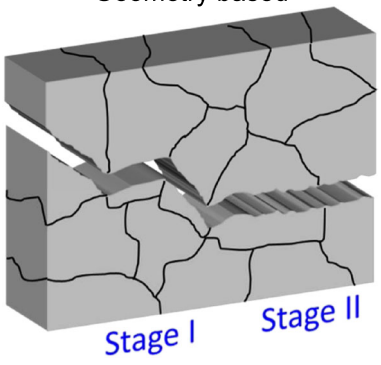
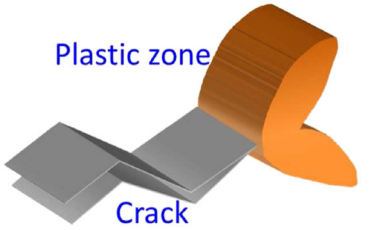


Fig. 10 A systematic classification of the predictive fatigue crack growth models.

Table 1 Examples fatigue crack growth models based on the fracture mechanics concepts

Type	Basis	Investigators	Major impact
<p>Linear elastic</p>  <p>Crack</p>	Elastic treatment of near-crack material	Paris ^{30,31} Forman ³³ Walker ³²	–Establishes empirical power laws for FCG characterization
<p>Geometry based</p>  <p>Stage I Stage II</p>	Geometry of crack growth in various stages	Suresh ^{34–36} Ritchie ³⁷	–Provides rationale for the observed power law relations –Derives constants for Paris's law (C and m) in terms of geometrical input
<p>Plastic accumulation</p>  <p>Plastic zone</p> <p>Crack</p>	Elasto-plastic consideration of cyclic crack growth	Tomkins ^{46,47} McClintock ^{44,45} Newman ^{52–55} Elber ^{48,49} Morrow ^{42,43} Antolovich ⁴¹ Sehitoglu ^{56–59}	–Considers plasticity based constitutive behaviours (e.g. closure effects in the wake and ahead of crack) in deriving FCG metrics

FCG, fatigue crack growth.

intensity stress factor range, ΔK_{th} , bound the lower end of the da/dN versus ΔK curve. The parameter ΔK_{th} has been established as the metric representing the FCG resistance. The exponent, m , is also considered as an extremely useful metric for comparing material damage tolerance to date. The universal usage of the Paris law to a wide spectrum of materials has essentially formed the basis for further research endeavours to rationalize the observed power law dependence from a physical perspective. A good number of researchers attempted to connect the constants C and m with material and/or loading parameters (as discussed in subsequent sections).

Given its far-stretching applicability, Eq. (1) has undergone a considerable number of refinements in the form of further incorporation of global loading parameters such as mean stress, load ratio (R) and static fracture toughness (K_C). Most noteworthy among such endeavours are those by Walker³² and

Forman *et al.*³³ The importance of their modification can be understood by the wide usage in industrial settings. It provides a design engineer with a quick estimation of the damage rate with relatively easily measurable global parameters.

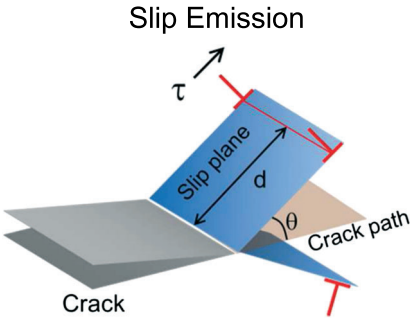
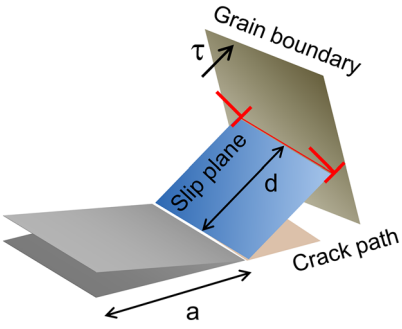
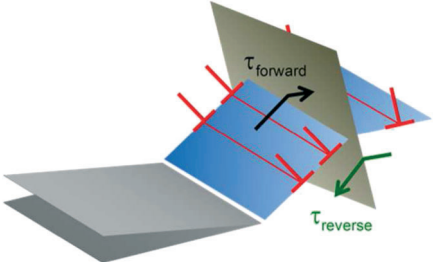
$$\frac{da}{dN} = f(\Delta K, R, K_C) \quad (2)$$

Walker and Forman *et al.*

Impact of linear elastic models

The primary impact of the LEFM-based models can be deemed as providing useful rules/equations for rapid assessment of damage trends. For instance, the widespread usage of the Paris law among the current practicing engineers can be attributed to its relative ease of application. The Paris-based characterization provides one with the

Table 2 Examples of fatigue crack growth models based on dislocation mechanics

Model type	Model basis	Investigators	Major impact
<p>Slip Emission</p> 	–Emission of slip from crack resulting in permanent tip extension	Gerberich ⁶¹ Weertman ^{63,64} Rice ⁶⁶ Yokobori ^{68,69} Lardner ⁶⁷ Needleman ^{70,71}	–Formulated stage II da/dN and mechanical K_{th} based on slip emission criteria
<p>Slip Blockage</p> 	–Blockage of crack-emitted slip by grain boundaries	Tanaka ^{75–77} Miller ^{84,85} Navarro ^{78–80}	–Predicted stage I FCG and microstructural K_{th} considering slip transfer resistance past grain boundaries
<p>Slip Irreversibility</p> 	–Irreversibility of crack-emitted slip under cyclic loading	Pippan ^{93,94} Krausz ⁹² Wilkinson ^{95,96} Sehitoglu ^{97–100}	–Formulated both stage I and II FCG metrics –Captured the role of interfaces precisely

FCG, fatigue crack growth.

important metrics – the threshold ΔK_{th} and the exponent m – which could most readily be used as important parameters to assess the damage behaviours. These equations are also excellent toolsets for pre-processing and post-processing of experimental data. Thus, the apparent simplicity in applying these models makes them widely applicable in the context of engineering design practices. These rules offer no input for the observed microstructural variations in the fatigue crack behaviours. Their predictive capability in terms of incorporating sub-structural phenomena is subsequently further improved by other models (e.g. geometrical or plasticity based theories). If a modern engineer or researcher wants to suggest process routes for improving fatigue resistance by tailoring microstructure, the LFM-based empirical laws need additional structural characterization.

GEOMETRICAL MODELS

With a view to elucidating the micromechanism as well as incorporating microstructural factors into FCG predictions, the geometrical theories emerged. We designate them ‘geometrical’ because the primary assumptions therein are associated with the geometry of the crack growth at various stages (with no plasticity input).

Suresh and Ritchie → rationalization of Paris-type power law

On analytical grounds, several researchers attempted to predict the da/dN on the basis of crack-path geometry. For example, Suresh^{34–36} considered the reduction of

the crack growth rate due to periodic deviations from a straight path and the associated contact of the flanks. The basic premise was that a kinked crack would require greater driving force, that is, ΔK in order to propagate than a straight crack of equivalent length. The da/dN for such a crack path was ultimately shown to be dependent only on the ΔK level, the length of the deflected portion of the crack L_{deflect} and the angle of deflection θ_{deflect} .

$$\underbrace{\frac{da}{dN} = f(\Delta K, L_{\text{deflect}}, \theta_{\text{deflect}})}_{\text{Suresh}} \quad (3)$$

Ritchie³⁷ furthered a model based on the notch analysis of the cracktip and applied it to the FCG threshold subjected to hydrogen diffusion (with a partial pressure, P_{H_2}). It was assumed earlier by Weiss and Lal^{38,39} that the crack would propagate if the nominal stress would be sufficiently high to exceed the static fracture strength, σ_{fracture} . Modifications in the effective radius⁴⁰ of the crack, $\rho^* = \rho^*(P_{H_2})$ as well as $\sigma_{\text{fracture}} = \sigma_{\text{fracture}}(P_{H_2})$ due to hydrogen ion absorption account for the corresponding variations in the ΔK_{th} levels. In addition, Arrhenius-type kinetics law was used to address the temperature (T) dependence therein.

$$\underbrace{\Delta K_{\text{th}} = f(R, \Delta K, \rho^*, \sigma_{\text{fracture}}, T)}_{\text{Ritchie}} \quad (4)$$

Impact of geometrical models

On carefully reviewing the foregoing models by Suresh and Ritchie, one can clearly perceive that their principal merit lies at the ability to rationalize the empirical crack growth data with some input representing the FCG geometry. Central to these theories is the postulation that the da/dN is governed by a ΔK -dependent power law of the form initially proposed by Paris and co-workers as in Eq. (1). Therefore, the primary objective thereof was to establish similar power laws with the Paris constant C and the exponent m now expressed in terms of mostly geometrical considerations. Motivated by the success of geometrical predictions, the consideration of the ever-present plasticity (both ahead and behind the cracktip), which is experimentally well known to have significant influences on the crack advancement, is addressed.

PLASTIC ACCUMMULATION MODELS

In general, plastic accumulation-based predictions acknowledge the considerable presence of the plastically deformed material in expressing the da/dN . These

models are particularly geared towards incorporating intrinsic and extrinsic effects (i.e. ahead and behind the cracktip, respectively) of dynamically evolving extent of the plasticity.

Antolovich, Morrow, McClintock and Tomkins → cyclic yielding and da/dN law

Antolovich and co-workers⁴¹ formulated da/dN based on a generic Coffin–Manson type low-cyclic fatigue damage formulation, that is, $(\Delta \epsilon_{\text{plastic}} + \Delta \epsilon_{\text{elastic}})/2 = \epsilon'_f (2N_f)^c + \frac{\sigma'_f}{E} (2N_f)^b$. They argued that the FCG would occur only when the macroscale plastic strain, on accumulation, is sufficiently high. Thus, they expressed the da/dN as a function of the empirical low-cycle fatigue properties as well as monotonic attributes $\Delta \epsilon_{\text{elastic}}$ (e.g. Young's modulus, E). Similarly, Majumdar and Morrow,^{42,43} on the basis of empirical equations of low-cycle fatigue, contended that the da/dN could be derived in terms of the macroscale Coffin–Manson parameters.

$$\underbrace{\frac{da}{dN} = f(\sum \Delta \epsilon_{\text{plastic}}) = f\left(\Delta K, \frac{\epsilon'_f}{(\sigma'_{\text{yield}})^2}, \frac{1}{E}, \frac{1}{\sigma'_f}, b, c\right)}_{\text{Antolovich and Morrow}} \quad (5)$$

On the other hand, McClintock^{44,45} assumed that if the local accumulated plastic strain at the cracktip exceeds a certain critical value, the crack starts advancing. Such a condition led to the establishment of a correlation between the crack opening displacement and the da/dN .

$$\underbrace{\frac{da}{dN} = \int_{r_{\text{plastic}}^{\text{cyclic}}} \Delta \epsilon_{\text{plastic}}^{\text{local}} = f\left(\Delta K^4, \frac{1}{E}, \frac{1}{\sigma'_{\text{yield}}}\right)}_{\text{McClintock}} \quad (6)$$

Similarly, Tomkins and co-workers^{46,47} attempted to predict the crack propagation on the basis of the decohesion of the near-tip material. The primary model input was a simple geometric assumption of the cyclic plastic zone size $r_{\text{plastic}}^{\text{cyclic}}$ and the macroscale plastic strain range $\Delta \epsilon_{\text{plastic}}$.

$$\underbrace{\frac{da}{dN} = f\left(\Delta K, r_{\text{plastic}}^{\text{cyclic}}, \Delta \epsilon_{\text{plastic}}\right)}_{\text{Tomkins}} \quad (7)$$

Elber, Suresh and Ritchie → early study of crack closure attributes

Elber and co-workers^{48,49} first suggested that FCG rate depends on the plastic history not only near the tip, but also in the wake. They unravelled the phenomenon of premature crack closure before the applied K level

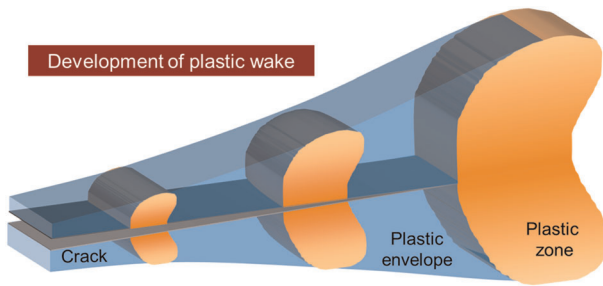


Fig. 11 Development of a plastic envelope in the wake of the progressing crack due to the ever-enlarging plastic zone first conceptualized by Elbar.^{48,49}

reaches K_{min} because of residual plastic deformation behind the cracktip. As the crack becomes progressively longer, the ΔK increases and so does the plastic zone (Fig. 11). Thus, an envelope of plastically deformed material is left behind the cracktip (the blue region). The extra material flows from the surrounding elastic bulk and accumulates on the crack faces, giving rise to the early contact of the crack faces even if the tensile load is still non-zero. As a result, the concept of the FCG driving force was re-defined as the load ratio R -dependent effective stress-intensity factor range, $\Delta K_{eff}(R) = K_{max} - K_{open}$.

$$\underbrace{\frac{da}{dN} = C(\Delta K_{eff}, R)^m}_{\text{Elber}} \quad (8)$$

In addition to the plasticity-induced crack closure, Suresh and Ritchie^{50,51} classified the crack contact scenarios in metallic materials as a result of – (i) oxide layer formation, (ii) viscous fluid penetration, (iii) phase transformation and (iv) surface asperities. All these extrinsic (i.e. behind the cracktip) phenomena were shown to contribute to the overall damage behaviour. The

controlling parameters of various types of closure-induced FCG were identified as: partial pressure of oxygen and hydrogen (P_{O_2} and P_{H_2}), crack opening displacement and load ratio (R).

$$\underbrace{\frac{da}{dN} = f(\Delta K_{eff}, R, P_{O_2}, P_{H_2}, CTOD)}_{\text{Suresh and Ritchie}} \quad (9)$$

Newman and Sehitoglu → predictions of crack closure

Newman and co-workers^{52–55} extensively simulated the history-dependent crack closure within finite element framework. They were able to capture the reduced degree of closure in plane strain compared with the plane stress. Plastic constitutive models were used to capture both near-tip and behind-tip permanent strains.

The mechanism of the extra material amassed on the crack faces (i.e. causing plasticity-induced closure) was studied by Sehitoglu and co-workers^{56,57} (Fig. 12). Under plane-strain conditions (i.e. for a very thick specimen), the material immediately ahead of the crack flows opposite and parallel to the crack growth direction in finite element simulations. On the other hand, farther away from the cracktip, the material flows towards the propagation direction. In essence, they pointed to the existence of the oppositely flowing materials in the vicinity of the crack faces. By contrast, for the plane-stress case (i.e. for a very thin plate), the material flows from the bulk perpendicular towards the crack flanks, resulting in a necking-like deformation.

In the finite element-based models both by Newman and Sehitoglu and their co-workers, the additional plasticity-related input parameters to predict the da/dN

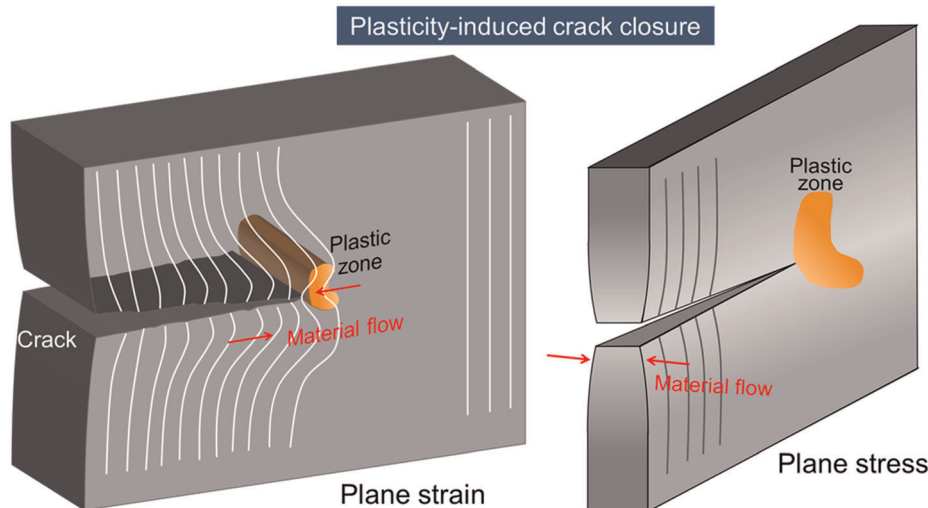


Fig. 12 The material flow from the bulk that accumulates on the crack flanks, thereby giving rise to the premature contact as noted by Sun and Sehitoglu.^{56,57}

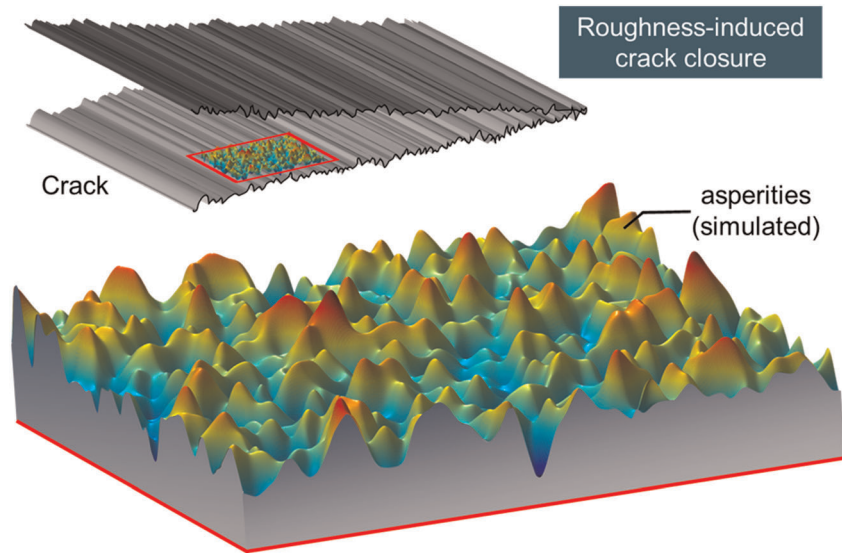


Fig. 13 Garcia and Sehitoglu^{58,59} modelled roughness-induced crack closure as a contact problem with random distribution of surface asperities.

levels were the plastic modulus H , and effective stress σ_{eff} , and hydrostatic stress σ_{hydro} .

$$\frac{da}{dN} = f \left(\Delta K_{\text{eff}}, R, \frac{\sigma_{\text{max}}}{\sigma_{\text{yield}}}, \frac{\sigma_{\text{eff}}}{\sigma_{\text{hydro}}}, \frac{H}{E}, \frac{\text{CTOD}}{h_{\text{asperity}}}, \rho_{\text{asperity}} \right) \quad (10)$$

In addition, Garcia and Sehitoglu^{58,59} investigated the roughness-induced crack closure by assuming Gaussian distribution of crack face asperities (Fig. 13). The closure phenomenon was modelled as a contact problem among the asperities. For the prediction of the roughness-induced closure, the average asperity height h_{asperity} and asperity density (per area) ρ_{asperity} were utilized.

$$\underbrace{\frac{da}{dN} = f \left(\Delta K_{\text{eff}}, R, \frac{\text{CTOD}}{h_{\text{asperity}}}, \rho_{\text{asperity}} \right)}_{\text{Sehitoglu}} \quad (11)$$

Impact of plastic accumulation models

The major contribution of these theories is undoubtedly the substantial incorporation of the plastic constitutive considerations into the realm of the otherwise empirically treated fatigue problems. For example, the earlier models concerned about the intrinsic plasticity effects (e.g. those by Antolovich, Morrow, McClintock and Tomkins) established that global material properties such as Young's modulus and cyclic yield strength could be used to predict the cyclic damage attributes. Such approaches were essentially important extensions over the LEFM/geometry-based theories, in that the analytical formulations were now more physically based than observation-based. Moreover, on discovering various closure

phenomena from experiments, the usefulness of the metric ΔK_{eff} was brought into attention. The plasticity-based FCG models can be further extended in applicability by accounting for the role of microstructural barriers to the plastic flow. To address such effects, one needs to include the mesoscale plastic deformation mechanisms themselves (such as dislocation slip activities) into the FCG modelling assumptions.

DISLOCATION MECHANICS-BASED FATIGUE CRACK GROWTH THEORIES

Exhaustive experimental studies have confirmed that FCG at the mesoscopic lengthscale is in fact governed by ubiquitous slip phenomena. It is now well accepted that depending on the history of dislocation slip (i.e. equivalent to the plastic zone size as treated in the continuum context), an advancing crack would behave as either microstructure-sensitive or not. Therefore, the FCG is a problem, which could most accurately be modelled by incorporating the variables controlling dislocation characteristics at the mesoscale. Slip-based theories essentially allow for the examination of ductile versus brittle tendencies, the role of interfaces as well as the irreversible damage. Upon a meticulous review, we deem it important to classify such models into three major categories, namely, (i) the dislocation emission, (ii) dislocation blockage and (iii) dislocation irreversibility.

DISLOCATION EMISSION MODELS

Rice and Thompson,⁶⁰ in their pioneering work, set a condition for the slip emission accounting for the

competition between the ductile and brittle fracture. Emission of slip was shown to have the effect of leaving a permanent displacement at the cracktip equal to the collective Burger's vectors.

Gerberich → establishing threshold criterion

A number of analytical models have been proposed to predict the condition for the crack growth onset (i.e. the threshold) on the basis of slip emanation. Most notable among these theories is the one by Gerberich.⁶¹ Generally speaking, the threshold condition in these models dictates that a crack would start advancing if the critical frictional stress $\tau_{friction}$ (i.e. which would be required to nucleate a dislocation) is exceeded. The other input parameters include the distance of the nucleated slip from the tip d and the angle between the crack and the slip paths θ . Similar condition was also examined by Sadananda⁶² and co-workers.

$$\underbrace{\Delta K_{th} = f(\tau_{friction}, d, \theta)}_{\text{Gerberich}} \tag{12}$$

Weertman, Rice and Needleman → predictions of da/dN

Weertman^{63,64} employed the slip distribution concept developed by Bilby, Cottrell and Swinden⁶⁵ (the so-called Bilby-Cottrell-Swinden model) to quantify the cracktip displacement (Fig. 14). The important contribution of this model was that the dislocation considerations at the

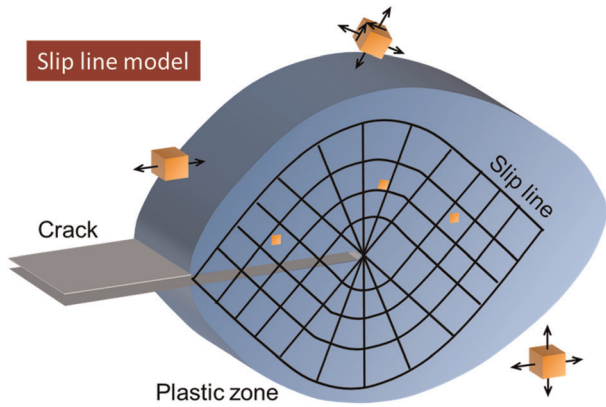


Fig. 15 Slip line model by Rice.⁶⁶

cracktip were shown to be suitably correlated with the global parameters such as the monotonic yield strength σ_{yield} and a critical hysteresis energy U^* . The significance of U^* is that the absorption of global hysteresis energy over cycles needs to overcome the critical U^* level in order for the crack to start propagating. Independently, Rice⁶⁶ reached a very similar conclusion regarding da/dN based on the near-tip plastic zone assumed to be consisting of continuous slip lines (Fig. 15). A material point well ahead of the cracktip was traced until it was first engulfed by the advancing plastic zone and then reached by the cracktip. The continuum stress fields in individual representative volume element (i.e. from the intersection of slip lines) were used to arrive at the expression for da/dN .

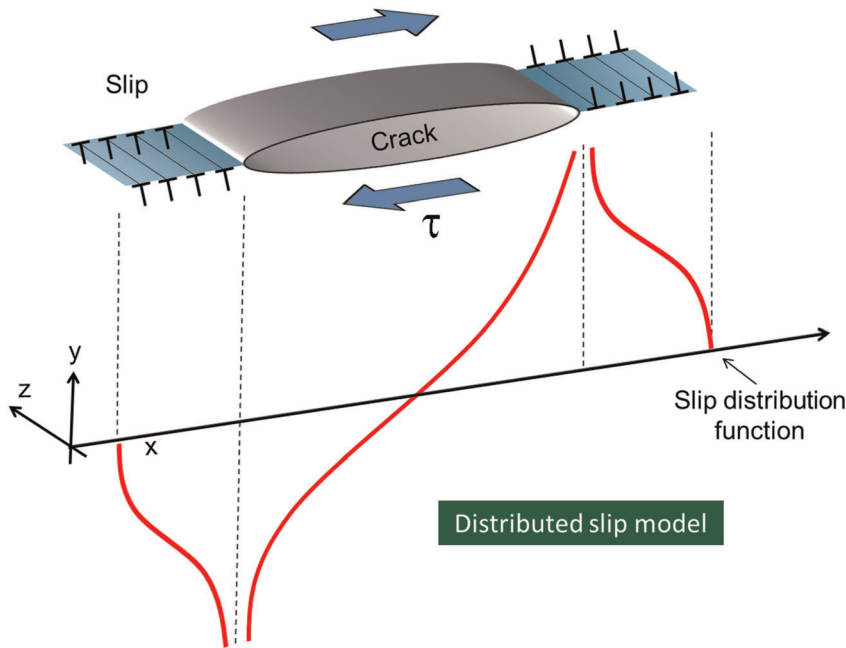


Fig. 14 The analytical da/dN model by Weertman^{63,64} based on the BCS slip distribution function.⁶⁵

$$\frac{da}{dN} = f \left(\underbrace{\Delta K, \frac{1}{\sigma_{\text{yield}}}, \frac{1}{U^*}}_{\text{Weertman and Rice}} \right) \quad (13)$$

Among other significant works are the ones by Lardner⁶⁷ and Yokobori.^{68,69} Lardner attempted to capture FCG by considering continuous slip distribution ahead of the crack. On the other hand, Yokobori and co-workers relied on discrete mathematical dislocations at the cracktip and predicted the da/dN based on the net Burgers vector of the emitted slip. Such models assist in directly examining the sensitivity of the local parameters (e.g. slip velocity, density etc.) on the crack propagation metrics. Essential among the input parameters for these theories were the magnitude of the Burgers vector \vec{b} , applied load frequency $f_{\text{frequency}}$ and the number of discrete slip emitted, n .

$$\frac{da}{dN} = f \left(\underbrace{\Delta K, |\vec{b}|, n, T, f_{\text{frequency}}}_{\text{Lardner and Yokobori}} \right) \quad (14)$$

More recently, Needleman and co-workers^{70,71} demonstrated the feasibility of incorporating the discrete dislocation dynamics principles in a finite element simulation framework. They simulated the growth of a crack under cyclic loading, driven by the motion of discrete dislocations of certain density ρ_{slip} (as acted upon by Peach–Köhler forces, $\vec{F}_{\text{Peach–Köhler}}$ by each other). This approach was capable of reproducing both the near-threshold as well as the stable propagation under different load ratio magnitudes.

$$\frac{da}{dN} = f \left(\underbrace{\Delta K, R, \rho_{\text{slip}}, \vec{F}_{\text{Peach–Köhler}}, \theta}_{\text{Needleman}} \right) \quad (15)$$

Impact of slip emission models

It is noteworthy that the dislocation emanation-based theories rely upon the fact the near-tip slip activities are under no influence of any slip-obstacles (e.g. grain/twin boundaries). As discussed earlier, such a situation would be possible during the stage II crack growth period when the history of massive accumulation renders the FCG rather microstructure-insensitive. Therefore, the slip emission-based models have proved greatly useful to predict the FCG metrics corresponding to the stable Paris regime. The applicability of these models to predict the microstructurally short crack growth behaviour can be further extended. As found experimentally, a stage I crack is considerably influenced by the presence of grain/twin boundaries as well as the host grain orientation, resulting in a tortuous growth path with highly fluctuating

rates.^{9,72,73} Essentially, the advancement of a short crack would be decided by the degree of shielding effects to the slip activities induced by interfacial defects.⁷⁴ The foregoing models pave the way for predicting such physical processes. Such considerations are addressed by the slip blockage-based FCG models discussed as follows.

DISLOCATION BLOCKAGE MODELS

Generally, these theories consider the resistance to the slip flow past a generic grain boundary (GB). Thus, the primary assumption of the slip blockage models is associated with overcoming the slip-shielding stress of an obstacle.

Tanaka, Navarro and de los Rios, Miller → predictions of stage I growth

Tanaka^{75–77} and co-workers proposed an analytical crack growth model based on the crack-emitted slip subjected to GB impedance. They considered the slip band to be represented by a continuous distribution of dislocations gliding against a uniform frictional stress. They assumed plastic slip associated with fatigue damage to be extending through grains, and GBs acting as slip barriers of given strength. As in Fig. 16, the model is capable of capturing the retardation of the advancing crack at the grain boundaries. The primary input therein was the friction stress required for the forward slip glide past a GB, that is, $\tau_{\text{friction}}^{\text{forward}}$ and the spacing between the cracktip and the boundary, d .

Navarro and de los Rios^{78–80} forwarded a similar FCG predictive theory unifying the short/long crack growth regimes. In their approach, the crack-emitted slip undergoes successive blocking a series of GBs (Fig. 17). It was shown that with increasing history of slip activities, the effective impedance of the grain boundaries is diminished. As a result, the crack growth gradually converges to the level equivalent to the stable stage II propagation. The model could faithfully predict the experimental short crack behaviour (particularly the fluctuating nature of the da/dN because of grain boundaries) as observed in some aluminium alloys^{81,82} and stainless steels.⁸³ It can also be noted that, upon encounters with a number of grain boundaries, the crack builds a history of slip activities and eventually becomes insensitive to such obstacles (i.e. corresponding to the stage II regime). Miller and co-workers^{84,85} examined also an advancing stage I crack passing through multiple grains and demonstrated the short crack growth characteristics subjected to GB-induced retardation. All these blockage models can be summarized as follows.

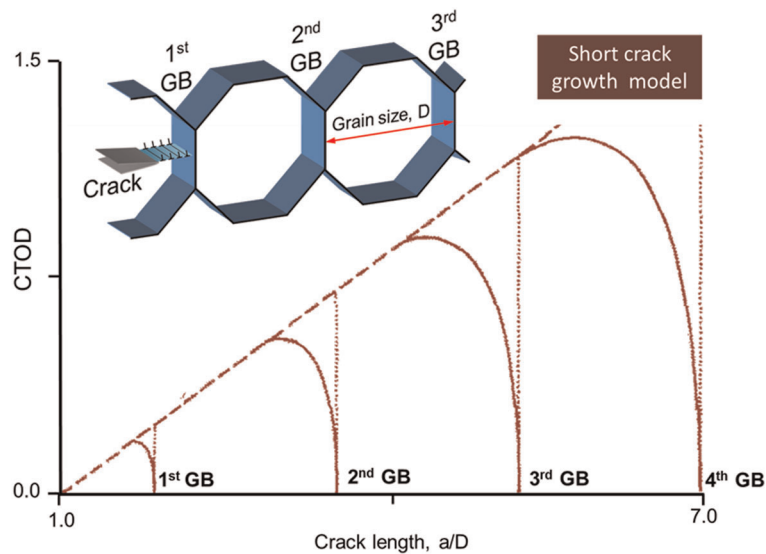


Fig. 16 The short crack growth model by Tanaka and co-workers.^{75–77} Retardation of the advancing crack at a series of grain boundaries was predicted.

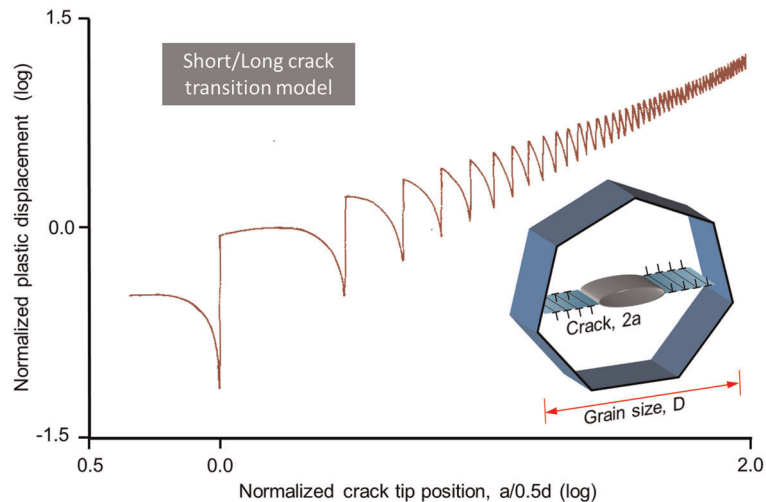


Fig. 17 Transition from the short crack to the long crack behaviour by Navarro and de los Rios.^{78–80}

$$\frac{da}{dN} = f\left(\Delta K, \tau_{\text{friction}}^{\text{forward}}, d\right) \quad (16)$$

Tanaka, Navarro and Miller

Impact of slip blockage models

The slip blockage-based theories were particularly impactful, in that they were able to predict the transition between the experimentally observed short/long crack thresholds.⁸⁶ This is essentially a significant improvement on the theoretical grounds. One immediate impact of these models is that the higher strength of slip obstacles, if possible to impart to the material, was predicted to be a beneficial microstructural attribute to achieve superior FCG resistance. Now, there exists a possibility for interesting extension of the slip blockage models considering the actual physics of the boundary-

affected stage I FCG. It is known experimentally that depending on the local stress and the slip geometry, the nature of the dislocation-boundary interactions may drastically differ.⁸⁷ In some cases, the GB may completely block the impinging slip and in some other, it may permit complete transfer (i.e. a cross-slip situation). Between these two extremities, there are myriad other possibilities of reaction outcomes.⁸⁸ Essentially, each reaction would be unique in terms of the degree of the resistance to the oncoming slip; and hence, the attendant crack behaviours in the long run.

The aforementioned slip blockage theories consider a generic nature of the GBs, which the crack would encounter. As observed experimentally, the crack growth rate may decelerate as it approaches certain type of boundaries and/or in certain orientation of the grain, but may proceed with no blockage in other cases.⁸⁹ In

some cases, the crack length corresponding to the threshold may span one or two or three grains, in others not. The aforementioned models have essentially assumed that the plastic zone is blocked by grain boundaries irrespective of the specific outcomes of slip-boundary interactions. To address such phenomena, one has to consider both the forward and the reverse flow of slip past a GB, which can be most conveniently quantified by considering the slip irreversibility.

DISLOCATION IRREVERSIBILITY MODELS

Fundamentally, this class of FCG models assumes that the cracktip extension occurs as a direct consequence of the irreversible trajectories of the crack-emitted slip. If the forward slip completely reverts to back the tip on the unloading half of the cycle, there would be no net crack growth whatsoever.

Krausz, Pippan and Sehitoglu → prediction of threshold and da/dN

Frong and Thomas^{90,91} and Wu, Koul and Krausz⁹² used the concept of irreversible slip at the cracktip resulting in the zigzag crack extension during the stage II growth period (Fig. 18). Under tension, the cracktip opens by emitting slip on the slip system 1 (red), which on unloading reverts back to the tip only partially, thus activating the parallel slip system 2 (blue). The open cracktip now slips on the system 2 during the rest of the unloading period resulting in the sharpening of the crack. Such process results in a differential between the forward and reverse displacements at the cracktip ($u_{forward}$ and $u_{reverse}$). The same mechanism is repeated on the cycle 2 for another pair of parallel slip systems. On the basis of the

forementioned mechanisms, these researchers proposed a da/dN model additionally incorporating the deformation kinetics (considering activation volume, V^*) of forward and reverse slip motions.

$$\frac{da}{dN} = f(\underbrace{\Delta K, u_{forward}, u_{reverse}, V^*, T}_{\text{Krausz}}) \tag{17}$$

Analytically, Pippan and co-workers^{93,94} advanced the idea of near-tip slip irreversibility by quantifying the trajectories of individual dislocations under cyclic loading. In their model, a series of elastically interacting dislocations are emitted from the crack during loading, which assume equilibrium positions under the balance of forces (Fig. 19). On unloading, these dislocations reverse their motions and attempt to return to the cracktip. The condition of the crack growth is established as a minimum of one residual Burgers vector left at the cracktip on each cyclic. This scenario would be possible when the emitted slip (i.e. during loading) is unable to return or annihilates with slip of opposite sign nucleated during the reverse loading. Pippan and co-workers were thus able to predict both the Paris regime and the threshold. The threshold behaviour in particular could not be captured via continuum theories such as the Rice's slip line model. The motions of forward and reverse dislocations were also investigated by Wilkinson and co-workers.^{95,96} They confirmed the important role of irreversible dislocation glide and the size of the dislocation free zone (x_{DFZ}) on the FCG metrics.

$$\frac{da}{dN} = f(\underbrace{\Delta K, x_i^{forward}, x_i^{reverse}, x_{DFZ}}_{\text{Pippan}}) \tag{18}$$

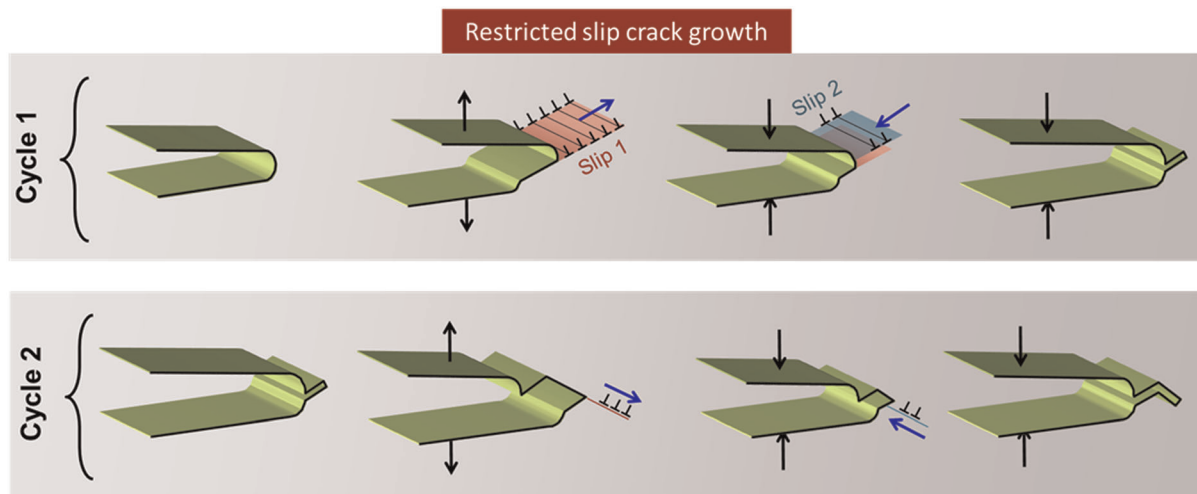


Fig. 18 Cyclic crack growth as a result of restricted slip as envisioned by Wu, Koul and Krausz.⁹²

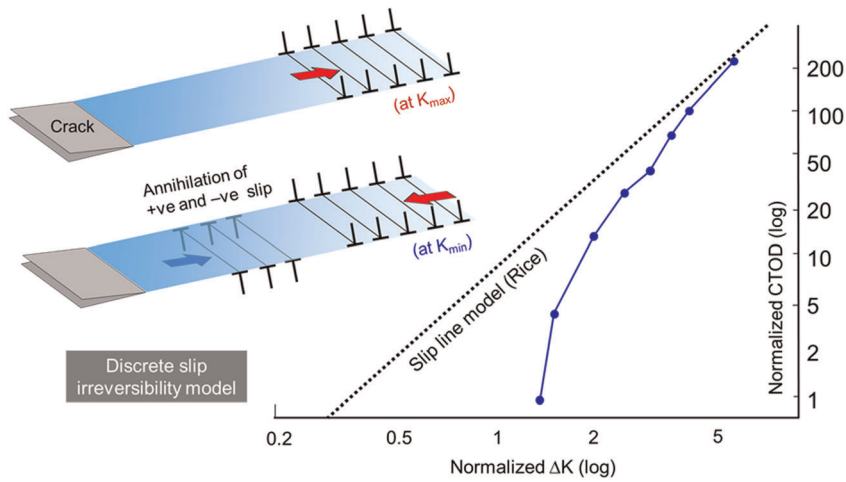


Fig. 19 Pippan’s model is based on the idea of the irreversibility of discrete slip.^{93,94}

The latest advancement in the slip-based modelling of FCG has recently been offered by Sehitoglu and co-workers^{97–100} (Fig. 20). Their particular contribution was to explore various slip-coherent boundary reactions and how they would greatly influence the stage I crack growth as well as the threshold scenario. As would be the most realistic case in nature, a certain boundary would influence the incident slip in a particular manner, which could be distinguished in terms of the residual dislocation created on the boundary \vec{b}_r . These researchers categorized the reaction types and the associated boundary penetration strength both for forward and reverse slip flow ($\tau_{friction}^{forward}$ and $\tau_{friction}^{reverse}$). This model particularly explored both boundary-specific and reaction-specific frictional stresses, which could be used to obtain the associated FCG metrics. They used the model to explore the role of nano-dimensions of a coherent twin on the da/dN . A trend was established in terms of the damage metric and twin-related geometrical parameters.¹⁰¹

$$\frac{da}{dN} = f(\Delta K, \underbrace{\tau_{friction}^{forward}, \tau_{friction}^{reverse}}_{\text{Sehitoglu}}, |\vec{b}_r|) \quad (19)$$

Impact of slip irreversibility models

Today, there exists a considerable number of experimental evidence that the slip irreversibility at the cracktip is the governing physical process that could fully account for any fatigue-related damage^{102–106} (e.g. strain localization leading to material separation at the very early stage or the subsequent advancement of the crack). To that end, these theories have particularly identified various controlling parameters to capture the degree of the cyclic slip irreversibility (e.g. dislocation trajectories, differential in forward and reverse displacement and extrinsic levels of frictional stresses). The concept of irreversible slip holds tremendous potential to capture any microstructural damage physics, thereby paving the way for indeed proposing a unified fatigue model.

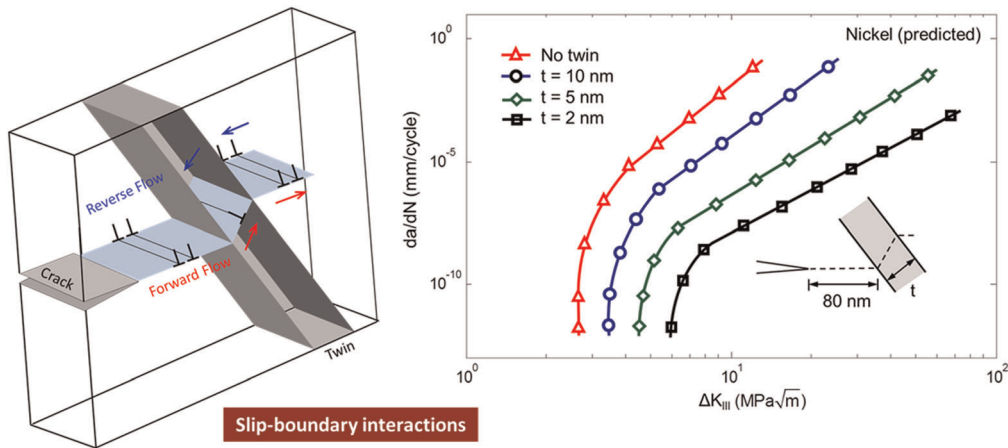


Fig. 20 The slip irreversibility-based model by Sehitoglu and co-workers.^{97–100}

With the advent of superior computer power, such an endeavour, is definitely not impossible today. One needs to determine the physical quantities underlying the inherent material propensity for slip versus any other mode(s) of plastic deformation. For example, computational materials scientists are unravelling the specifics of dislocation slip, which has been unprecedented so far (e.g. quantifying the energy barrier for slip from the discrete lattice level). Definitely, the irreversibility of discrete plasticity could open up a number of possibilities where it would be possible to merge the classical theoretical ideas with the modern energy barrier concepts. Future challenges include further unfurling of the discrete lattice level quantities, which the current irreversibility-based models can incorporate for further refinements. To that end, there are already significant developments already under way discussed as follows.

LATEST DEVELOPMENTS – ATOMISTICS

The last several years have witnessed a considerable rise in the understanding of the atomistic effects related to crack propagation. There are studies that have captured different near-tip damaging processes with atomic-scale resolution (e.g. slip emission, void formation/coalescence, crack branching etc.). Later, we describe briefly some recently emerging FCG studies using molecular dynamics (MD) simulations (also summarized in Fig. 21).

For nanocrystalline materials with grain size on the order of 10 nm, the FCG is found to occur via void

formation at and around triple joints as unravelled by Horstemeyer and co-workers,^{107–109} Nishimura and Miyazaki¹¹⁰ and Farkas *et al.*¹¹¹ Rountree *et al.*¹¹² reported a change in crack growth mechanism (e.g. branching, slipping and cleavage) depending on the crystal orientation. Zhou *et al.*¹¹³ modelled the FCG in presence of nano-sized coherent twins, and extracted the da/dN metrics from atomistic simulations. Machova and co-workers^{114,115} examined various near-tip plastic phenomena in body centered cubic iron. Warner and co-workers^{116,117} proposed a coupled atomistic-discrete dislocation framework where the cracktip was atomistic, while the surrounding medium was assumed as a continuum (via finite element methods). From these atomistic studies, new functional dependence of crack growth has emerged at the nanoscale for a number of materials of interest.¹¹⁸ For example, the da/dN is found to be dependent on the strain-rate ($\dot{\epsilon}$), Schmid factor (m_{Schmid}), single crystal orientation (\vec{g}_{hkl}), vacancy generation rate ($\dot{\rho}_{vacancy}$) and the density of interfacial obstacles ($\rho_{interface}$).

$$\frac{da}{dN} = f\left(\Delta K, \frac{1}{\dot{\epsilon}}, m_{Schmid}, \tau_{friction}, \vec{g}_{hkl}, \dot{\rho}_{vacancy}, \rho_{interface}\right)$$

Horstemeyer, Farkas, Machova, Rountree, Chen, Miyazaki and Warner

(20)

Benefitting from advanced computational materials science tools, the foregoing endeavours have unearthed unprecedented knowledge of nanoscale materials behaviour underlying the FCG, otherwise impossible to obtain

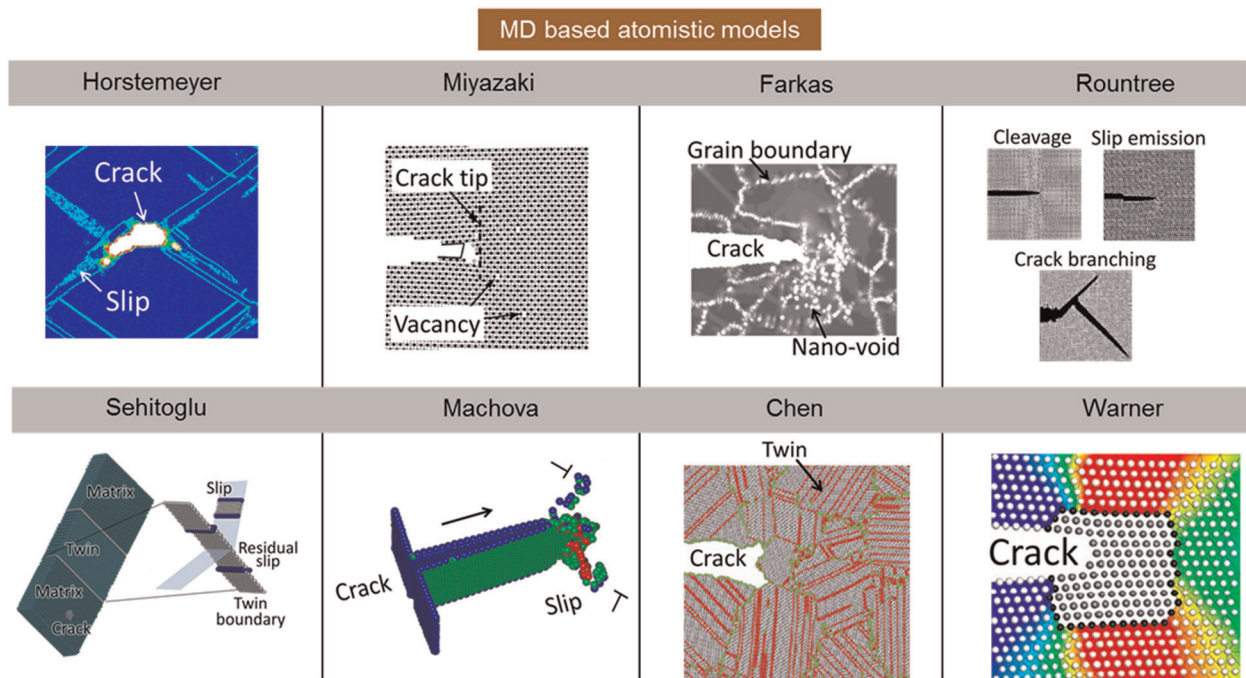


Fig. 21 Some recently emerging atomistic simulation-based fatigue crack growth models. MD, molecular dynamics.

from experiments. These studies have demonstrated the feasibility of extracting lattice scale parameters of importance, thus opening up new frontiers of research.

One must, however, take considerable caution in interpreting atomic scale simulations particularly in the continuum context. Currently, there are some well-known artefacts inherent in the MD-based modelling.¹¹⁹ These side-effects may factor in spuriously while extrapolating certain MD results to the continuum behaviours, if not careful. MD deformation, for example, is characterized by rather high strain-rates (on the order of 10^8 s^{-1} or even higher), thus unrealistically raising the nominal stress levels to several gigapascals. Such speedy deformation at the nanoscale may give rise to the mechanisms, which may not occur in nature under similar conditions. Moreover, further complications can emerge because of the presence of free surface (depending on boundary conditions). Free surfaces with dangling bonds may introduce undesired energy flow into the bulk material given the few nanometers lengthscale of a typical simulation representative volume element. Finally, some simulation-obtained metrics (e.g. elastic modulus, cohesive energies) are also subjected to the accuracy of the curve-fitted pair-potential containing all the materials description.¹²⁰ In other words, one must be careful regarding what parameter to calculate from atomic simulations and how to scale it to the continuum level via appropriate mesoscale normalizations. As an example of such normalization scheme, one can extract periodic energy profile (i.e. Peierls landscape), which is immune to the foregoing artefacts,^{121–123} and then convert it into mesoscale frictional stresses (discussed in more details in the next section).

DISCUSSION AND CONCLUDING REMARKS

Initiation versus propagation

Per the most commonly practiced engineering guidelines, the study of metal fatigue has long been treated as two separate problems: (i) crack initiation (i.e. the appearance of a detectable stage II crack of a few millimetres length as revealed by conventional non-destructive techniques) and (ii) crack propagation (i.e. stable incremental lengthening of the discernible stage II crack up to the final fracture). Traditionally, initiation-based characterizations are conducted by Coffin–Manson–Basquin type equations (i.e. stress–strain versus life curves), while propagation studies are Paris law-based (da/dN versus ΔK). The reason for such separation is the observation that initiation and propagation behaviours respond differently to both loading and material variables^{124,125} (e.g. grain size, farfield stress levels). For example, at low farfield stress (i.e. high cycle fatigue, $N > 10^6$), a large fraction of the fatigue life is spent upon the macro-crack initiation, which

mechanistically is in fact the stage I growth period over a finite cluster of grains. On the other hand, with increased stress levels (i.e. low-cycle fatigue), the stage II crack propagation dominates the total lifespan. Similarly, alteration in material variable such as grain refinement is observed to hugely improve the initiation life, while considerably deteriorating the propagation (i.e. stage II) resistance.¹²⁶

These empirical findings strongly consolidated the separate treatment of crack initiation and propagation leading inevitably to distinct symposia and conferences for decades. However, such separation of communities is in fact diminishing recently in view of the latest revelations discussed as follows. If one delves deeper into the mechanistic processes of these seemingly distinct damage phenomena, interesting similarities are found in the form of slip activities. The physics behind material separation at the microscopic level, that is, stage I crack formation is due to the irreversible to-and-fro motions of glissile dislocations as studied extensively by Essmann, Mughrabi and co-workers.^{127,128} The irreversible bulk dislocation activities manifest themselves at the free surface or grain interfaces in the form of persistent slip bands leading to stage I crack nucleation. Other sites for slip accumulations (i.e. crack nucleation sites) are pre-existent stress concentrators such as grain boundaries and inclusions. Now, it is the very same process of slip localization at the cracktip that also drives the stage I propagation to evolve into the stage II until the final failure. Evidently, the crack initiation and propagation (as in their conventional definitions) share the same mechanistic foundation at the microscopic lengthscale. This is exactly where, as one can perceive, the possible unified treatment of crack formation and progression could be performed on modelling grounds. For example, the influences of the farfield stresses and grain size/distribution could be theorized in terms of how slip responds to the variations thereof. In that regard, significant progresses have been made in quantifying the governing parameters for dislocation slip in the recent decade.

Promising arenas for future research

From slip perspective, the lattice resistance to dislocation glide (i.e. the Peierls barrier) is energetically represented by the so-called unstable stacking fault energy γ_{us} , first conceptualized by Vitek.¹²² Subsequently, Rice¹²¹ and later Tadmor and Hai¹²⁹ laid the foundation for utilizing γ_{us} for the slip emission condition from the cracktip under static fracture condition. As discussed earlier, the fundamental slip-mediated irreversible processes underlying material separation and damage procession are essentially similar. In the fatigue context, the fault energy considerations certainly hold considerable promise in terms of bridging the initiation and propagation processes. Further benefit of using a slip-based energy criterion lies

at the immense promise of exploiting the latest atomistic modelling tools most appropriately, circumventing the aforementioned artefacts. For example, recent advances note that the parameter γ_{us} subjected to alloying and/or an increased presence of interfaces could be extracted precisely using combined MD and quantum mechanical simulations (e.g. density functional theory).^{88,130} Mesoscale normalizations could be applied to convert γ_{us} into corresponding frictional stresses to be used in continuum formulations. Such an approach has the potential of capturing the inherent material propensity in terms of crystal defects, the dynamics of which essentially governs the material constitutive responses at the macroscale. Given the identification of various controlling parameters at different lengthscale, the incorporation of latest atomistic understanding would bring forth further improvements in the modelling synergy in foreseeable future. Thus, within a uniform theoretical framework, one can examine the microscale slip behaviours leading to material separation as well as the ensuing progression subjected to a variety of microstructural environments.

Today at our disposal, we possess an assortment of modeling tools to address the physical processes of damage at various lengthscale. For instance, the principles of the continuum mechanics can directly correlate with the experimentally measurable damage metrics. At the mesoscale (i.e. at the single grain level), one can employ dislocation dynamics^{131–133} simulations to predict the macroscale constitutive response. Smallest of all is the atomic scale where, as we have pointed out earlier, one can examine the inherent lattice properties related to damage accumulation. A rigorous review covering the microstructural effects on fatigue has recently been conducted by Pineau and co-workers¹³⁴ to which interested readers are referred. The possible unification of all these approaches into one depends on the inherent shortcomings of individual methods and how information from one lengthscale is translated to the others. More research is required to fine-tune the strategies to avoid, for example, the artefacts and uncertainties of atomistic simulation methods. Thus, in terms of extending the multiscale approach (i.e. spanning continuum, mesoscale and atomistic phenomena) of fatigue evaluation for modern engineering, applications need a combined treatment. Today, commercial finite element-based simulation packages are available to address the engineering component analyses with accuracy. It would of course be worthwhile to work towards developing a combined atomistic (representing discrete lattice effects) and continuum (addressing the macroscale effects) simulation package available to modern engineers for immediate use. To that end, one ought to develop methods to incorporate the foregoing theoretical developments into a technological tool. Such a tool would provide unprecedented capability for a modern design engineer.

For instance, in view of improving the overall fatigue properties, the ideal design goal in fabricating metals and alloys is to optimize the microstructural variables for enhanced resistance to both crack initiation and crack propagation. It remains to be seen how the recent developments in the computational materials science would give rise to physically based materials design principles replacing the century-old empirical approaches. Such an accomplishment would certainly empower modern engineers to decide on what desired attributes to impart to the microstructure so as to achieve superior fatigue qualities.

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