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Hybrid discrete dislocation models for fatigue crack growth

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ABSTRACT

A framework for accurately modeling fatigue crack growth in ductile crystalline solids is necessarily multiscale. The creation of new free surface occurs at the atomistic scale, where the material's cohesive strength is controlled by the local chemistry. On the other hand, significant dissipation during fatigue crack growth takes place at a size scale that can be modeled appropriately by conventional continuum mechanics. The intermediate size scale where the discreteness of dislocations comes into play is the main origin of the hysteresis needed for fatigue and of the high stresses required for atomistic separation to take place. We focus on recent developments which permit analyses of fatigue crack growth involving the direct coupling of disparate size scales. Although no analyses have been carried out directly coupling size scales from the atomic to the conventional continuum, the ingredients to do so are in place. We provide background that illustrates the key role played by the intermediate discrete dislocation size scale and review steps that have been taken to permit direct size scale coupling. The prospects and modeling needs for further developments are also discussed.

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1. Introduction

Fatigue crack growth is the growth of a crack under cyclic loading conditions at a driving force that is smaller than is required for the same crack to grow under monotonic loading conditions. For crystalline metals, there is a threshold driving force below which fatigue crack growth does not occur or, more likely, occurs at a rate too low (say less than 10^{-8} mm/cycle) to be of concern in applications. For increasing values of driving force, the average crack growth rate at first increases steeply and subsequently enters the Paris law regime, see e.g. Suresh [1]. Near the threshold plastic deformation is confined to a relatively small volume in the vicinity of the crack tip. As the crack driving force increases, the plastically deformed volume emanating from the crack tip increases but effects such as those arising from net Burgers vector (geometrically necessary dislocations) and the discreteness of dislocation sources still come into play in the near crack tip region.

Typically, analyses of fatigue crack growth are carried out using a fatigue crack growth law that is specified *a priori*. In contrast, the focus here is on modeling where crack growth can arise naturally as a consequence of the solution to an initial/boundary value problem.

A variety of continuum theories have been proposed to rationalize fatigue crack behavior in the Paris law regime. In some cases, e.g. [2,3], it is presumed that the fatigue crack growth rate is proportional to the cyclic crack opening displacement which implies a Paris exponent of two. Damage accumulation models, e.g. [4,5], give rise to a Paris exponent of four. More recent continuum plasticity based models have been developed, see e.g., [6–8], which can lead to a wider range of behaviors but at present the continuum based models have yet to account either for the wide range of Paris exponents observed experimentally or for the observed scaling with material properties, e.g. [9–11].

Dissipation is necessary for fatigue. For an elastic system (i.e., the structure, component or specimen together with the imposed loading is appropriately modeled as elastic), failure either occurs during the first cycle or not at all since the system traverses the same states in each cycle. Hence, the description of dissipation is key for modeling fatigue crack growth. The dissipation affecting fatigue crack growth occurs over many scales: fatigue crack growth rates in metals are environmentally sensitive, for example, oxide

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formation on new crack surfaces can affect the course of fatigue crack growth; dissipation in the near-tip dislocation structures that develop under cyclic loading lead to a short crack effect and to a dependence on material properties, for example yield strength, that differs from what classical continuum descriptions of plasticity predict; for larger plastic zone sizes significant dissipation occurs away from the near crack tip vicinity. In general, more than one of these scales plays a significant role during the course of fatigue crack growth so that a multiscale modeling framework is needed for a predictive theory. Such a framework does not exist at present but significant steps are being taken.

The mesoscale, where discrete dislocation effects need to be accounted for, plays a central role in mediating between atomic scale effects and dissipation processes that can be modeled appropriately using conventional continuum descriptions. The organized dislocation structures near a crack tip give rise to much higher stress levels to drive atomic scale processes than are predicted by conventional continuum plasticity, e.g., [12,13]. Computational discrete dislocation modeling of threshold conditions of fatigue crack behavior originated in the studies of [14,15]. Deshpande and co-workers [13,16–18] supplemented that work in a series of fatigue crack growth studies using the framework of [19] for formulating and solving general boundary value problems with discrete dislocation plasticity. The presence of a fatigue threshold and Paris law behavior emerged as a natural outcome of the boundary value problem solution. As the same formulation has been used to also analyze crack growth under monotonic loading conditions, the crack growth behaviors under monotonic and cyclic loading conditions can be compared. Furthermore, this framework permits fatigue crack growth in multi-phase materials to be modeled which is important since in structural metals fatigue cracks can initiate in brittle second phase particles and then propagate into the ductile matrix.

Here, we briefly review some discrete dislocation plasticity predictions for fatigue crack growth. Then, we present some recent steps taken to carry out multiscale analyses of fatigue crack growth, where discrete dislocation plasticity is directly coupled to an atomistic or conventional continuum formulation. Finally, we discuss limitations of the current framework and prospects for future developments.

2. Some discrete dislocation predictions

As noted in [12], dislocations play a dual role in the fracture process under monotonic loading. On the one hand, plastic flow caused by the motion of dislocations delays crack initiation and increases the resistance to crack growth. On the other hand, it is the local stress concentrations associated with discrete dislocations in the vicinity of the crack tip that leads to stress levels of the magnitude of the cohesive strength, causing the crack to propagate. This dual role is key for fatigue in crystalline metals – the dissipation from dislocation motion provides the irreversibility, while the high stresses associated with the dislocation structures that form near the crack tip precipitate crack growth.

Here, we briefly summarize the results from a series of crack growth analyses under cyclic loading conditions using discrete dislocation plasticity [16–18,13,20]. Plastic deformation is described through the motion of large numbers of discrete dislocations, which are treated as singularities in an isotropic elastic solid. Distinct from the treatments by [14,15], in our approach the material model is independent of the presence of a crack. The fracture properties of the material are embedded in a cohesive surface constitutive relation, so that crack initiation and crack growth are stress as well as deformation driven. A key aspect of the formulation is that the plastic stress–strain response and the evolution of the disloca-

tion structure, as well as crack growth are outcomes of the solution of the boundary value problem. Furthermore, the only distinction between an analysis of monotonic crack growth and fatigue crack growth is that in fatigue the remote loading is specified to be an oscillating function of time. In all these studies, a crack is assumed to be present from the beginning; the study of fatigue crack initiation within the same framework has been proposed [21] but the number of cycles that can be computed is limited by the computational resources required.

2.1. Theory

A brief overview of the theoretical framework is presented; background and further descriptions are given in [16–18,13,20] and references cited therein. Initially, the crystal is assumed to be free of mobile dislocations, but to contain a random distribution of dislocation sources and point obstacles. The rules for dislocation nucleation and motion use the Peach–Koehler force as the driving force. The sources mimic Frank-Read sources and generate a dislocation dipole when the magnitude of the Peach–Koehler force exceeds a critical value for a specified period of time. The obstacles, which represent small precipitates or forest dislocations, pin dislocations and release them once the Peach–Koehler force attains a specified obstacle strength. Annihilation of two dislocations with opposite Burgers vector occurs when they approach each other within a critical annihilation distance. Dislocation motion is assumed to occur only by glide with no cross slip. The magnitude of the glide velocity $v^{(k)}$ of dislocation k is taken to be linearly related to the Peach–Koehler force $f^{(k)}$ through the drag relation $f^{(k)} = Bv^{(k)}$. There is no special dislocation nucleation from the crack tip.

In the small-scale yielding studies of [16,17,13], loading is prescribed in terms of displacements corresponding to the isotropic elastic mode I singular field remote from the crack tip; [18,20] analyze a finite-size specimen under remote uniaxial tension. There is a single cohesive surface that lies in front of the initial crack. At each time step, an increment of the remote loading (the mode I stress intensity factor $\dot{K}_1 \Delta t$ for small scale yielding) is prescribed. At the current instant, the stress and strain state of the body is known, and the Peach–Koehler forces on all dislocations can be calculated. On the basis of these forces the dislocation structure is updated, which involves the motion of dislocations, the generation of new dislocations, their mutual annihilation, their pinning at obstacles, and their exit into the open crack. After this, the new stress and strain state can be determined.

The field quantities, i.e. the displacement u_i, the strain ϵ_{ij} and the stress σ_{ij} are determined using the superposition method in [19],

$$u_i = \tilde{u}_i + \hat{u}_i, \quad \epsilon_{ij} = \tilde{\epsilon}_{ij} + \hat{\epsilon}_{ij}, \quad \sigma_{ij} = \tilde{\sigma}_{ij} + \hat{\sigma}_{ij}. \quad (1)$$

The (~) fields are the superposition of the singular fields of the individual dislocations in their current configuration while the (^) fields represent image fields that correct for the actual boundary conditions and include the response of the cohesive surface. The sum of the (~) and the (^) fields in (1) gives the solution that satisfies all boundary conditions. Since the (^) fields are smooth in the region of interest, the boundary value problem for them can be solved using a standard finite element method.

Both reversible and irreversible cohesive traction–displacement relations have been used. As the cohesive surface ahead of the crack separates, the magnitude of the traction increases, reaches a maximum and then approaches zero with increasing separation. In a vacuum, there is no oxidation of the newly formed surface and it is expected that this relation is followed in a reversible manner. When the newly formed surfaces oxidize, the cohesive relation will

not be followed in a reversible manner. The effect of the formation of the oxide layer and the subsequent surface contact during unloading is modeled by specifying unloading from and reloading towards the monotonic cohesive law to occur according to a linear incremental loading/unloading relation.

A reference stress intensity factor K_0 is introduced that provides a convenient normalization for the imposed stress intensity factor. It is defined in terms of the work of separation of the cohesive surface, ϕ_n, by $K_0 = \sqrt{E\phi_n/(1-\nu^2)}$. Crack growth in a linear elastic solid (with Young's modulus E and Poisson ratio ν) with the given cohesive properties takes place at $K_I/K_0 = 1$.

2.2. Predictions of fatigue crack growth in single crystals

In the small-scale yielding calculations of [16,17,13], the applied stress intensity is varied between $K_{\min}$ and $K_{\max}$.

In [16,17] the plane strain calculations are carried out for single crystals with three slip systems oriented at $\pm 60°$ and $0°$ to the initial crack line. Crack growth is restricted to occur along the initial crack line and, hence, crack growth takes place along the $0°$ slip plane. Symmetry about the initial crack line is assumed. The fatigue threshold results obtained in [16], and summarized in Fig. 1, lead to the conclusion that crack growth under cyclic loading occurs if and only if (i) the cyclic amplitude $\Delta K_I := K_{\max} - K_{\min}$ exceeds a critical value ΔK_{th}^*, and (ii) the maximum stress intensity $K_{\max}$ exceeds a critical value $K_{\max}^*$. With a reversible cohesive constitutive relation, which models conditions in a vacuum, this can be rationalized as follows: For sufficiently low $K_{\max}$, no dislocations are generated and the system is elastic. Therefore, for fatigue to occur with a reversible cohesive law, $K_{\max}$ must exceed some minimum $K_{\max}$ denoted by $K_{\max}^*$. For $K_{\max} \gg K_{\max}^*$, interactions within the now dense dislocation structure act to retard dislocation motion. Accordingly, a minimum cyclic stress intensity factor range ΔK_I is needed to induce dislocation motion during unloading and reloading. Thus, in this regime, a critical ΔK_{th}^* is needed. For an irreversible cohesive relation, which models conditions in an oxidizing environment, contact plays an important role [16] but this does not qualitatively change the picture.

Beyond the threshold fatigue crack growth is predicted [17], with a dependence of crack growth rate (da/dN) on cyclic amplitude that is similar to the Paris law behavior seen experimentally, see Fig. 2. The effective stress intensity range ΔK^{eff} responsible for
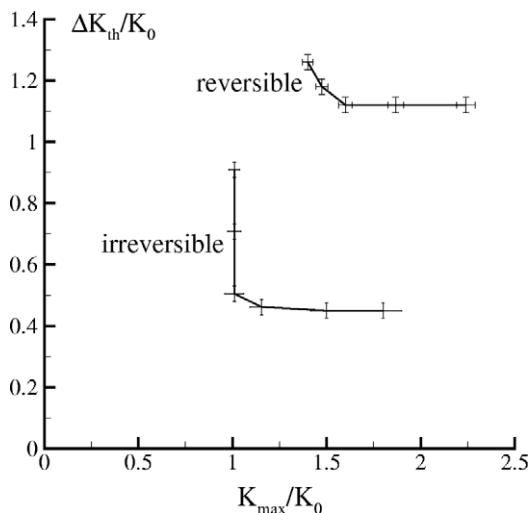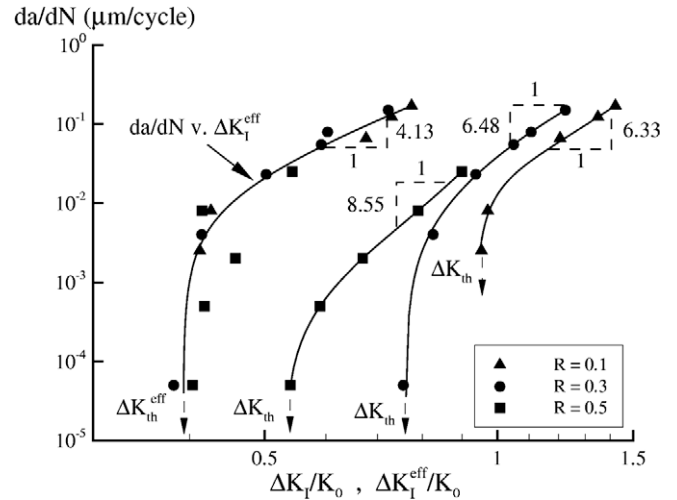

Fig. 2. The cyclic crack growth rate $\log(da/dN)$ versus $\log(\Delta K_I/K_0)$ and $\log(\Delta K_I^{eff}/K_0)$ for an interface crack. From [17].
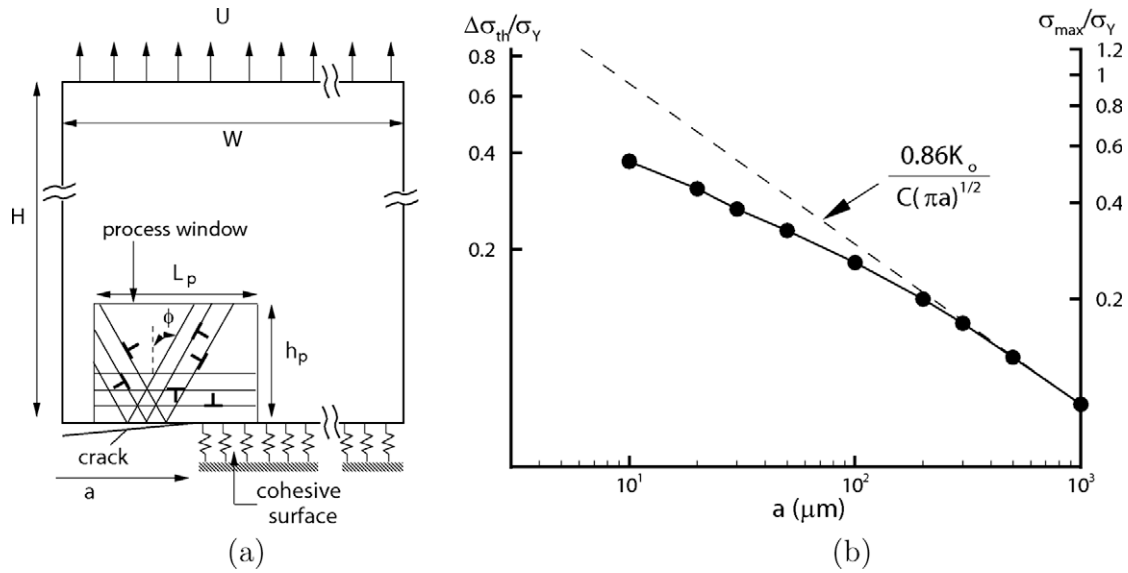
crack growth is defined by $K_{\max} - K_{op}$ where K_{op} is the stress intensity factor at which the crack faces first separate upon reloading. The effect of crack closure is more pronounced at the lower values of ΔK_I so that ΔK_{th}^{eff} is much less than ΔK_{th}.

The fatigue threshold behavior of short cracks has been studied by [18] using geometrically similar edge cracked single crystal specimens (see Fig. 3a) subjected to remote tension fluctuating between $\sigma_{\min}$ and $\sigma_{\max}$. The crystal has three slip systems, $\phi^{(1)} = -35.3° \phi^{(2)} = 35.3°$ and $\phi^{(3)} = 90°$ (see Fig. 3a) so that one slip system is oriented parallel to the initial crack line. As seen in Fig. 3b, for a crack shorter than 300 µm, the deviation from ΔK-governed fatigue increases with decreasing crack size, with the fatigue threshold for smaller cracks tending to be governed by $\Delta\sigma$ rather than by ΔK. A consequence is that short cracks can grow under cyclic loading conditions even when $K_{\max}$ is less than the stress intensity at which the crack would grow in an elastic solid. However, in these cases, values of $K_{\max}/K_0 < 1$ are consistent with $\sigma_{\max} < \sigma_Y$ (the yield strength). In [18] $K_{\max}/K_0$ was written as $K_{\max}/K_0 \approx \sigma_{\max}\sqrt{a/(E\phi_n)}$. For realistic parameter values (e.g. $\phi_n \approx 1\,\mathrm{J/m^2}$ for a wide range of materials), it turns out that $\sqrt{E\phi_n/a} \approx \sigma_Y$ for a 10 micron crack size.

At least in the near-threshold and Paris law regimes, the studies cited here predict that fatigue crack growth rates are relatively independent of the yield strength of the material, but scale with the elastic modulus. This rather surprising observation has been borne out in experimental studies on a variety of metallic alloys. Consistent with experimental data, the discrete dislocation plasticity results in [13] show that $\Delta K_{th}^{eff}/E$ is rather independent of the normalized yield strength σ_Y/E. In contrast, conventional continuum plasticity models predict that fatigue crack growth is sensitive to the value of the yield strength, see e.g. [3,5].

2.3. Fatigue crack growth in multi-phase materials

A wide variety of structural alloys contain brittle particles dispersed in a ductile metallic matrix. While such particles are sometimes added for structural purposes, more often they arise during processing. These particles, or inclusions, are often undesirable byproducts of the material fabrication because fracture can originate by particle cracking followed by propagation into the surrounding ductile matrix. In particular, under cyclic loading conditions, cracks formed during processing or during the initial

Fig. 1. Discrete dislocation predictions for the variation of ΔK_{th} with the applied $K_{\max}$. From [16].

Fig. 3. (a) Edge-cracked specimen used to study short-crack behavior. The calculations are carried out for fixed ratios $H/W = 12.5$ and $a/W = 0.1$ for various crack lengths a. (b) Predicted fatigue threshold, $\Delta\sigma_{th}/\sigma_Y$, versus crack length a (corresponding values of σ_{max}/σ_Y are shown on the right axis). From [18].
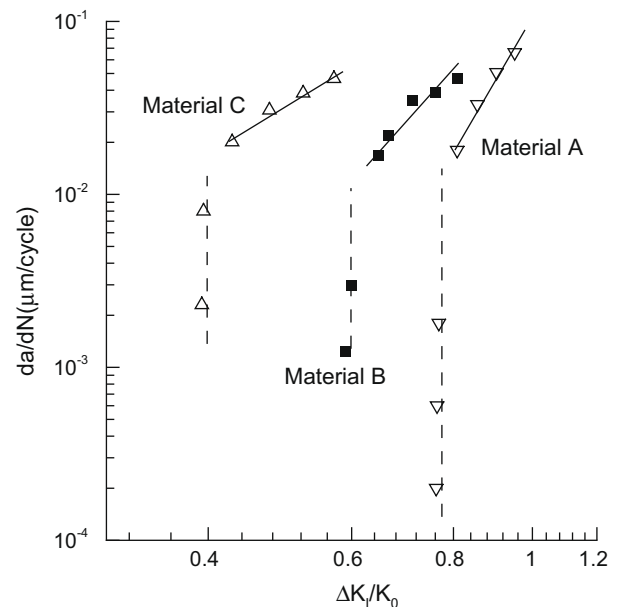
stages of loading will grow and ultimately lead to failure of the structure or component.

A planar single crystal (elastically isotropic with a Young's modulus E_m) reinforced by a 10 μm isotropic elastic particle (Young's modulus E_p) containing an initial crack was considered in [20]. The particle was taken to be completely cracked so that the initial crack length is equal to the particle size. Crack growth into the surrounding crystal was modeled via a cohesive framework. The presence of the elastic particle influences crack growth due to the effects of: (i) the modulus mismatch on the crack tip stress intensity; (ii) this stress intensity on the evolution of plasticity; and (iii) the blocking of slip at the particle-matrix interface. These effects were investigated separately and sequentially by considering the three cases summarized in Table 1: (i) material A, an initially-cracked single crystal, which should thus show only small crack effects; (ii) material B, a particle with the same elastic properties as the matrix, $E_p = E_m$ but no dislocation activity inside the particle, which should show the effects of slip blocking only; and (iii) material C, a particle that is elastically stiffer than the matrix, $E_p = 5E_m$, which should show the joint effects of modulus mismatch and slip blocking.

Fatigue crack growth calculations for the three materials are shown in Fig. 4. The calculations reveal a threshold for fatigue crack growth and a transition to a Paris law behavior, both depending on the existence of the elastic particle and the modulus mismatch. For a matched-modulus particle (Material B), the threshold is reduced by 25% relative to the single crystal (Material A) and this is attributed to slip blockage by the particle. For the high-modulus particle (Material C), the threshold is reduced by 50% relative to Material A and this is due to both slip blockage and the enhanced stress intensity factor due to the elastic mismatch. These results show that fatigue crack growth from mi-

Fig. 4. Discrete dislocation predictions of fatigue crack growth in a single crystal initiated from a 10 μm elastic, cracked particle. From [20].

cron-scale particles is strongly influenced by plasticity size effects, elastic mismatch, and particle constraints on plastic flow.

2.4. Current limitations of the discrete dislocation approach

There are a variety of idealizations in the discrete dislocation calculations of fatigue crack growth reported to-date that need to be relaxed to obtain quantitatively useful predictions. For example, for numerical reasons, the K_0 that is used is about a factor of two smaller than representative of metals like aluminum, a high loading rate is used to reduce the computing time; the analyses are carried out for pure mode I loading with symmetry assumed about the crack plane, while in single crystals mixed mode loading conditions generally prevail at the crack tip; the analyses have been two-dimensional, with both three-dimensional dislocation effects

Table 1
The three material systems analyzed by [20] for a cracked elastic particle (p) in a plastically deforming matrix (m).

Material	E_p/E_m	Particle
A	1	No
B	1	Yes
C	5	Yes

and three-dimensional crack growth effects neglected; and the effects of crack tip blunting are not taken into account in the small strain analyses. Also, the calculations have been carried out for small amounts of straight ahead crack growth in a single crystal, whereas experimental data typically are for larger amounts of crack growth in polycrystalline materials. These are not restrictions in principle; both the discrete dislocation framework and the cohesive surface framework are extensible.

Fatigue crack growth rates are sensitive to the environment and accounting for environmental effects means accounting for chemistry in the crack tip region. This in turn requires an atomistic rather than a phenomenological cohesive model of the creation of new free surface. Also, most of the limitations mentioned in the previous paragraph have the effect of giving rise to values of ΔK_{th} that are relatively low and the Paris law exponents values rather high. For increased values of crack growth resistance the region over which significant plastic dissipation occurs increases. Even in a two-dimensional context, discrete dislocation plasticity calculations of fatigue crack growth require large amounts of computer time. Limiting the size of the region that needs to be analyzed with discrete dislocation plasticity has the potential to significantly reduce the required computer time and enable calculations of larger amounts of crack growth. In the next Section we discuss some initial steps taken to carry out multiscale analyses of fatigue crack growth.

3. Hybrid fatigue modeling

Modeling of fatigue via discrete dislocation plasticity captures a range of physically important fatigue phenomena, as shown above, but this comes at a high computational cost and a limited range of plasticity. Multiscale modeling by coupling of a discrete dislocation region to a continuum plasticity region is thus one direction for extending discrete dislocation plasticity approaches by permitting much larger plastic zone sizes at greatly reduced computational cost. To date, discrete dislocation analyses of fatigue crack growth have used a cohesive zone model to handle material separation at the smallest scales, which is an approximation that condenses atomic scale deformation, dissipation, and irreversible phenomena into a simple description. Multiscale modeling by coupling of a discrete dislocation region to a smaller atomistic region around the crack tip is thus a direction for enhancing the fidelity of the small-scale material description. In principle, all three scales (atomistic, discrete dislocation, and continuum plasticity) can operate simultaneously within a single computational framework, with the method/refinement used at each material point selected by consideration of the key operative mechanisms that must be captured at various distances from the crack tip.

An illustration of the scales involved in the problem is given in Fig. 5. At present, a full integration of methods has not been achieved but both the atomistic-discrete-dislocation and discrete-dislocation-continuum-plasticity multiscale methods have each been developed. Here we thus discuss some recent progress in multiscale modeling at both large and small scales with an emphasis on modeling of fatigue crack growth and related irreversible processes.

3.1. Discrete dislocation plasticity coupled to continuum slip crystal plasticity

Any effort to directly couple discrete dislocation plasticity and a continuum plasticity description needs to address a variety of issues and here we discuss the approach to tackle these issues taken in [22]. The formulation is restricted to small deformations and the material in a region near the crack tip is described by discrete dis-
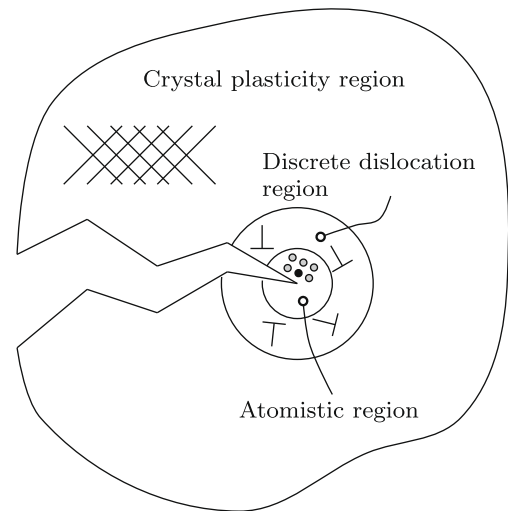

Fig. 5. Illustration of the hybrid multiscale approach. The crack tip region at the nanometer scale is modeled using atomistic mechanics, gradient plasticity effects are captured using a discrete dislocation domain at the micron scale, and the large scale dissipative plasticity is modeled using crystal plasticity at larger scales.

location plasticity while outside this region the material is described by conventional (size-independent) continuum slip crystal plasticity.

The material response in the two regions needs to be calibrated so that there is a consistent representation of material response at the interface between them. Obviously such a calibration is not unique. In [22] plane strain tension calculations were carried out for specimens large enough so that the dependence on specimen size was weak and the crystal plasticity constitutive parameters were chosen to match the rate-dependent discrete dislocation plasticity response.

Matching of displacements at the interface can also only be approximate because the discrete dislocation plasticity displacement field has jumps due to slip whereas the continuum plasticity displacement field is smooth. In [22] the discrete dislocation displacement field at the interface was numerically smoothed using

$$u_i = \hat{u}_i + \frac{1}{S_r}\int_S w\tilde{u}_i ds, \quad S_r = \int_S wds, \tag{2}$$

where $\hat{u}_i$ and $\tilde{u}_i$ are defined in Eq. (1), where w is a weight function and S_r is a representative surface element of the interface S.

Due to the singular nature of the $\tilde{u}_i$ field, dislocations are not allowed to reach the interface since this would give rise to a stress concentration at the interface that would drive unphysical plastic flow in the continuum plasticity region. The weight function w and the offset of dislocations from the interface implicitly introduce numerical length scales which need to be chosen in a way that minimizes their effect on the predicted results. In [22] these length scales were arrived at by numerical experimentation.

The presumption of the formulation in [22] is that all effects of net Burgers vector (geometrically necessary dislocations) are accounted for in the discrete dislocation plasticity region.

In [22] it was found that the discrete dislocation region could be reduced from a size of 30×30 μm to 10×5 μm with nearly no loss in accuracy of the crack growth versus applied load relation but with a reduction of a factor of 14 in the computer time required.

Fig. 6 shows some preliminary results using this approach to analyze fatigue crack growth under mode I small-scale yielding conditions. The crack is subjected to cyclic loading for various values of $R = K_{min}/K_{max}$ and $\Delta K/K_0 = (K_{max} - K_{min})/K_0$ where K_0 is the
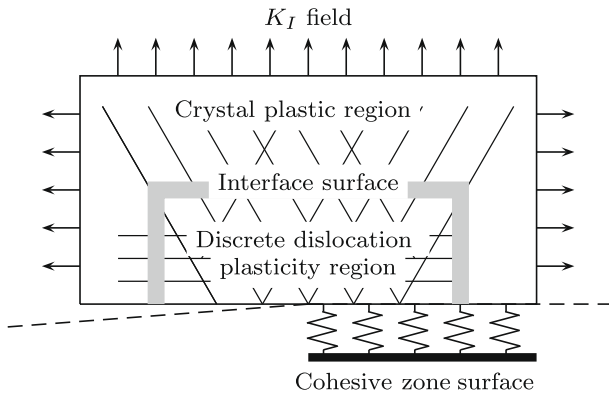
Fig. 6. Schematic of the boundary value problem for mode I crack growth under small-scale yielding conditions.

stress intensity factor at which a mode I crack starts to propagate in a linear isotropic elastic solid.

The material parameters used in these simulations are those used in [22] except that here the cohesive zone is taken to be irreversible, as in previous discrete dislocation plasticity fatigue calculations, e.g. [16,17]. The crack growth for cyclic loading is shown in Fig. 7 and it clearly illustrates the near threshold properties of the mode I crack for a range of different load levels. The highest load level in Fig. 7 corresponds to a maximum stress intensity factor of $K_{\max}/K_0 = \Delta K/(1 - R)K_0 = 2.1$ whereas the lowest load level corresponds to $K_{\max}/K_0 = 1.19$. As expected the amount of crack growth increases with increasing R and $\Delta K/K_0$. Fatigue crack growth analyses for high R-values are especially computationally intensive because of the relatively large plastic zone size.

Although aspects of the formulation in [22] (e.g. the interface continuity conditions) are applicable in three dimensions, there are inherently three-dimensional issues that must be addressed to develop a fully three-dimensional formulation. For example, in three dimensions part of a dislocation loop can cross the interface between the discrete dislocation plasticity and continuum plasticity regions.

3.2. Coupled atomistic-discrete-dislocation model (CADD)

The use of a cohesive zone for handling material separation in discrete dislocation modeling of fracture and fatigue permits capturing of the fundamental material strength and fracture energy.
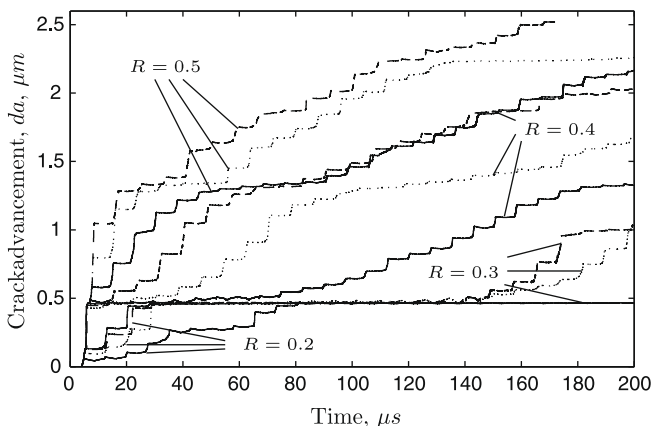

Fig. 7. Crack propagation versus time for a mode I crack. The crack is subjected to cyclic loading and loaded for different R-values in the range from 0.2 to 0.5. Solid lines correspond to $\Delta K/K_0 = 0.95$, dotted lines corresponds to $\Delta K/K_0 = 1.0$ and dashed lines corresponds to $\Delta K/K_0 = 1.05$. From [23].

In addition, with the introduction of irreversibility, the cohesive zone can capture features associated with contact and surface oxidation. The cohesive zone also absorbs dislocations. However, the cohesive zone representation does not nominally include other atomistic scale phenomena that occur and modify the nanoscale deformation. Such phenomena include crack tip dislocation emission, dislocation emission from grain boundaries or interfaces along which the crack might be growing, detailed interaction of dislocations with the highly deformed material around the crack tip, the interaction of chemical embrittlement with the local crack tip field, and non-crystalline deformation mechanisms and diffusion. One strategy for handling such phenomena is to perform separate atomistic studies and extract effective cohesive zone models that capture the energy, strength, and dissipation of these phenomena, see e.g. [24]. This approach will generally neglect, however, the interactions of the dislocations generated in the bulk of the material with the crack region. An alternative approach is to develop a multiscale model in which the atomistic and discrete dislocation regions are intimately connected, which has been accomplished in a method termed the coupled atomistic-discrete-dislocation (CADD) model [25,26].

As with the coupling of discrete dislocations and crystal plasticity, several hurdles must be overcome in coupling a fully atomistic description of deformation to one that handles only the dislocation defects residing in an underlying continuum elastic medium.

First, the material response in the two domains must be calibrated, with the atomistic model being the reference material. The continuum elastic constants, the possible dislocation Burgers vectors and slip planes, Peierls stresses, dislocation mobility versus Peach–Koehler force, and the stacking fault energies for partial dislocations, if present, are all obtained from separate atomistic models using the same atomistic interatomic potentials. The description of the discrete dislocations is thus identical aside from the absence of an atomistic core, which need not be resolved atomistically. Phenomena that are related to the atomic cores, such as dislocation junction and dislocation annihilation must be studied atomistically and introduced as constitutive rules into the discrete dislocation model.

Second, the matching conditions for displacements and tractions at the atomistic-continuum interface must be developed. There are a number of methods for handling this aspect of coupling, with a recent review evaluating many of them on an equal footing [30]. Because the atomistic material is non-local, i.e. the interatomic potentials generally extend beyond near-neighbor interactions, the concept of continuum tractions is not strictly valid. Thus, the most accurate methods use displacements of so-called pad atoms residing in the continuum domain and having displacements computed by a continuum finite element formulation to interact through the interatomic potentials with the true atoms in the atomistic region. This approach ensures continuity of displacements at the interface and preserves the correct forces on atoms near the interface.

Third, the transfer of atomistic dislocations into the continuum regime and vice-versa must be handled. Atomistic dislocations, with a highly non-linear core region, cannot approach too close to the interface with the linear-elastic continuum lest large spurious forces be generated. While these interactions can be reduced they cannot be eliminated, [27]. Thus, dislocations in the atomistic regime are detected prior to reaching the interface at a distance where spurious forces are negligible (typically 5–20 Å). Upon detection, a dislocation is transferred to the continuum by the introduction of a dislocation dipole with the negative dislocation introduced atomistically at the site of the detected dislocation and the positive dislocation introduced as a discrete dislocation in the continuum domain. The negative atomistic dislocation annihilates the original dislocation, leaving only the positive disloca-

tion in the continuum. Transfer of dislocations from the discrete regime into the atomistic regime is accomplished by the reverse process.

The CADD method has been applied to a number of problems in deformation and fracture, but no explicit fatigue crack growth problems have been investigated. To demonstrate the potential utility of the method for fatigue, we discuss two examples demonstrating irreversible deformation behavior caused by atomistic-scale phenomena that could contribute to fatigue crack nucleation and/or propagation.

As a first example, we examine dislocation nucleation at a crack tip. This phenomenon is well-studied at the atomistic scale, but the behavior of the emitted dislocations upon unloading has not been widely analyzed. Irreversible behavior can arise generally because the nucleation process is not an equilibrium one. In fcc metals, emission of the first partial dislocation is controlled by the unstable stacking fault energy γ_{us}, with the required stress intensity scaling as $K_{Ie} \approx \sqrt{\mu \gamma_{us}}$ where μ is the shear modulus. Once emitted, the equilibrium position of the partial dislocation is governed by a balance between the applied force, the image force, and the stacking fault force caused by the stacking fault energy γ_s. Within elasticity theory, the equilibrium dislocation position distance d satisfies

$$d = \frac{K_{eff}^2 b^2}{8\pi\gamma_s^2}\left(1 + \sqrt{1 - \frac{2\mu\gamma_s}{(1-v)K_{eff}^2}}\right)^2 \qquad (3)$$

where $K_{eff} = K_I \cos^2(\theta/2)\sin(\theta/2)$, b is the Burgers vector and θ is the angle between the crack plane and the slip plane. When γ_{us} is much higher than γ_s, the dislocation will emit at a high value of K_I, and move far from the crack tip. On unloading, the dislocation moves back toward the crack tip but is not absorbed at the crack tip until K_I is well below K_{Ie}. This irreversible behavior is shown explicitly in Fig. 8 for a dislocation emitted from a crack tip in nickel, for the geometry shown in Fig. 9. The first partial is nucleated at $K_{Ie} = 0.38$ eV/Å$^{5/2} = 0.61$ MPa$\sqrt{m}$ and quickly moves to a distance $d = 180$Å that is well outside the atomistic domain. With increased applied load, the dislocation moves further from the crack tip. Upon reduction of the applied K_I, the dislocation then moves back toward the crack tip, passes back into the atomistic region, and is eventually re-absorbed at $K_I \approx 0.24$ eV/Å$^{5/2} = 0.38$ MPa$\sqrt{m}$. The position
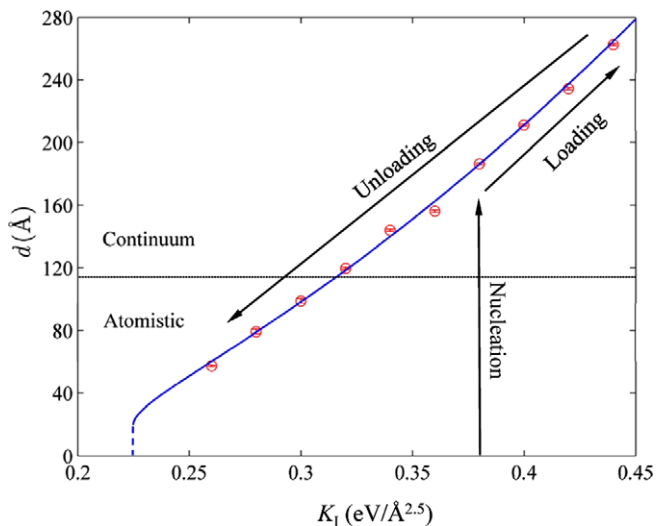
versus K_I as computed by CADD and as predicted theoretically are in good agreement. During unloading under cyclic conditions, the emitted dislocation remains in the material and influence other dislocations in the system at applied loads where it did not previously exist. After the first cycle, the dislocation motion is reversible if it is not re-absorbed into the crack tip. If it is re-absorbed, then there is a load-unload hysteresis cycle.

As a second example, we consider dislocation interactions at a grain boundary and the associated irreversible deformation. This example is not directly related to crack tip fatigue, but demonstrates behavior that should be introduced into fatigue simulations of polycrystals at the discrete dislocation level. We select one illustrative case: edge dislocations impinging on a symmetric $\Sigma - 11(113)$ boundary in aluminum. In this study [29], a discrete dislocation source is placed in the continuum domain several microns from the grain boundary and emits discrete dislocations under the action of a simple shear stress; a schematic of the geometry is shown in Fig. 10. The applied load drives dislocations toward and into the grain boundary, a small section of which is modeled atomistically. In the simulation, dislocations simultaneously exist in the discrete dislocation domain, in the atomistic domain but some nanometers away from the grain boundary, at the grain boundary, and along the grain boundary, in both atomistic and continuum regions due to the formation and motion of grain boundary dislocations. In this particular case, when dislocations impinge on the grain boundary, the dislocation/grain-boundary interaction leads to the formation of a grain-boundary–dislocation source that emits dipole pairs of grain boundary dislocations. If only one lattice dislocation has absorbed into the grain boundary, the process can be fully reversible under reverse loading as seen in Fig. 10a where the grain boundary dislocations have recombined and the absorbed lattice dislocation is reappears in the bulk crystalline grain. However, if five lattice dislocations have been emitted from the grain source, and two pairs of grain boundary dislocations have been emitted, the emission generates a complex deformation at the grain-boundary/lattice-dislocation interaction region that is not fully reversible. Upon reducing the applied shear to zero, the grain boundary dislocation return to the region of their origin but do not fully annihilate, but rather drive the beginning of transmission of a dislocation into the neighboring grain and generate nanoscale damage at the grain boundary. In general, under all but the simplest conditions, irreversible phenomena occur that will also influence bulk lattice dislocations in the discrete regime. The defects formed by the dislocation/grain-boundary interaction may also serve as the nuclei for fatigue crack nucleation. These phenomena are difficult to capture with standard cohesive zone models at larger scales, and we expect that, at a minimum, the properties of the cohesive zone would need to evolve with deformation to capture the true atomistic phenomena observed in these calculations.

4. Modeling needs and prospects

The discrete dislocation framework discussed above has proven capable of modeling aspects of fatigue crack growth in ductile crystalline materials – such as the lack of dependence of the fatigue crack growth rate on the flow strength – that are difficult, if not impossible, to model using any other currently available framework. However, much remains to be done before truly predictive fatigue crack growth predictions can be obtained. The physical description needs to be extended in several directions and advances in computational methodology are needed to permit representative loading conditions to be simulated.

The most obvious idealization adopted to-date in all the fatigue crack growth calculations carried out using discrete dislocation plasticity, including all the hybrid calculations, is that the calcula-

Fig. 8. Dislocation distance from the crack tip along a slip plane, as predicted by a continuum model and as simulated using CADD during a single load-unload cycle. Note the hysteresis due to the initial nucleation of the dislocation (1 eV/Å$^{5/2}$ = 1.6 MPa$\sqrt{m}$).

tions have been carried out within a two-dimensional plane strain context. The two-dimensional context precludes, for example, consideration of variations along the crack front and, perhaps more importantly, precludes consideration of three-dimensional dislocation mechanisms. On the other hand, much progress was made in the development of fracture mechanics for monotonic loading
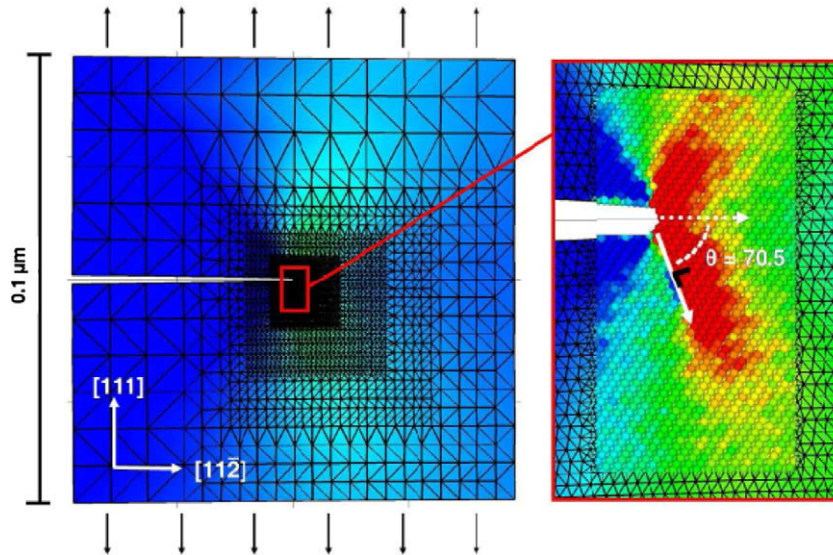
Fig. 9. CADD simulation cell for crack-tip partial dislocation emission in fcc metals, showing large scale continuum region and atomistic-scale crack tip region. Contours show vertical strain under an applied stress intensity. From [28].
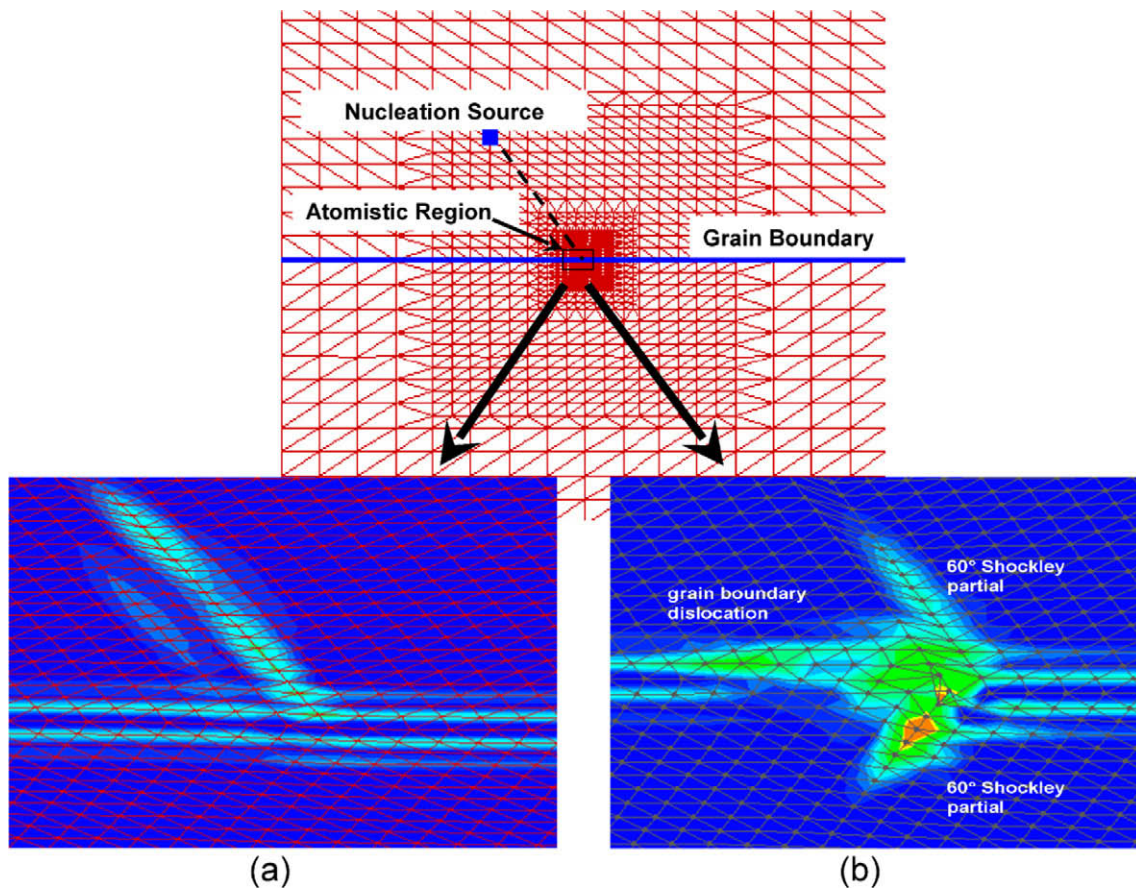
Fig. 10. Schematic of CADD model for study of dislocation/grain-boundary interactions, where a small region of 2000 atoms at the intersection of the dislocation source slip plane and the grain boundary is modeled atomistically while the remainder of the model (which would contain 200,000,000 atoms if done with full atomistic resolution) is modeled using the discrete dislocation method. (a) re-emission of a single edge dislocation into the bulk grain during unloading after absorption and (b) equilibrium structure after unloading for a 5-dislocation pile-up impinging on the grain boundary, showing grain boundary dislocations are unable to completely recombine and instead generate new partial dislocations the boundary and damage within the boundary. Colors denote atomistic potential energy, with blue lowest, and thus help visualize the deformation. From [29].

based on two-dimensional analyses and methods have been developed for including at least some three-dimensional physics in two-dimensional discrete dislocation calculations [31]. Also, some steps have been taken to develop a fully three-dimensional capability for solving general discrete dislocation plasticity boundary value problems, e.g. [32,33], but what can be computed currently is still rather limited. For a multiscale analysis, there are additional modeling challenges; for example, the passing of a dislocation loop between modeling frameworks. In addition to the modeling challenges for developing a three-dimensional multiscale framework, major advances in computers and computational methods will be needed since even two-dimensional discrete dislocation plasticity analyses of fatigue crack growth require substantial computing resources.

Another modeling limitation is that the analyses to-date have been restricted to single crystals. More typically, fatigue crack growth in a polycrystalline material is of interest in applications. However, it is often the case that during much of the fatigue life the crack and the plastic zone are confined to a single grain. On the other hand, during the early stages of fatigue crack growth, the crack is growing in mode II (shear) rather than in mode I (tension) as modeled in the analyses discussed here. Additionally, after some crack growth, the plastic zone impinges on or crosses grain boundaries so that the single crystal idealization is no longer appropriate. The characterization of grain boundary-dislocation interactions is an open issue for a variety of mesoscale analyses as well as for fatigue crack growth but progress is being made, e.g. [27,34].

The analyses discussed here have presumed that the dislocations nucleate from sources inside the material and have been carried out assuming a cleavage mode of fatigue crack growth. Dislocations can also nucleate from the crack tip and, at least in some circumstances, the crack tip is the main source of dislocations, see e.g. the discussion in [15]. Including a physically based model of this type of nucleation in full boundary value problem discrete dislocation plasticity analyses, which would allow consideration of a more deformation driven mode of crack growth, would be an important step.

Fatigue crack growth is strongly affected by the environment, for example a surface oxidation layer can have a strong effect, so that the direct coupling to an atomistic description of the crack tip region as in the CADD framework is very important. The CADD framework is capable of incorporating a quantum mechanical description of the near tip region, which is key for the accurate representation of chemistry, but at a significantly increased computational cost. Thus, increased computational efficiency is needed to permit accurate modeling of environmental effects on fatigue. Another, computationally less demanding route, is to use quantum mechanical calculations to develop phenomenological cohesive relations that model the effects of chemistry. It remains to be seen whether or not a phenomenological relation can accurately represent chemical–mechanical interactions in the vicinity of a crack tip under cyclic loading.

Discrete dislocation plasticity is inherently statistical for two reasons. First, the crack growth response varies with the specific location of dislocation sources and obstacles for distributions having the same density. Secondly, numerical solutions of the dynamics of discrete dislocations can exhibit chaotic behavior [35], so that extremely small differences in initial conditions can give rise to different locations of dislocations in the crack tip region, which in turn can affect crack growth. The implication of these for the statistics of fatigue crack growth remains to be elucidated.

Even in the two-dimensional plane strain context substantial computational challenges remain. In a wide variety of cases of interest, cohesive strengths can approach theoretical strengths. A consequence of this is that cohesive lengths become very small

so that extremely fine finite element meshes, grid sizes of the order of a few nanometers, are required. Furthermore, in order to calculate micrometers of crack growth many loading cycles are needed. Numerical techniques to limit the high resolution discretization to the near crack tip region, such as moving mesh methods and special higher order crack tip elements, are being explored to limit the computing time.

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