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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.

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 dislocation 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 $\dot{K}_I \Delta t$ 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],

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

The ($\tilde{}$) fields are the superposition of the singular fields of the individual dislocations in their current configuration while the ($\hat{}$) fields represent image fields that correct for the actual boundary conditions and include the response of the cohesive surface. The sum of the ($\tilde{}$) and the ($\hat{}$) fields in (1) gives the solution that satisfies all boundary conditions. Since the ($\hat{}$) 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