

MATERIAL DISSOLUTION AT THE CRACK TIP

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Abstract

Despite a long-documented history of environmental effects, an understanding of the controlling mechanisms remains clouded. At fault are several challenges. First, multiple mechanisms can act simultaneously, e.g., dissolution, oxide fracture, oxide formation, material redeposition, and hydrogen embrittlement. Second, the scale of the material separation process on which the environment acts is atomistic, inhibiting direct observation. Considering these challenges, atomistic modeling can serve as a powerful probe to illuminate the mechanisms governing environmental effects and providing a means to study the material separation processes under the action of isolated mechanisms. Here, we report on the results of atomistic simulations specifically constructed to illuminate the role of material dissolution at the tip of a long crack. In cases of both brittle and ductile materials, we find that material dissolution can free arrested cracks. Beyond this, we find material dissolution to play a dole role, accelerating crack growth in the cases of brittle materials under sub-critical loading and accelerating crack tip blunting in the case of ductile materials. We find the result to be largely independent of loading magnitude and type, i.e. static vs fatigue. In total these results provide guidance for the development of continuum scale crack growth rules.

1. Introduction

The identification of the mechanisms that control environmentally assisted fatigue crack growth has been a long standing challenge. Without knowledge of the mechanisms, there is limited basis for materials design. Given the scale that the mechanisms opporate, direct observation via microscopy is limited. Given the multitude of mechanisms that might opporate, inference from higher scale laboratory measurements is frustrated. It is from this context that we have employed atomistic-based simulations to isolate and study the action of one potential mechanism for environmental crack growth, examing at the scale which controls the technological relevant case of near threshold crack growth.

The results are obtained via a recent implementation of the concurrent, multi-scale coupled atomistic-discrete dislocation (CADD) model that incorporates a small, high resolution atomistic domain embedded inside a larger continuum domain governed by a self-consistent boundary condition. Mechanical equilibrium is obtained using LAMMPS for the atomistic region and FEniCS for the continuum region. This computational model is referred to as LF-CADD and it enables the simulation of substationally greater deformation histories and spatial domain sizes than would be possible with atomistic simulation alone.

2. Results

Our results indicate that the effect of dissolution can be dual natured depending on the material. For a ductile material (one that nucleates dislocations from crack tips under increasing load), dissolution acts to blunt the crack, increasing crack opening. This occurs by the formation of surface steps whose propagation acts to open the crack for cases of both static and cyclic loading. The rate of crack opening is greater than the rate of crack growth, which suggests a blunting effect in a ductile material.

Alternatively, for a more brittle material (where crack tips can nucleate dislocations and/or cleave depending upon their geometry), dissolution enhances crack growth. Its action was found to occur via two distinct mechanisms. At low static loadings and loading amplitudes, cracks propagate slowly and continuously while maintaining a small crack opening. Similar to the ductile material, this occurs by the formation and propagation of surface steps. However, in contrast to the ductile material, the surface steps are of opposite character. At larger static loading and loading amplitudes, crack growth under the action of

dissolution can occur by sudden burst events associated with effect of dissolution on atomic scale crack tip geometry.

The below figure shows atomistic details of crack surface steps formed in ductile and semi-brittle materials subjected to dissolution and cyclic loading. Red hollow circles correspond to the site of surface step formation, with red arrows pointing in the direction of step propagation. For discussion it is useful to characterize the crack geometry into three parts: (A) top surface, (B) bottom surface, and (C) crack front. For the case of dissolution in a ductile material (a), a surface step is formed on the bottom crack face, which acts to open the crack and leads to crack blunting. For the case of dissolution in a semi-brittle material at low loads (b), a surface step is formed on the crack front face, leading to continuous and slow growth while maintaining a narrow crack. For the case of dissolution in a semi-brittle material at higher loads (c), cleavage (bursting) happens when the dissolution produces atomically sharp features at the crack tip. In the below figure grey atoms are free (bulk) atoms in the atomistic window. Red atoms are pad atoms and remain fixed during each iteration of the mechanical relaxation. Stress intensity factors are normalized by the critical stress intensity factor for the nucleation of the first dislocation upon loading crack in a pristine crystal. In all cases shown, the loading ratio is 0.25.

