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An atomistic investigation into the nature of near threshold fatigue crack growth in aluminum alloys

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ABSTRACT

Despite decades of study, the atomic-scale mechanisms of fatigue crack growth remain elusive. Here we use the coupled atomistic–discrete dislocation method, a multiscale simulation method, to examine the influence of dislocation glide resistance on near-threshold fatigue crack growth in an aluminum alloy. The simulations indicate that the threshold increases with an increase in dislocation glide resistance, and that a transition in the crack growth direction can occur when dislocation nucleation is inhibited by other nucleated dislocations. Three main mechanisms of fatigue crack propagation are observed: cleavage along the primary slip plane, crack extension by dislocation emission, and crack extension by opening along lattice defects.

1. Introduction

Aluminum alloys continue to serve as the primary material system for many critical components in aircraft structures. Accordingly, a key aspect of aircraft safety involves the prediction of fatigue crack growth in these materials. This technological motivation has spurred the growth of a vast library of experimental and theoretical studies on fatigue crack growth over the past decades. Nonetheless, one critical aspect of the phenomenon has remained particularly unclear, i.e. the atomistic mechanism by which the crack tip propagates forward under cyclic subcritical loadings.

Considering the atomic nature of crack tip processes, modeling must be atomistic in nature. However, interpreting atomistic modeling results relative to fatigue crack growth in real alloys involves many significant challenges. One of the largest challenges is the limited spatial domain that is typical of atomistic models. Simulations having a small spatial domain can artificially influence the movement of dislocations away from the crack tip and ultimately bias crack tip behavior [1–8]. Discrete dislocation (DD) dynamics simulations are not generally plagued by this problem as they can accommodate a much larger spatial domain, while still explicitly modeling every dislocation. However, DD models do not explicitly represent the atomic scale complexities that occur at a crack tip [9–13], and thus cannot illuminate the atomic mechanisms by which a crack tip propagates.

In this work, a concurrently coupled atomistic–discrete dislocation multiscale method (CADD) is used to resolve the shortcomings of tradition atomistic and DD simulations with the specific goal of illuminating the atomic scale mechanisms that occur at a crack tip during fatigue crack growth. The model consists of an aluminum crystal with a crack, loaded in mode I. Upon loading, dislocations nucleate at the crack tip in the atomistic region of the model. In most cases, the dislocations then glide into the nearby DD region, where their motion is inhibited by an imposed glide resistance (friction force). The imposed glide resistance is the primary variable studied in this work, and is the sole feature of the model that connects it

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Nomenclature

$\mathbf{F}$	atomic force vector
x, y, z	coordinate axes
γ_0	maximum damping coefficient
$d(x, y)$	distance between an atom and an interface
x_{min}	minimum x value in atomistic region
x_{max}	maximum x value in atomistic region
y_{min}	minimum y value in atomistic region
y_{max}	maximum y value in atomistic region
E^c	total energy of continuum region
$\hat{\boldsymbol{\sigma}}$	stress solution from finite element analysis
$\hat{\boldsymbol{\epsilon}}$	strain solution from finite element analysis
$\hat{\mathbf{u}}$	displacement solution from finite element analysis
$\tilde{\boldsymbol{\sigma}}$	stress from infinite medium dislocation fields
$\tilde{\boldsymbol{\epsilon}}$	strain from infinite medium dislocation fields
$\tilde{\mathbf{u}}$	displacement from infinite medium dislocation fields
Ω_c	continuum domain
$\partial\Omega_T$	boundary to continuum domain
$\mathbf{T_0}$	traction boundary condition applied to continuum domain
$\mathbf{r}$	position vector of dislocation
B	mobility factor
f	Peach Koehler force
$\mathbf{b}$	Burgers vector
$\mathbf{n}$	vector normal to dislocation glide plane
C_{11}, C_{12}, C_{44}	elastic constants of model aluminum
R	load ratio, minimum load divided by the maximum load
da/dN	Change in crack length per loading cycle
ΔK_I	Mode I stress intensity range, maximum Mode I stress intensity minus the minimum Mode I stress intensity
ΔK_I^{th}	threshold Mode I stress intensity, below this value no crack growth is observed

to aluminum alloy response, i.e. no alloying elements are included in the atomistic region and thus direct interactions between the crack tip and alloying elements and precipitates are not considered. By studying the relationship between dislocation glide resistance and crack tip response under cyclic loading, this work aims to illuminate the effect of aging on fatigue crack growth, something for which experimental results exist.

The manuscript focuses on two key components of the results emerging from our models. The first is the identification of the atomistic mechanisms by which a crack tip propagates forward in a ductile metal subjected to cyclic loading. The second is the dependence of the crack tip mechanisms on dislocation glide resistance, which gives insight into the mechanism by which experimentally observed near threshold fatigue crack growth rates are influenced by the aging of alloys.

2. Methods

A concurrent multiscale simulation approach is used to connect an atomistic region encompassing an aluminum crack tip with a discrete dislocation region capable of capturing dislocation pileups microns in length. In this way, the detailed atomistic processes occurring at the crack tip can be simulated under the presence of a realistic stress filed created by a distribution of dislocations. Dislocations on the primary slip plane are restricted from gliding freely away from the crack tip by a friction force applied homogeneously throughout the discrete dislocation portion of the simulation.

2.1. CADD concurrent multiscale method

The underlying theory of the multiscale method is built upon the coupled atomistic-discrete dislocation (CADD) framework of Shilkrot et al. [14,15]. The CADD coupling methodology consists of solving two distinct problems, involving an atomistic and continuum region that are coupled by self-consistent displacement boundary conditions. The atomistic region is composed of a set of atoms bounded by a set of interface atoms/nodes as seen in Fig. 1. The DD continuum region is approximated by finite elements and thus the fields associated with it are a function of the corresponding nodes. The interatomic force, **F**, experienced by each atom within the atomistic region and at the interface results from interactions not only within the atomistic region and its bounding interface, but also interactions with pad atoms that extend into the continuum. The forces are then used to dynamically relax the atomic positions. Unlike the atoms in the atomistic and interface regions,