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Investigation of crack tip dislocation emission in aluminum using multiscale molecular dynamics simulation and continuum modeling

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ABSTRACT

This work investigates the dislocation nucleation processes that occur at the tip of a crack in aluminum under a broad range of crystallographic orientations and temperatures. A concurrent multiscale molecular dynamics – continuum simulation framework is employed. The results are then interpreted using a Peierls continuum model that uses finite temperature material properties derived from molecular dynamics simulation. Under ramped loading, partial dislocation nucleation at the crack tip is found to lead to both full dislocation emission and twinning, depending upon the orientation, temperature, and magnitude of the applied load in the simulation. The origins of the dependencies are made apparent by the Peierls continuum model. The continuum model suggests that in many instances dislocation nucleation from the crack tip can be considered to be a strain rate independent process, yet still temperature dependent through the temperature dependence of the stacking fault energies and elastic constants.

1. Introduction

The ability to accurately model material failure is a key parameter to the analysis and design of advanced engineered systems. In practice, failure models are typically phenomenological in character, based on experimentally measured macroscopic quantities, such as ultimate strength, limit strain, and toughness. While phenomenological failure models have merits, their application to situations outside of the data set to which they were trained can lead to catastrophic errors. As a result, the engineering research community has long pursued the development of more robust failure models that are more closely linked to the underlying physics. Thanks to continually increasing computing resources, improved algorithms, and advanced simulation methodologies (atomistic, phase field, finite element, mesoscale models, etc.), the prospect for further improvement remains strong.

The physics of material failure in engineering alloys begins at the atomic scale, where interatomic decohesion and defect formation, propagation, and interaction occur. At the microstructural scale, the net effect of these mechanisms emerges as

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Nomenclature

a_o	lattice constant of aluminum at 0 K (a_o=0.405 nm)
b_p	magnitude of the Burgers vector of a Shockley partial dislocation
C_{11}, C_{12}, C_{44}	single crystal elastic constants
d_{FE}	size of the finite element domain in the Embedded Statistical Coupling Model (ESCM) model
d_{MD}	size of the molecular dynamics domain in the ESCM model
F	energy factor
H	thickness of the molecular dynamics domain in the ESCM model used in the simulations
h	interplanar spacing between the slip planes in aluminum
k_B	Boltzmann constant
K_I	mode I stress intensity factor
K_{IC1}	stress intensity factor for leading partial dislocation nucleation
K_{IC2}	stress intensity factor for complementary partial dislocation nucleation
K_{IT}	stress intensity factor for trailing partial dislocation nucleation
K_I^{LSL}	stress intensity factor below which a stable state for the leading partial dislocation does not exist
K_{IC1}^{AT}	stress intensity factor for leading partial dislocation nucleation without thermal activation
K_{IC2}^{AT}	stress intensity factor for complementary partial dislocation nucleation without thermal activation
K_{IT}^{AT}	stress intensity factor for twinning partial dislocation nucleation without thermal activation
K_I^P	most probable stress intensity factor for partial dislocation nucleation
K_{II}^{eff}	resolved stress intensity factor on the active slip plane
$K_{II}^{eff^*}$	resolved shielded stress intensity factor on the active slip plane
$K_{II\ crit}^{eff^*}$	resolved shielded stress intensity factor on the active slip for partial dislocation nucleation
Q_{2D}	activation energy per unit length from Peierls continuum model
Q_{3D}	total activation energy
r	distance from the crack tip
r_p	distance from crack tip to partial dislocation
s	shear stress on the slip plane due to slip
T	system temperature
U	energy of an infinite linear elastic solid with a sharp crack
U_o	energy of an infinite linear elastic solid with a sharp crack with no slip
γ_{ssf}	stable stacking fault energy
γ_{usf}	unstable stacking fault energy
γ_{stf}	stable twinning fault energy
γ_{utf}	unstable twinning fault energy
Δ	relative shear displacement between two atomic planes
$\vec{\delta}$	slip discontinuity in continuum model
δ_e	magnitude of edge component of a slip discontinuity
δ_s	magnitude of screw component of a slip discontinuity
ε	applied far-field uniaxial strain
θ	slip plane inclination angle with respect to the crack plane
Φ	local slip discontinuity energy penalty
μ	shear modulus
ν	Poisson's ratio
τ	shear stress on the slip plane in the direction of $\vec{\delta}$
φ	angle between the slip direction and the normal to the crack front in the slip plane
ξ	distance from the crack tip
Ψ	generalized stacking fault energy
ω	expected rate of thermally activated event
ω_o	attempt frequency of thermally activated event

microcracking and crystal plasticity. Ultimately these processes result in macroscopic failure, amenable to traditional continuum plasticity and fracture mechanics. The goal of physics based modeling is to acknowledge and understand this hierarchy. By doing so, it aims to be more predictive, robust, transferable, and potentially provide the insight necessary for creating new materials with improved properties.

Successful physics based failure modeling requires a sound understanding of the controlling mechanisms. A technologically important and illustrative example is the prediction of crack growth in engineering alloys. Crack growth in metals occurs via interatomic decohesion at the crack tip, a mechanism that is in competition with crack tip plasticity in the form of dislocation nucleation and propagation. Additional complexity exists in face-centered-cubic (f.c.c.) alloys, where crack tip dislocation emission can consist of either crystallographically restoring plastic slip in the form of full dislocations or crack tip twinning due to the nucleation of successive partial dislocations (Weertman and Weertman, 1992). While both mechanisms are associated with plastic deformation, they can ultimately lead to drastically different crack tip behavior, influencing the overall material toughness. Accordingly, a key step, necessary for the development of predictive physics based crack growth models in f.c.c. metals, is to develop a comprehensive understanding of the competition between crack tip twinning and full dislocation emission.

Modeling this competition presents a particular challenge in that it is sensitive to strain rate, temperature, and crystallographic orientation (Farkas et al., 2001; Hai and Tadmor, 2003; Yamakov et al., 2006; Warner et al., 2007; Warner and Curtin, 2009; Venables, 1963). This paper reports on the authors' attempts to more comprehensively understand the