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Role of nanotwins on fatigue crack growth resistance – Experiments and theory

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ABSTRACT

The study of near-threshold fatigue crack growth has long remained an empirical field due principally to the highly microstructure-sensitive nature thereof. The primary challenges have been to forward physical model(s) informed by the governing micromechanism(s), which would be able to predict the experimental behaviors devoid of empiricism. Today, we have sophisticated experimental techniques (e.g. digital image correlation, electron microscopy) as well as atomistic simulation tools (e.g. molecular dynamics) at our disposal to finally revisit the century old fatigue problem in the light of physical phenomena therein. This paper is geared towards achieving such a feat with a very special type of materials, nano-twinned alloys, as the candidate materials, which are of great recent interest due to their reportedly superior damage properties. Specifically, we investigate how the microstructural features (e.g. slip transfer mechanism at coherent twin boundaries, twin thickness/spacing, frictional stress, pre-existent near-tip slip density) can be modulated to improve the damage resistance. The results suggest that these parameters considerably affect the crack propagation impedance (as quantified in terms of ΔK_{eff}^{th}). A thorough discussion of the current findings and the most recent literature developments in this regard are provided.

1. Introduction

1.1. Motivation and objective

Nanotwinned metals and alloys are novel emerging materials that are drawing considerable research interests thanks to their superior mechanical properties [1–3]. Given their considerable promise, their fracture and fatigue properties have come under scrutiny only in the recent years [4–6]. Quite interestingly, the damage tolerance of these nanotwinned materials is found to be demonstrably improved compared to the more conventional counterparts. In this context, we note the importance of further studies, specifically addressing the microstructure-sensitive crack growth regime. In particular, it would be of great interest to establish the relevant factors governing the near-threshold crack advance mechanism(s) in the presence of nano-scale twins. Essentially, the very nature of the problem necessitates a synergistic approach between sophisticated experimental characterizations and the requisite theoretical underpinnings at the microscopic level. Recently, there have been considerable developments in connecting atomic scale physical process to the macroscale deformation behaviors [7–9]. To that end, we first probe into the experimental crack propagation behavior(s) of nanotwinned Ni–2.89 wt.% Co alloy, and then rationalize the findings with a physical theory. Our modeling strategy is twofold involving both non-continuum and continuum analyses: (1) studying the role of coherent twin boundaries on the crack-emitted slip (via atomic-scale simulations), and (2) examining the cyclic crack advancement metrics influenced by nano-sized twins (via continuum scale simulations).

1.2. Experimental damage properties

As the crack tip is a source of dislocations [10] and dislocation patterns evolving under cyclic loading are directly related to the twin thickness [11], it is reasonable to expect that twin volume fraction will affect the fatigue damage impedance of nanotwinned metals/alloys. Singh et al. [12] reported that decreased inter-twin spacing results in a substantial improvement of fatigue crack growth resistance in nanotwinned Cu. Similar enhancement in the damage properties was also noted by Sangid et al. [13] for the case of electrodeposited nanotwinned Ni–Co alloys. In

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Nomenclature

FCG, CTB	fatigue crack growth, coherent twin boundary
MD, GSFE	molecular dynamics, generalized stacking fault energy
HT	heat treated
EAM	embedded atom method
DIC	Digital Image Correlation
da/dN	FCG rate
a	crack length
N	number of cycles
b_r	magnitude of residual Burgers vector
K, $K_{\max}$, K_{open}	stress intensity factor (SIF), maximum SIF, opening SIF
$\Delta K, \Delta K_{\text{th}}, \Delta K_{\text{eff}}^{\text{th}}$	SIF range, threshold SIF range, effective threshold SIF range
k_{IIIa}, k_{IIIe}	local applied SIF, critical SIF to emit slip
R	load ratio
G	shear modulus
E^{misfit}, E^{elastic}	misfit and elastic energy
ν	Poisson's ratio
d	lattice constant
t, s	twin thickness, twin spacing respectively
θ	angle between crack and slip paths
r	radial distance measured from the crack tip
p	Paris law exponent
C	Paris law proportionality constant
T	T stress
Tw	twin coordinate frame
n^C	number of crystal dislocations, number of pre-existent dislocations
n^{emit}	number of dislocations emitted from the crack tip
n^{res}	number of residual dislocations
Δu	irreversible crack tip displacement in Burger vector's direction
$\varepsilon^{\max}$	maximum strain at the crack tip plastic zone
ε^{irr}	irreversible strain at the crack tip
x, y	horizontal and vertical positions of dislocations respectively
$\sigma_F, \sigma_F^{\text{Barrier}}$	unobstructed and obstructed slip glide stress

particular, the electron microscopy of fatigued Ni–Co alloys indicated a widespread presence of slip-mediated plasticity subjected to the twins. The foregoing literature findings strongly suggest that the mechanistic origin of the observed near-threshold damage properties can be attributed to the outcome of massive slip–twin interactions. Particularly, we note that the cyclic crack increment would be directly proportional to the degree of crack-emitted slip irreversibility, which would be governed by a specific outcome of the slip–twin interaction [14–16]. In other words, the greatest resistance to the cyclic crack growth would intuitively originate from the case of slip–twin interception with the least extent of slip irreversibility. Hence, it is imperative to pinpoint such slip interception mechanism to better understand the mechanistic origin of the reportedly superior damage impedance of nanotwinned materials.

1.3. Theoretical developments

Considerable progress has been made in understanding the role of CTBs on transferring dislocation slip [17,18]. Early literature noted that a CTB can allow: (1) full transmission of slip with no residual slip on the interface (i.e. the cross-slip through the boundary), (2) partial transmission when an interfacial residual slip develops and (3) no transmission whatsoever (i.e. the incorporation onto the boundary) [19]. These interaction outcomes are strongly dependent on the local stress state and the geometry of the approaching slip [20]. The effects of these reaction outcomes on the fatigue crack propagation properties have most recently been addressed by Chowdhury et al. [16,21,22]. Particularly, they considered the case of non-zero residual dislocation, and demonstrated how the irreversibility of the associated slip trajectory would be influenced.

Earlier, Pippan et al. [23,24] devised a continuum dislocation model to demonstrate the importance of considering irreversibility of discrete slip (in the presence/absence of obstacles) to quantify fatigue threshold metrics. A complete analysis of the cyclic slip–barrier interaction outcomes i.e. the role of residual slip, from a non-continuum standpoint could provide useful mechanistic insight in this regard. It can be inferred from the Chowdhury et al.'s study [16,21,22] that a lower magnitude of residual slip promotes the overall slip reversibility, and hence decelerates the attendant crack growth rate.

Given the foregoing background, the cross-slip of a screw dislocation is particularly noteworthy, and bears important mechanistic implications regarding the fatigue crack growth resistance. The cross-slip at a twin boundary would occur with the least amount of frictional resistance due to the absence of residual slip [19]. Most notably, under cyclic loading, the lattice impedances for forward and reverse cross-slip would essentially be similar, unlike other reaction types (where reverse glide would be more difficult due to the residual dislocation) [16]. In other words, the cross-slip can be associated with the least irreversible dislocation trajectory during fatigue loading.

1.4. Current approach

In light of the foregoing discussion, one can identify the governing factors for the near-threshold crack growth properties of nanotwinned materials, namely, the characteristic twin dimensions (i.e. thickness and spacing), the initial dislocation density and slip–twin interaction types. This paper aims to analyze the effects of these factors in cross-slip configuration. First, fatigue crack growth experiments are performed on electrodeposited nanotwinned Ni–2.89 wt.% Co before and after heat treatment. We characterize the threshold stress intensity factor range and the ensuing Paris regime of nanotwinned Ni–Co for both cases. Then, we employ a high magnification, *in situ* DIC technique to quantify the degree of axial, cyclic irreversible strain at the crack tip. Transmission electron microscopy (TEM) is utilized to note the microstructural differences between the pre- and post-heat treated materials. On theoretical grounds, we conduct molecular dynamics (MD) simulations to investigate the cross-slip of a crack-emitted dislocation across a CTB. Particularly, the energy barrier for cross-slip is quantified and then used in a Peierls–Nabarro formalism [25,26] to extract the associated lattice friction stress. Thus-computed friction stresses are used as an important ingredient in a continuum scale dislocation motion simulation. These fatigue crack growth simulations, informed by the atomistically calculated glide strengths are then used to isolate the role of twin boundaries on the damage metrics of the Ni–Co alloys. In essence, we propose a generic modeling platform to test the role of friction stress, twin dimension and pre-existent dislocation density (in the near-tip area) on the damage resistances in terms of the effective threshold stress intensity range. In doing so, no