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SciVerse ScienceDirect
Acta Materialia 61 (2013) 2531–2547
Acta MATERIALIA
www.elsevier.com/locate/actamat

Modeling fatigue crack growth resistance of nanocrystalline alloys

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Received 18 November 2012; received in revised form 16 January 2013; accepted 17 January 2013
Available online 15 February 2013

Abstract

The description of fatigue crack growth in metals has remained an empirical field. To address the physical processes contributing to crack advance a model for fatigue crack growth (FCG) has been developed utilizing a combined atomistic–continuum approach. In particular, the model addresses the important topic of the role of nanoscale coherent twin boundaries (CTB) on FCG. We make the central observation that FCG is governed by the dislocation glide resistance and the irreversibility of crack tip displacement, both influenced by the presence of CTBs. The energy barriers for dislocation slip under cyclical conditions are calculated as the glide dislocation approaches a twin boundary and reacts with the CTB. The atomistically calculated energy barriers provide input to a mechanics model for dislocations gliding in a forward and reverse manner. This approach allows the irreversibility of displacement at the crack tip, defined as the difference between forward and reverse flow, to be determined. The simulation results demonstrate that for both refinement of twin thickness and a decrease in crack tip to twin spacing FCG resistance improves, in agreement with recent experimental findings reported in the literature.

Keywords: Fatigue; Nanocrystalline; Nickel; Damage tolerance; Coherent twin

1. Introduction

Current assessment of materials for damage tolerance is based on methodologies that were developed more than 40 years ago. These methodologies are empirical and “rule based”, such as the well known ASME Design Code [1] that treats combined fatigue and creep damage. Today it remains a challenge to predict material degradation under fatigue loading conditions utilizing scientific principles. Compared with unidirectional deformation, fatigue introduces irreversibilities that are characteristic of cyclical deformation. These irreversibilities are a strong function of the crystal structure, the alloy composition, and the interface interactions. Nanocrystalline materials with twin boundaries [2–10] have attracted considerable attention recently, and possess combined strengthening attributes with higher ductility. On the other hand, their fatigue damage tolerance characteristics have received less consideration, and the present paper is geared towards building a framework for the modeling of fatigue crack growth in nanomaterials.

A number of studies have elucidated the strengthening mechanisms in nanocrystalline materials under monotonic loading conditions [2–4,11–15]. Fatigue studies of nanocrystalline metals displaying higher endurance limits [16–20] compared with their coarse grained counterparts have also been undertaken. Recent works have also demonstrated superior damage tolerance [5,21] in the presence of nanoscale twins, hence the prospect of enhanced overall fatigue resistance with combined monotonic strength holds considerable promise. In particular, Singh et al. [5] demonstrated that introducing nanotwins with a gradually diminishing lamellar spacing in ultrafine grained (UFG) Cu substantially improved damage tolerance metrics such as the threshold stress intensity range ΔK_{th} and, most significantly, the

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http://dx.doi.org/10.1016/j.actamat.2013.01.030

near-threshold crack growth rate $\mathrm{d}a/\mathrm{d}N$. Moreover, studies by Sangid et al. [21] on electro-deposited nanocrystalline nickel–cobalt alloys with a high volume fraction of annealing twins in the grains further corroborated the existence of superior fatigue crack growth (FCG) impedance. While these studies point to the significance of coherent boundaries on FCG behavior, understanding the mechanistic origin of such microstructure-driven phenomena necessitates a detailed study informed by the underlying atomistics, capturing the operative cyclical crack tip plasticity at the appropriate length scale. The current paper has developed a model for subcritical FCG behavior combining atomistic and continuum considerations in the presence of twin lamellae of nanoscale thickness and spacing. The advantage of the model is that there are no adjustable parameters (fitting constants) and crack propagation occurs due to the irreversibility of plastic flow at crack tips.

A fatigue crack advances because of the irreversible glide of dislocations emitted by the crack-tip, the degree of which dictates the net plastic displacement per cycle [22–30]. Pippan et al. [27–29] showed that crack tip displacement under forward and reverse loading does not cancel out because of dislocation annihilation, resulting in fatigue crack advance. We note that microstructural factors that would influence the degree of glide irreversibility must also alter the FCG rates. Specifically, microstructural obstacles, such as coherent twin boundaries (CTBs) and grain boundaries (GBs), in the neighborhood of an advancing crack mean that the slip reversibility is difficult to ascertain. The extent of irreversibility imposed by these obstacles is a function of the nature of the slip–interface interactions. At the same time, the presence of such interfaces influences the resistance to slip propagation τ_o (i.e. the difficulty of plastic flow advancing past the obstacle, manifested as an elevation of the unstable fault energy γ_{us}). γ_{us} is the maximum fault energy during slip established from the block-like motion of an upper surface relative to a lower one. Inevitably, its extrinsic (modified) level will change due to the intersection of slip with interfaces. The resulting crack growth rate $\mathrm{d}a/\mathrm{d}N$ is related to the slip paths, residual dislocations, and conservation of the Burgers vectors as influenced by the twin width and spacing.

Fig. 1 depicts the forward slip emission from an advancing fatigue crack and its interaction with a CTB. The nature of the slip–CTB interaction is a function of the type of incident dislocation (pure edge, pure screw or mixed). Residual dislocations with a total Burgers vector b_r are an outcome of these reactions, which depend on the interface orientation and the resolved shear stresses of the incoming and outgoing slip systems [31,32]. Variations in such slip–twin reactions would ultimately modify the glide path irreversibility. The fatigue crack growth resistance is expected to change with the four factors shown in Fig. 1, the irreversibility (denoted p), the intrinsic stress τ_o related to the gamma surface (Generalized Stacking Fault Energy), and the twin thickness t and twin spacing d. If the irreversibility p is 0 no crack growth can occur. We show that the irreversibility is dictated by the gamma surface differential upon forward and reverse flow at the crack tip.

The prevalence of twins, as in the case of the Ni–Co alloy seen in the transmission electron microscopy (TEM)

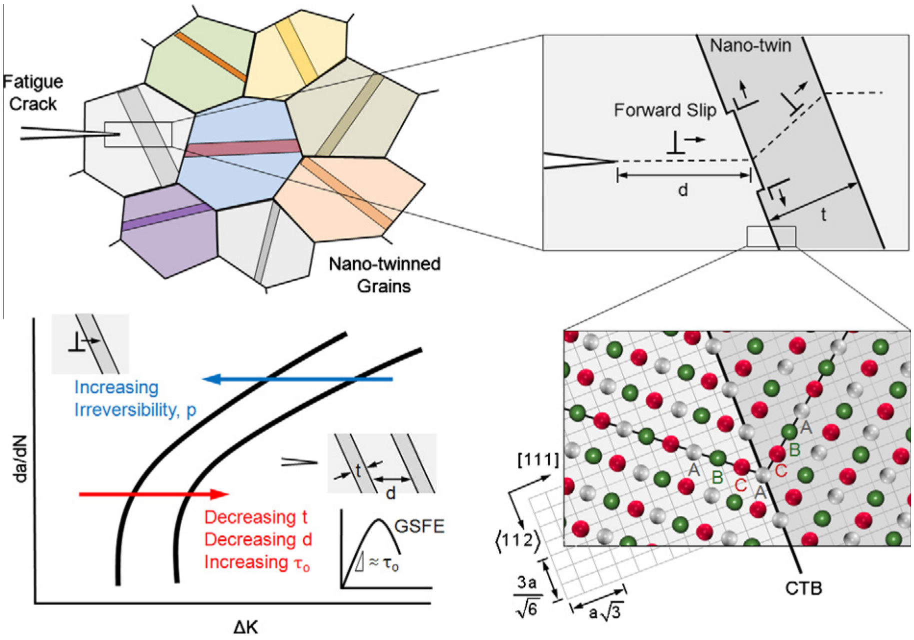

Fig. 1. Schematics representing the focus of the investigation in this paper. In forward load an advancing fatigue crack emits dislocations (pure screw type under mode III loading) which interact with a nanoscale twin. Slip-coherent twin boundary (CTB) interactions dictate the FCG mechanism. The current work studied the isolated role of twin lamellae width (t) and the crack to twin spacing (d) on the FCG behavior in a single nanotwinned grain. The coherency of the twin boundaries allows glissile motion of dislocations on the CTB, unlike incoherent GB. Factors that influence fatigue crack growth behavior are summarized. In addition to t and d, the glide strength, τ_0 and the irreversibility, p, under cyclical loading influence fatigue crack growth rates.