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Recent advances in modeling fatigue cracks at microscale in the presence of high density coherent twin interfaces

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ABSTRACT

This concise review chronicles recently emerged fatigue crack growth behaviors of nanomaterials with prevalent Σ3 boundaries and the related modeling endeavors. Experimentally, these nano-twinned materials demonstrated remarkably high damage tolerance, which is a significant countertrend to the previous nanocrystalline literature. To explore the physical rationale, various slip transfer mechanisms at a coherent twin-matrix interface are investigated using crystal simulations. The role of different slip-interface reactions is identified as modifying the cyclic slip irreversibilities, which in turn drives the crack advancement. As the residual Burgers vector from a reaction attains maxima, the associated fault energetics is predicted to saturate, which is an important discovery regarding the damage mechanism. Consequently, a generic computational recipe for theorizing material degradation is established, using reaction-specific Peierls stresses as crucial input. A general agreement between predictions and experiments lends sufficient credence to the adopted modeling approach. We also survey relevant literature and point out promising avenues for future research.

1. Background

In this paper, we aim to update the readers on the recent developments regarding: (a) engineering coherent interfaces in microstructure so as to achieve superior fatigue resistance and (b) the modeling strategies based on interfacial plasticity to predict damage metrics therein.

Superior mechanical attributes due to interface coherency

Rapid innovations in today's industrial sectors are pushing the boundaries for advancing next generation materials. Due to extreme operational ceilings, the current service components (e.g. in aeronautical structures) warrant a favorable combination of high strength, ductility and cracking resistance. A desired synergy of these properties could be achieved through modulating the microstructure which can be characterized by techniques such as electron diffraction and microscopy (Fig. 1). For instance, increasing the interface density (i.e. grain refinement via thermo-mechanical treatments) has so far remained the most popular strategy to impart ultra-high strength [1–5], however, at the significant expense of cracking resistance and ductility. The empirical correlations among these attributes are schematically presented in Fig. 1 with dotted lines (red[1], blue and green) for conventional materials.

Quite intriguingly, recent literature suggests that raising the interface density, while maintaining high coherency, can indeed meet an unprecedented amalgam of all the desirable attributes listed above [6]. The most promising candidates to have actually manifested such a feat are the nano-twinned metals and alloys with a prevalence of Σ3 interfaces, which is the most coherent of all boundaries. The coherency of a boundary can be interpreted as the degree of atom-by-atom registry between the crystals from both sides. In addition to superior toughness [7,8], remarkably high fatigue crack growth resistance therein has been reported lately [9,10]. On summarizing the experimental literature, it can be inferred that a finer twin lamellar thickness and/or spacing is more beneficial in obstructing damage propagation than the coarse-twinned counterparts (experimentally obtained data based on Ni-2.9%Co alloy and pure Cu [9–11] shown in Fig. 2). It is interesting to note that this behavior is in contrast with the fatigue crack growth responses of conventional nanocrystalline materials [12–16]. It is imperative to recall that a pronounced deterioration

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[1] For interpretation of color in Figs. 1 and 4, the reader is referred to the web version of this article.

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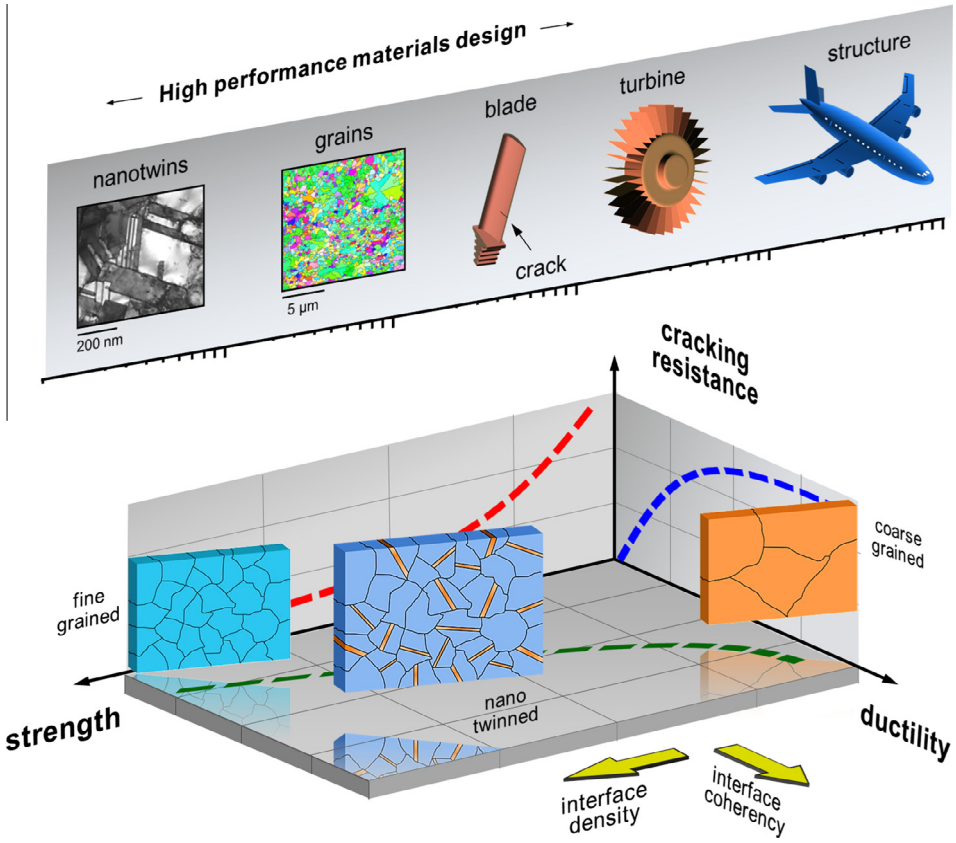

Fig. 1. Achieving superior mechanical attributes in terms of strength, ductility and cracking resistance via nanoengineering.

in the crack propagation impedance was earlier found as a result of densely packed (incoherent) boundaries in nano-grained metals. A careful study of nano-twinned and traditional fine-grained materials behaviors strongly indicates that interface coherency indeed plays a pivotal role in imparting not only high toughness but also improved cracking attributes. Moreover, unlike the conventional nano-sized grains, the nano-twins are found to be quite stable upon thermomechanical treatments [10,11]. Table 1 summarizes the literature results in this regard.

While rationalizing monotonic attributes is quite straightforward (e.g. in terms of slip inhibition), the fatigue cracking is a rather complicated phenomenon to address. Theorizing such a

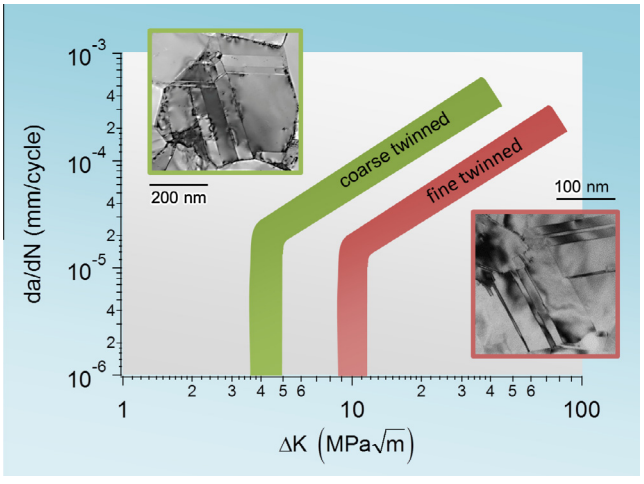

Fig. 2. Comparison of experimental literature [9–11] on nanotwinned NiCo alloys and pure Cu – a correlation between the twin lamellar thickness (and/or spacing) and the damage trends has been noted.

problem entails a detailed exploration of the underlying damage micromechanisms and pinpointing the governing parameters at the nanoscale [17], which we discuss as follows.

Damage characteristics in nano-twinned microstructure and the controlling variables

Of all failure modes, the fatigue is of paramount concern since catastrophic fracture can occur under cyclic loads well below the static safety margin [18]. Repeated loading induces irreversible slip accumulation at the microscopic stress concentration sites (e.g. surface extrusions/intrusions), ultimately triggering material separation i.e. crack formation [19]. The entire spectrum of the ensuing crack progression is generally understood as the microstructure-sensitive stage I and microstructure-independent stage II (Fig. 3). In a nano-twinned environment, a stage I crack would advance by slip irreversibilities subjected to coherent Σ3 boundaries as elaborated below.

It is well accepted today from exhaustive sets of experiments that the generic fatigue crack growth mechanism in ductile metals is microscopically controlled by pervasive slip activities [20]. For instance, depending on the extent of dislocation slip, an advancing crack would behave as either microstructure-sensitive or not. Therefore, the damage propagation problem could most accurately be modeled by pinpointing the variables controlling slip characteristics at the mesoscale. It is imperative to note that the inherent material response to slipping can be traced back to the discrete lattice effects such as the Peierls energy valley contributions. These effects are thus important to include in any physically based fatigue modeling endeavor as we set out to outline in this article.

Characterization-wise, a stage I crack growth rate, *da*/*dN*, would undergo fluctuating values due to intermittent encounters with multiple boundaries (red curve in Fig. 4). With a history of

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Table 1
Summary of literature findings on fatigue crack growth behaviors in nanomaterials.

Materials	Microstructure	Principal investigators	Experimental discovery	Proposed mechanism
Pure Cu	Nano-twinned (lamellar thickness/spacing: 30–80 nm)	[9]	Increased crack growth resistance with twin refinement	Enhanced plasticity accommodation by Σ3 interfaces
NiCo alloys	Nano-twinned (lamellar thickness/spacing: 15–60 nm)	[10,11,23,67,80]	High damage impedance due to twin refinement (Paris exponent ~1.3 and ΔK_{th} ~10 MPa $\sqrt{m}$)	Reduced slip irreversibilities due to Σ3 interfaces
Pure Ni	Nano-grained with no twin (average grain size: 10–70 nm)	[12–16]	Marked deterioration in cracking resistance	Combined effect of grain growth, void coalescence and reduced tortuosity

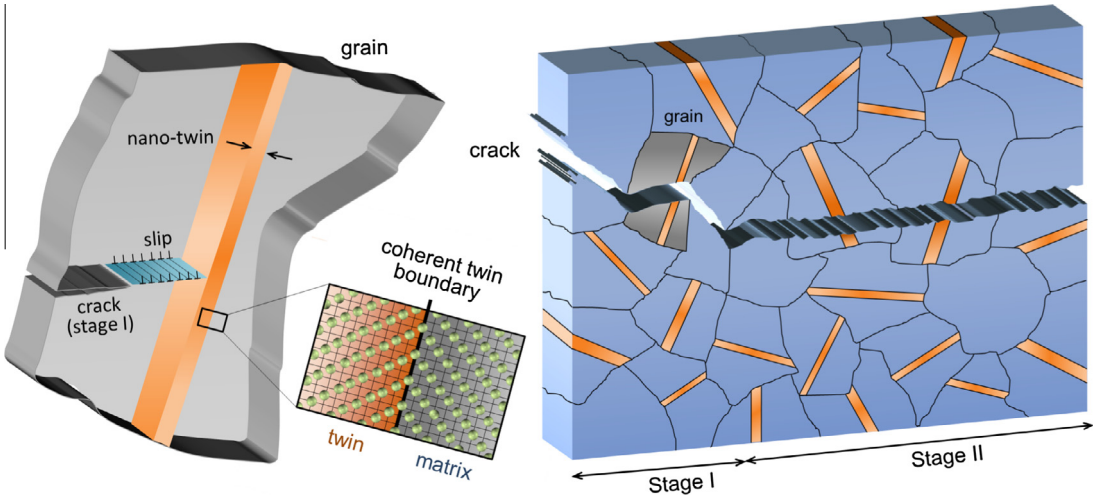

Fig. 3. Fatigue crack growth in presence of nano-twins with coherent Σ3 boundaries.

irreversible slip accumulation, the crack ultimately reaches a boundary-insensitive stage II with a large plastic zone (as can be seen by digital image correlation in Fig. 4). The relative span of the earliest crack propagation period is crucial, in that it is inherently decided by the specific nature of slip- Σ3 boundary reactions from grain to grain. Conventional engineering practice regards the stage I growth as an incubation period prior to the appearance of a macroscopically visible stage II crack on overcoming the so-called mechanical ΔK_{th} (blue curve in Fig. 4). Therefore, any tailored microstructure (e.g. with high density of twin boundaries) prolonging the initial growth period would be translated into an overall improvement in the material cracking resistance. From modeling perspective, the early growth regime presents itself as a unique conduit for examining the role of these interfaces on the damage tendencies.

We note that the variables governing a stage I crack in nano-twinned microstructure are: (a) host grain orientation, (b) local stress state, and (c) the distribution of twin boundaries. From modeling standpoint, the most convenient way to incorporate the aforementioned crystallographic factors is in terms of the irreversible slip trajectories [21–23]. For example, prior to a microscopic crack intercepting the nearest interface, the slip would emanate on the maximum Schmid factor system(s) and interact therewith. Depending on the nature of the slip/interface reaction, the extent of the irreversibility would vary substantially. Since the crack growth rate, da/dN, is directly proportional to the degree of irreversibility, one can examine the role of the aforementioned crystal variables on the cracking resistance using such an approach. For a microstructurally small crack, the physical lengthscale of the per-cycle cracktip extension is several lattice spacings, decided by the collective Burgers vectors of irreversible slip. Evidently, such a behavior can only be understood by considering the near-tip microplasticity at the crystal level. We model crack advancement mechanism based on irreversibility of crack-emitted slip undergoing interfacial plasticity. The modeling and experimental results (to be discussed next) are all based on fcc Ni-2.9%Co alloy. It should be noted that similar investigation is also performed on pure Cu, Ni and Al [24,25].

2. Modeling – crystal phenomena affecting fatigue

Role of slip emission in dictating the ductile versus brittle fracture was first brought into attention by Rice and Thomson in their pioneer work [26]. Subsequently, a number of models ventured into predicting fatigue crack growth on the basis of cracktip slip phenomena [27–29]. Today, one can build upon these foundational works, bolstered by the modern computational science tools, to address the interface-affected fatigue problem.

To that end, let us first consider a pre-existent stage I crack in presence of a nanometer thick annealing twin as depicted in Fig. 5. During propagation, the crack emits a series of dislocations which glide forward to intercept the nearest coherent twin boundary (CTB). In what manner the crack advancement would be affected by the presence of the CTB depends entirely on (a) the specific outcome of slip-CTB reactions, (b) the associated fault energetics and (c) the Peierls stress level. We outline the particulars of their roles as follows.

2.1. Importance of crack-emitted slip transfer at interfaces

The specific nature of how the crack-emanated slip would transmit past a twin boundary would considerably affect the attendant growth rate. Early literature noted that a CTB has the unique ability to permit complete/partial/no transfer of the incident slip ($\vec{b}_{incident}$) [30–35] as extensively substantiated both on experimental and theoretical grounds. The criteria for slip transfer mechanisms at a generic grain boundary have been first proposed from

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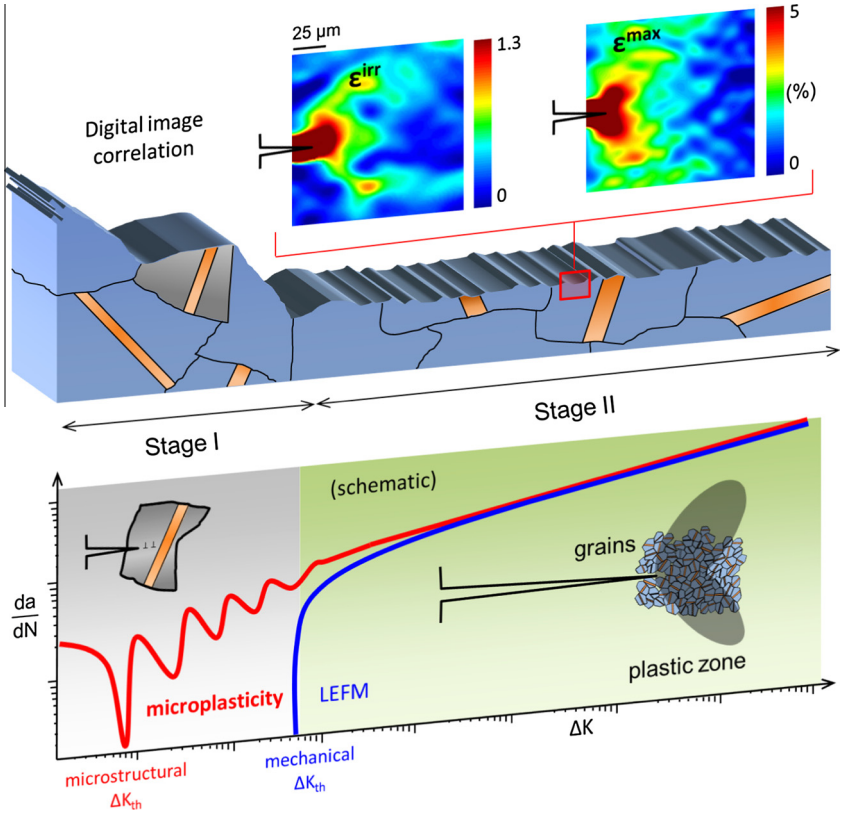

Fig. 4. The stage II near-tip strain localization due to irreversibility is studied via DIC [11] and *da*/*dN* determined. Stage I crack growth behavior (red) can be predicted using microplasticity concepts.

experimental studies [36] as: (a) maximization of local resolved shear stress, (b) minimization of the angle between incident and outgoing slip planes and (c) minimization of residual Burgers vector ($\vec{b}_r$). Recent atomistic simulations by Dewald and Curtin [37,38] unraveled further ramifications to these rules, particularly addressing the role of local variations in stress and geometry at and around an interface. With the aid of molecular dynamics simulations, we categorize five distinct types of slip-CTB interactions that are most likely to occur following the aforementioned rules: (a) incorporation (i.e. twinning and/or de-twinning) [30,39–41], (b) transmission [32,42], (c) multiplication [43], (d) transmission and incorporation [33,44,45], and (e) blockage by a Lomer lock formation [46,47]. The governing conditions for these reactions (Table 2) are identified as: (a) the local stress state i.e. the relative Schmid factors on the twin boundary, incident, and outgoing slip systems ($m_{incident}$, $m_{boundary}$ and $m_{outgoing}$) and (b) the geometry of the intercepting slip i.e. edge/screw/mixed [48]. Each reaction culminates in a different type of residual slip, $\vec{b}_r = \vec{b}_{incident} - \vec{b}_{transferred}$ (onto the CTB), which acts as a unique signature for a specific reaction. The reactions represent the initial interaction mechanisms when the very first slip reaches the pristine interface. Since $m_{incident}$, $m_{boundary}$ and $m_{outgoing}$ are unchanged for a particular loading state, the reactions fundamentally remain the same for subsequent incidence. Only the intermediate reaction steps differ, however, to a minor extent. We note that these atomistic slip transfer mechanisms are based on quasi-static volume element of fcc lattice with periodic boundary conditions (i.e. representing bulk material). The materials range from Cu, Ni, Al and Ni-2.9%Co.

The nature of various slip transfer outcomes bears important mechanistic implication regarding the damage growth [49]. Different local stress situations are bound to arise at twin boundaries from one grain to another in a polycrystalline environment. This would give rise to a distribution of the foregoing straining mechanisms. For example, it is only reasonable to deduce that in strongly textured material a particular type of reaction, as favored by the local conditions, would be predominant. On the same rationale, a random grain distribution would pose equal probability of all mechanisms. Experimentally, a stage I crack is known to decelerate as it approaches a boundary within a certain grain, but may proceed with no blockage in other cases [50]. The reason is attributable to the fact that different reactions impart different resistances to the crack-emitted slip, and hence influence the attendant crack growth rate. Thus, the categorization of the slip transfer mechanisms can be deemed as the necessary groundwork for a mechanistic study of microstructure-sensitive damage propensities. Recent literature noted the use digital image correlation (DIC) to extract $\vec{b}_r$ for an assortment of grain boundaries [51]. These experimental observations suggested that the magnitude of $\vec{b}_r$ is inversely proportional to the transferred strain. In other words, an increasing magnitude of $\vec{b}_r$ is indicative of enhanced slip penetration strength past the interface.

Therefore, aside from the qualitative classification, one needs to quantify the degree of resistances that individual reactions pose as a precursor to theorizing CTB-affected cracking. As a first step towards that objective, we compute unstable stacking fault energy (γ_{us}) corresponding to various straining mechanisms at the CTB. The principal impact of doing so is that the extrinsic levels of γ_{us} could most conveniently be incorporated into Peierls-Nabarro framework to predict the associated frictional stresses. The prediction scheme is discussed below.

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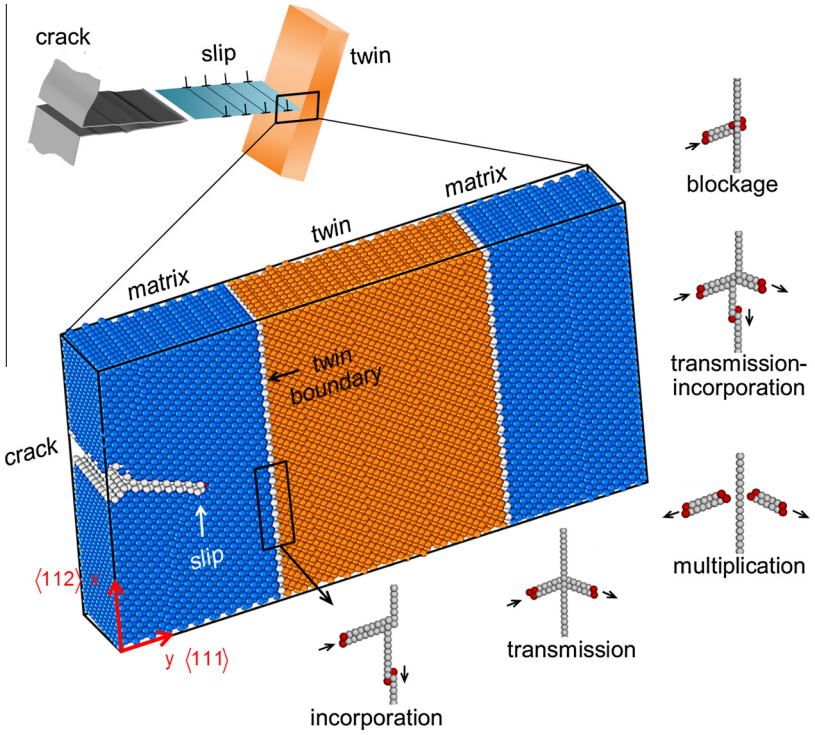
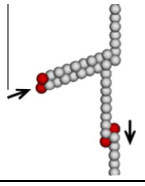
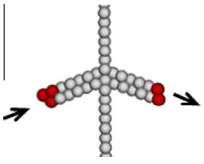
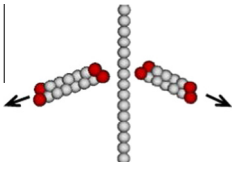
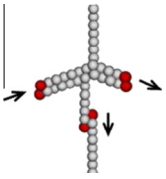
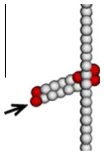


Fig. 5. Various outcomes of slip-coherent twin boundary depending on the stress state and slip geometry [48].

Table 2
Summary of slip-twin boundary interactions under certain applied stress states, and the Schmid factors on incident, boundary and outgoing slip planes ($m_{incident}$, $m_{boundary}$ and $m_{outgoing}$ respectively).

	Incorporation	Transmission	Multiplication	Transmission-incorporation	Blockage by Lomer lock
					
Applied stress state	$\begin{bmatrix} 0 & \sigma_{xy} & 0 \\ \sigma_{yx} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & \sigma_{xz} \\ 0 & 0 & 0 \\ \sigma_{zx} & 0 & \sigma_{zz} \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & \sigma_{xz} \\ 0 & 0 & 0.5\sigma_{yz} \\ \sigma_{zx} & 0.5\sigma_{yz} & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & \sigma_{xy} & 0 \\ \sigma_{xy} & 0 & 0 \\ 0 & 0 & \sigma_{zz} \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & \sigma_{yy} & 0 \\ 0 & 0 & 0 \end{bmatrix}$
Incident dislocation (full) type	Screw	Edge	Mixed	Mixed	Mixed
$m_{incident}$	0.39	0.41	0.34	0.46	0.31
$m_{boundary}$	0.5	0.00	0.22	0.5	0.00
$m_{outgoing}$	–	0.41	0.34	0.46	0.16

2.2. Unstable stacking fault energy, γ_{us}

First conceptualized by Vitek [52], the γ surface in its entirety is traditionally understood as the energy density (per area) versus atomic displacement curves obtained upon rigidly shearing two atomistic crystals (Fig. 6). A more physical interpretation thereof dictates that the γ energetics constitutes the energy cost to create a particular crystal fault with a specific degree of lattice shearing as originating from the inherent atomistic bonding landscape. For example (Fig. 6), the unstable stacking fault energy (γ_{us}) along the direction $\langle 1\,1\,2 \rangle$ signifies energy barrier for nucleating an intrinsic stacking fault [53]. Early experimental literature [54–56] has noted that that fault energetics has a significant role on the fatigue behaviors. On theoretical grounds, the parameter γ_{us} has been pioneered as a vital metric for the fracture criterion by Rice, Tadmor and their co-workers [57–59]. The applicability of γ_{us} in fatigue modeling context is also equally important, as we show, although its use therein has remained relatively un-explored until now. The primary constraint has been the unfeasibility of its experimental determination as the associated lattice structure represents a metastable state. Such a configuration constitutes an intermediate step in the pathway of a stable and tangible defect (i.e. slip) formation, thus necessitating its *in-situ* quantification with atomic scale resolution. Accomplishing such a feat is beyond the scope of existing experimental measurement techniques. Nonetheless, with the advent of improved atomistic simulations we now have at our disposal the ability of accurately capturing the crystals at quasi-equilibrium state both temporally and spatially.

To that end, we demonstrate how the extrinsic levels of γ_{us} could be utilized as a unique signature in solving the role of particular interface on influencing fatigue cracking. With a view to doing

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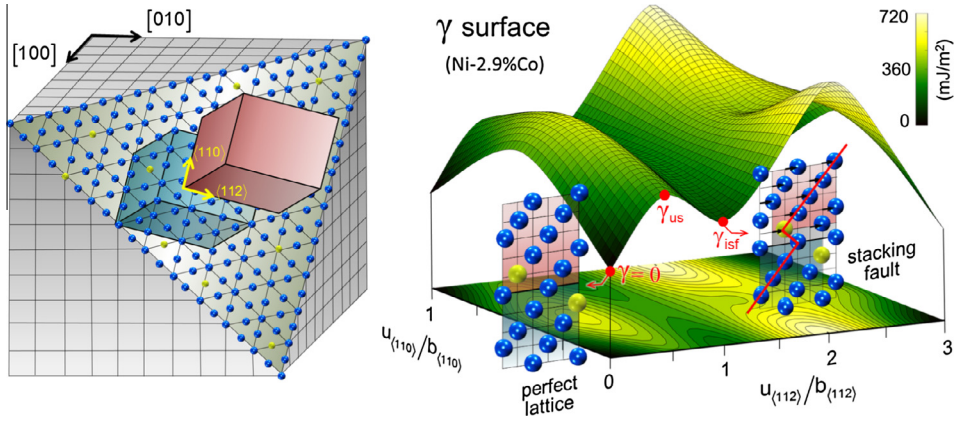

Fig. 6. The γ surface of Ni-2.9%Co alloy (blue atom → Ni, lime green atom → Co) [48].

so, the magnitudes of γ_{us} corresponding to various slip-CTB reactions (in a Ni-2.9%Co alloy as an example material [48]) are computed utilizing an embedded atom method pair-potential [60]. We provide a theoretical framework to incorporate these γ_{us} levels, representing crack-emitted slip subjected to encounters with a CTB, into fatigue.

As discussed earlier, the crack-emitted slip undergoes unique transfer mechanism at the coherent interface. Utilizing atomic scale calculations, we unravel the correlation among the number of incident slip (n_{slip}), the reaction-specific γ_{us} and the magnitude of residual Burgers vectors, $\vec{b}_r$. The data on Ni-2.9%Co material from [48] are presented in Fig. 7. As the oncoming slip continues to impinge on the CTB, the γ_{us} evolves non-linearly from a bulk level (γ_{us}^{bulk}) to saturated magnitudes (γ_{us}^{sat}) for individual interactions. The area under the entire γ surface is also known as the so-called misfit energy, E_{misfit}, which represents the total energy expenditure to be overcome in order for slip to occur. We utilize this concept along with the elastic interaction energy between an incident slip and the residual slip to establish a work-energy balance (to be discussed in next section).

For the fatigue crack growth problem, important strategies could be devised from the computed correlation and the associates magnitudes of the variables (n_{slip}, b_r and γ_{us}). From a non-continuum perspective, a prevalence of twin boundaries in the microstructure would be manifested as a substantial increase in the overall Peierls energy landscape. Thus, the average Peierls energy barrier would be strongly dictated by specific strain transmission outcome. For an advancing crack, a higher magnitude of driving force would be required to sustain adequate dislocation emission. For example, higher magnitudes of γ_{us} means a greater degree of shielding effects to the approaching slip and the crack in the long run. A reduced γ_{us} would render the to-and-fro slip glide past the interface relatively easier, thus promoting the reversibility of overall slip trajectories. In order to incorporate these considerations into a crack growth formalism, one ought to convert the maximum values of γ_{us} (i.e. γ_{us}^{sat}) values into the corresponding mesoscale frictional stresses.

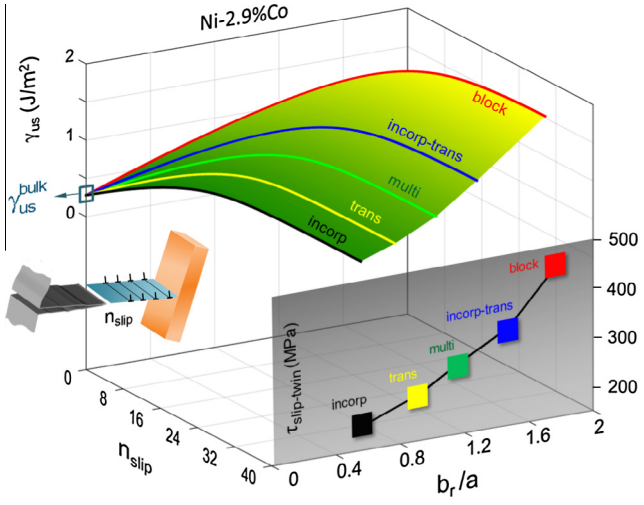

Fig. 7. Evolution of slip energy barrier (γ_{us}) from bulk to saturation for various transfer mechanisms (note that a zero b_r case represents cross-slip). Corresponding frictional stresses at saturation [48].

2.3. The important role of lattice friction stress

The lattice friction stress (also known as the Peierls stress) represents the dislocation nucleation/glide resistance [61,62]. This parameter has remained a crucial factor in signifying the degree of shielding to the crack growth [63–65]. Some early works pioneered its use in setting the crack growth threshold condition [66]. The threshold was dictated by the criterion that a crack would start advancing if the frictional impedance at the cracktip is exceeded by means of external driving forces. The modification from the intrinsic (i.e. representing the free glide) level to that under influence of grain boundaries in the fatigue context was explored by Tanaka, Navarro and their co-workers [64,67]. One consequence on the modeling endeavors of such assumption was that an increased friction was predicted to be beneficial towards fatigue resistance. In order to establish the role of various slip transfer mechanisms on fatigue, one ought to extract the corresponding barrier stress.

The necessary theoretical framework for predicting the friction stress has been well documented in the literature [62,68,69]. Peierls and Nabarro [61,70] have originally laid the groundwork for using the periodic energy-displacement as the primary input to predict the associated friction stress. In their original treatment, sinusoidal relationship was assumed on an ad hoc basis. It is well established today that the area underneath whole spectrum of the γ surface (as represented by the γ_{us} as the peak energy) constitutes the total atomistic energy expenditure for slip movement.

When a newly approaching slip is about to intercept the boundary, it ought to overcome two energy contributions: (a) the misfit energy, $E_{misfit} = E_{misfit}(\gamma_{us})$ which is the energy cost for shearing discrete lattice (i.e. the total area underneath the γ surface surface) and (b) the residual (elastic) energy, $E_{residual} = E_{residual}(b_r)$ which represent the elastic interaction between incident and the residual

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slip. Thus, the required applied stress $\tau_{slip\text{-}twin}$ to move the dislocation towards the boundary by ∂d can be derived from the work-energy balance as in Eq. (1) [48].

$$\underbrace{b_{incident}\tau_{slip\text{-}twin}\partial d}_{\text{applied work}} = \underbrace{\partial E_{misfit} + \partial E_{residual}}_{\text{total energy expense}} \quad (1)$$

Fig. 8 illustrates the above considerations. To generalize Eq. (1) for any interception mechanism, let us consider the net $\vec{b}_r$ to be consisting of component $(\vec{b}_r)_i$ located at r_i ($i = 1, 2, 3\ldots$). Upon mathematical manipulation, we have the following Eq. (2) for the final expression for the $\tau_{slip\text{-}twin}$.

$$\tau_{slip\text{-}twin} = max\left\{\frac{1}{b_{incident}}\frac{\partial E_{misfit}(\gamma_{us}^{sat})}{\partial d}\right\} + \frac{1}{db_{incident}}\sum_i \frac{\mu(b_r)_i^2}{4\pi}\ln\left(\frac{D}{r_i}\right) \quad (2)$$

where D is the size of the crystal (i.e. the grain diameter); μ the shear modulus; x position of dislocation. The D/r_i ratios are taken to be constant (1/500), given the fact that such a value amounts to the classical expression [62]: $\sum_i \frac{\mu(b_r)_i^2}{2}$. It is noteworthy here that positions of the residual slip (with respect to the original reaction) with increased incidence differ from case to case. In case of any locations thereof, the proper r_i values should be chosen reflecting the positions of the individual components of the net residual slip. Using Eq. (2), the $\tau_{slip\text{-}twin}$ values for various slip transfer mechanisms are predicted as listed in Fig. 7. Physically, the stress $\tau_{slip\text{-}twin}$ means the combined contribution of the Peierls stress and the elastic interaction stress (to be overcome) between the incident and the residual slip. In Eq. (2), the interplay between a partial dislocation connected by a stacking fault and the boundary is reflected by the captured γ_{us} magnitudes. This is attributed to the fact that the γ_{us} values are calculated by tracing the potential energy differential of a selected group of "tracing" atoms [23,48] as a dissociated dislocation with an extended core (i.e. with a stacking fault in-between) approaches the tracing atoms.

We point out here that in pure fcc materials the intrinsic lattice resistance is believed to be significantly low. This fact is experimentally indicated by small critical resolved shear stress values in single crystals of fcc metals (e.g. Ni, Cu and Al having 9–13.5 MPa [71,72], 2.1–3.2 MPa [73,74] and 0.78–1.3 MPa [75,76] respectively). However, the widespread presence of twin boundaries has demonstrably increased the average Peierls energy peaks (as reflected in terms of enhanced γ_{us} at the interface), thus resulting in a much larger $\tau_{slip\text{-}twin}$ (Fig. 7).

The impact of the aforementioned $\tau_{slip\text{-}twin}$ model can be understood by its considerable potential for extension towards any grain boundary type. The requisite input could be obtained from similar atomistic analysis. The details are expected to differ; however, the fundamental methodology would be essentially similar [56]. For example, in the earlier literature [77,78], the energy barrier γ_{us} for different boundary types are studied extensively and utilized in a crack nucleation modeling framework. For the twin boundary related fatigue crack propagation problem, next we configure a dislocation mechanics based framework, utilizing the frictional stress as a vital constituent, to solve for damage metrics.

3. Modeling fatigue crack advancement by means of slip irreversibility

Simulation-wise, nano-materials (with a grain size on the order of 10 nm) are found to undergo cyclic cracking due to void formation at and/or around triple joints [79–81]. Some other researchers also modeled [82,83] the single crystal orientation dependence on the type of damage mechanisms. It is now well known experimentally that the slip irreversibility at the crack constitutes the most generic physical process that drives the fatigue damage propagation [84]. In the early literature, a number of theoretical undertakings attempted to address the cracking problem on the basis irreversible of plastic flow [21,22,85]. The principal assumption therein is that irreversible slip at the cracktip gives rise to a differential between the forward and reverse

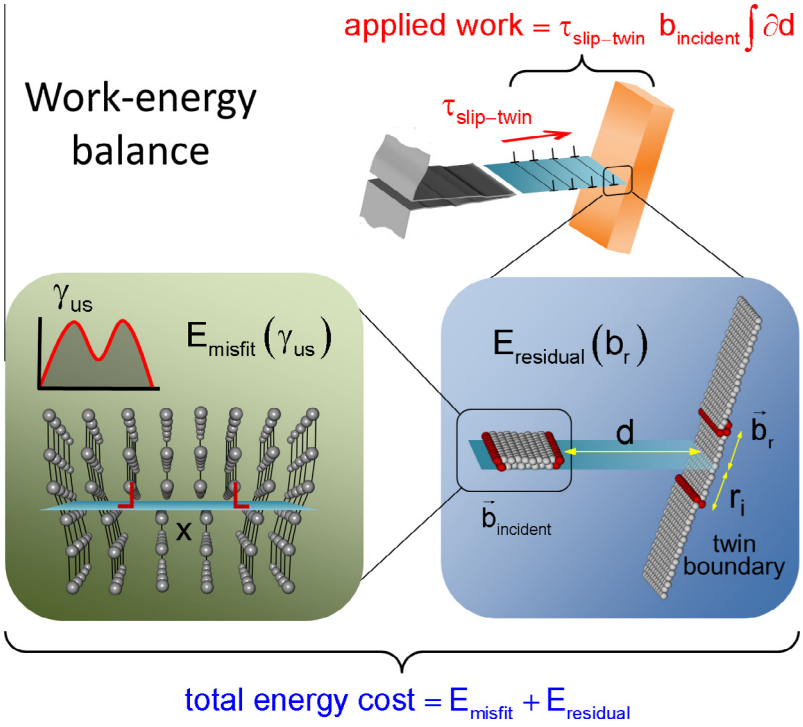

Fig. 8. The total energy expenditure in order for an incident slip, $\vec{b}_{incident}$, to overcome: E_{misfit} and $E_{residual}$.

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displacements ($u_{forward}$ and $u_{reverse}$ respectively) [85]. Considering the discrete nature of slip, the trajectories of individual slip can also be quantified [22,86,87] where a series of mathematical dislocations are emitted from the crack. They return to the tip on reversing the load. The crack growth criterion is established as a minimum of one residual Burgers vector left at the cracktip on each cycle. Building on these modeling breakthroughs, the concepts of interface-affected $\tau_{slip\text{-}twin}$, as outlined previously, could be incorporated therein to study the influence of CTB on the da/dN behaviors as we discuss below.

Fig. 9 illustrates the current concept of predicting da/dN on the basis of irreversible slip trajectories now informed by the specific nature of the slip-boundary interactions. The fundamental idea is the crack emits n_{slip} number of slip during loading, which intercepts the twin in a forward and reverse manner on loading/unloading [23]. The cracktip thus displaces by an amount, $u_{forward} = f(x_i^f, \tau_{Peierls}^f, t)$ where x_i^f the slip positions during forward loading, $\tau_{Peierls}^f$ the frictional stress (either free or boundary-induced glide, whichever is appropriate) for forward flow, and t twin lamellar thickness (or inter-twin spacing) [23]. On unloading, slip starts reverting back to the cracktip (followed by elastic relaxation) during which either of the two following possible scenarios can transpire. Slip of opposite sign (designated "−ve") can emit during the load reversal and thus annihilate the returning "+ve" slip. Another possibility is that no −ve slip nucleates and +ve slip returns. In any case, the cracktip displacement is now, $u_{reverse} = f(x_i^r, \tau_{Peierls}^r, t)$, where the x_i^r is reverse slip positions and $\tau_{Peierls}^r$ friction stress during reverse flow. The terms $u_{forward}$ and $u_{reverse}$ are obtained as follows [25]:

$$du = \frac{1}{2\mu}\int \tau \partial x \tag{3}$$

Eq. (3) represents the generic expression for the cracktip displacement. Considering the discrete nature of slip, we derive the forward and reverse displacements as in Eqs. (4) and (5).

$$u_{forward} = \frac{1}{2\mu}\sum_{i}^{n_{slip}} x_i^f \tau_i^f \tag{4}$$

$$u_{forward} = \frac{1}{2\mu}\sum_{i}^{n_{slip}} x_i^r \tau_i^r \tag{5}$$

At any stage of loading, the shear stress components acting on the i-th dislocation can be written as, $\tau_i = \tau_{applied} - \tau_{image} - \tau_{pile\text{-}up}$ [86], which when equal to free glide $\tau_{Peierls}$ (or $\tau_{slip\text{-}twin}$ at the boundary) can be used to solve for x_i^f and x_i^r. The force balance is established among the applied, image and pile-up stresses. It should be noted that the frictional stresses for forward/reverse cases are distinguished in view of the fact that residual slip may create a considerable differential thereof. This formalism could be applied for mode I, II and III cracks considering either edge or screw type dislocations. The dislocation positions to be utilized in computing displacements $u_{forward}$ and $u_{reverse}$ are obtained from the force balance [25,88]. The acting shear stress terms are balanced against the friction stress as in Eq. (6).

$$\underbrace{\frac{K}{\sqrt{2\pi x_i}}}_{applied} - \underbrace{\frac{A}{2x_i}}_{image} \underbrace{- A\sum_{j\neq i}^{j=n_{slip}} \sqrt{\left(\frac{x_j}{x_i}\right)}\frac{1}{x_j - x_i}}_{pile\text{-}up} - \tau_{Peierls} = 0 \quad (i = 1,2,3\ldots n_{slip}) \tag{6}$$

where A is $\mu b/2\pi(1-\nu)$ and $\mu b/2\pi$ for edge and screw dislocations respectively (ν is Poisson's ratio). Eq. (6) is numerically solved for the all the slip at a given instance of loading (i.e. a particular value of the applied stress intensity factor, K). Then, finally da/dN is computed as follows:

$$\frac{da}{dN} = u_{forward} - u_{reverse} \tag{7}$$

Following the aforementioned methodology, in Fig. 10, the da/dN for a stage I crack is predicted (using frictional stresses corresponding to slip transmission case in pure Ni, as an example [25]). The computed dislocation positions at K_{max} and K_{min} are shown when the crack is far from the twin boundary and also when very close to the twin boundary. The model is able to capture the retardation of the crack at the interface. The ΔK corresponding to the minimum da/dN (i.e. equal to one Burgers vector cracktip extension) can be deemed as the effective threshold, $\Delta K_{th,eff}$, an important metric representing inherent cracking resistance [89]. This predicted metric represents the intrinsic cracking resistance as induced by a coherent twin boundary for particular twin lamellar thickness (35 nm).

Based on a very similar modeling approach, the experimental threshold behaviors for the coarse- and fine-twinned Ni-2.9%Co alloys is predicted [11] (considering cross-slip at the twin boundary) as shown in Fig. 11. The colored bands represent the modeled threshold values accomplished via varying the initial dislocation density between the cracktip and the twin boundary (starting from an initial value of $10^{12}/cm^2$), twin lamellar thickness (t) and inter-twin spacings (ranging from 25 nm to 55 nm). The

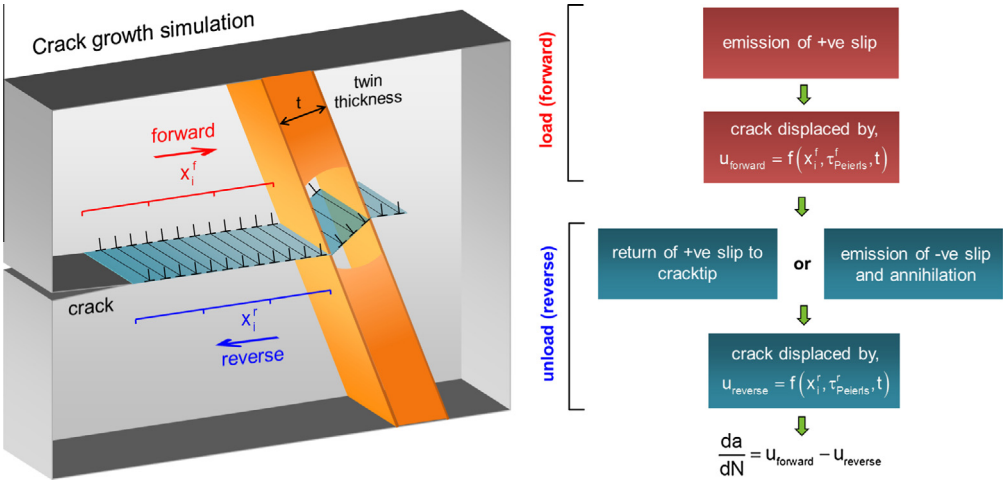

Fig. 9. Crack progression as a result of differential between forward and reverse slip positions influenced by coherent twin boundaries [24,25].

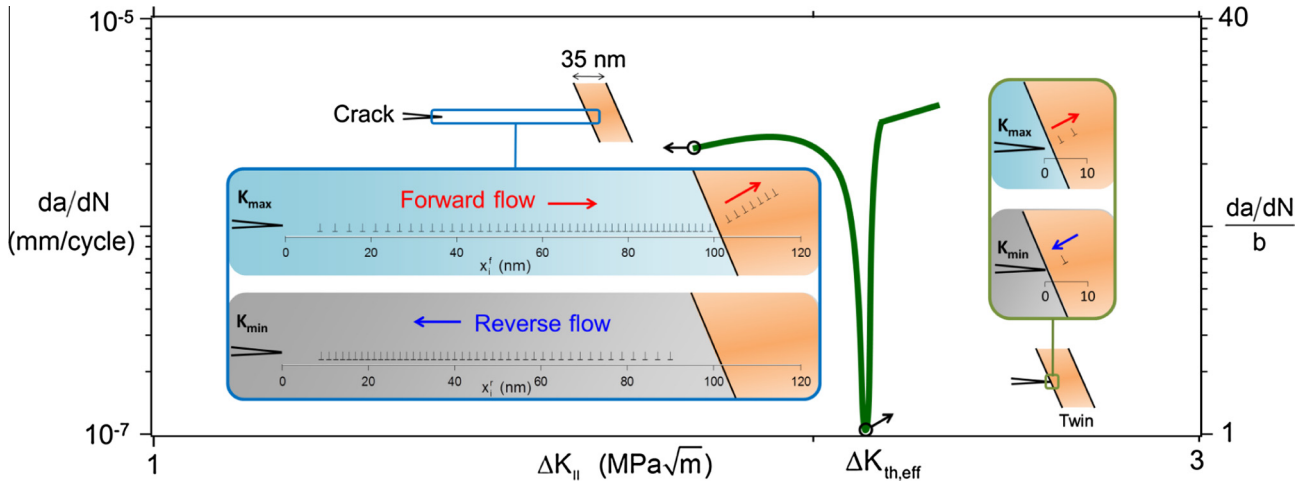

Fig. 10. Positions of dislocations during a stage I crack growth (simulated). The ΔK corresponding to a da/dN equal to one Burgers vector (1b) constitutes the so-called microstructural ΔK_{th} for a coherent twin boundary [25].

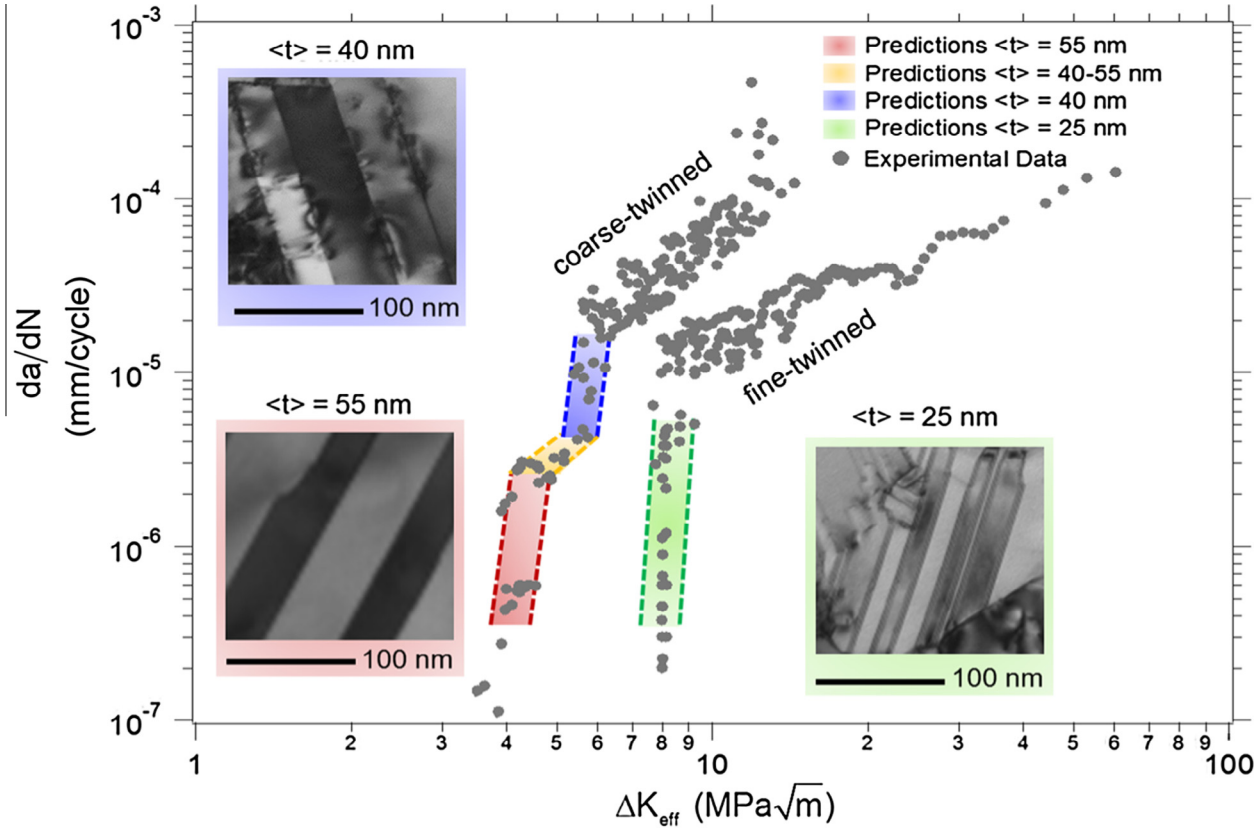

Fig. 11. Prediction of experimental threshold behaviors of coarse-twinned (due to heat treatment) and fine-twinned NiCo alloy [11].

good agreement between the theory and the experiment is achieved. Most importantly, the model input considered as the mechanistic in nature as discussed throughout the entire paper. The current model can be employed to study the microstructure-independent stage II growth regime as well [23]. The condition is to allow a considerably large degree of slip emission by increasing the driving force i.e. ΔK. In such a case, due to high pileup stress, the interface would offer little resistance, thus giving rise to the post-threshold behaviors.

The most significant impact can be deemed as the elimination of a significant number of adjustable parameters in theorizing fatigue by including a mechanistic basis. Microscopic damage processes are considered to ultimately arrive at macroscale comparable with experiments. Although certain approximations related to continuum fields of dislocations are adopted, further refinement in this regard remains a promising future endeavor.

4. Summary and conclusions

On the whole, we have discussed the improved fatigue cracking behaviors of nano-twinned materials compared to conventional materials as recently noted in the literature. The modeling strategies to solve coherent interface-affected fatigue crack growth problem are outlined. Particularly, the importance of considering the

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slip transfer mechanisms at the interfaces (as emitted by the crack) is emphasized. A step-by-step formalism to extract the associated slip energy barriers for individual strain transmission mechanisms is outlined and the importance thereof is discussed. The modeling approach involves conversion of fault energetics into corresponding friction stresses. In addition to the current problem in hand, we have asserted that such methodology holds considerable promise for addressing any other types of grain boundaries as well. For example, there exists literature listing computed γ_{us} for a variety of interface types. The fault energetics remains to be used in such a fatigue model to provide the damage metrics for a material rife with the respective boundaries. The model promotes a generic framework to incorporate the parameters such as $\vec{b}_r$, γ_{us} and $\tau_{Peierls}$, t, to represent the exact nature of material microstructure (in terms of interface type and distribution). Thus, such knowledge will be particularly invaluable, in that one can readily estimate the trend in the damage resistance for a given polycrystalline material with a prevalence of certain interface types. In addition, the adopted atomistic approach suggests future avenues of theorizing near-tip nano-scale damage mechanism in other classes of materials (e.g. transforming alloys [90,91]) although the details of analyses may differ.

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References

[1] R. Gu, A. Ngan, Dislocation arrangement in small crystal volumes determines power-law size dependence of yield strength, J. Mech. Phys. Solids 61 (2013) 1531–1542.
[2] K. Kumar, H. Van Swygenhoven, S. Suresh, Mechanical behavior of nanocrystalline metals and alloys, Acta Mater. 51 (2003) 5743–5774.
[3] H. Gleiter, Nanostructured materials: basic concepts and microstructure, Acta Mater. 48 (2000) 1–29.
[4] M.A. Meyers, A. Mishra, D.J. Benson, Mechanical properties of nanocrystalline materials, Prog. Mater Sci. 51 (2006) 427–556.
[5] R.A. Andrievski, Nanostructures under extremes, Uspekhi Fizicheskikh Nauk. 184 (2014) 1017–1032.
[6] A. Pineau, A.A. Benzerga, T. Pardoen, Failure of metals III. Fracture and fatigue of nanostructured metallic materials, Acta Mater. (2015).
[7] K. Lu, L. Lu, S. Suresh, Strengthening materials by engineering coherent internal boundaries at the nanoscale, Science 324 (2009) 349–352.
[8] L. Lu, X. Chen, X. Huang, K. Lu, Revealing the maximum strength in nanotwinned copper, Science 323 (2009) 607–610.
[9] A. Singh, L. Tang, M. Dao, L. Lu, S. Suresh, Fracture toughness and fatigue crack growth characteristics of nanotwinned copper, Acta Mater. 59 (2011) 2437–2446.
[10] M.D. Sangid, G.J. Pataky, H. Sehitoglu, R.G. Rateick, T. Niendorf, H.J. Maier, Superior fatigue crack growth resistance, irreversibility, and fatigue crack growth–microstructure relationship of nanocrystalline alloys, Acta Mater. 59 (2011) 7340–7355.
[11] S. Alkan, P. Chowdhury, H. Sehitoglu, R.G. Rateick, H.J. Maier, Role of nanotwins on fatigue crack growth resistance – experiments and theory, Int. J. Fatigue 84 (2016) 28–39.
[12] T. Hanlon, E. Tabachnikova, S. Suresh, Fatigue behavior of nanocrystalline metals and alloys, Int. J. Fatigue 27 (2005) 1147–1158.
[13] B.L. Boyce, H.A. Padilla II, Anomalous fatigue behavior and fatigue-induced grain growth in nanocrystalline nickel alloys, Metall. Mater. Trans. A 42 (2011) 1793–1804.
[14] P. Cavaliere, Fatigue properties and crack behavior of ultra-fine and nanocrystalline pure metals, Int. J. Fatigue 31 (2009) 1476–1489.
[15] Y. Yang, B. Imasogie, G. Fan, P.K. Liaw, W. Soboyejo, Fatigue and fracture of a bulk nanocrystalline NiFe alloy, Metall. Mater. Trans. A 39 (2008) 1145–1156.
[16] J. Xie, X. Wu, Y. Hong, Shear bands at the fatigue crack tip of nanocrystalline nickel, Scripta Mater. 57 (2007) 5–8.
[17] L. Guo, T. Kitamura, Y. Yan, T. Sumigawa, K. Huang, Fracture mechanics investigation on crack propagation in the nano-multilayered materials, Int. J. Solids Struct. 64 (2015) 208–220.
[18] H. Mughrabi, Fatigue, an everlasting materials problem-still en vogue, Procedia Eng. 2 (2010) 3–26.
[19] H. Mughrabi, Cyclic slip irreversibilities and the evolution of fatigue damage, Metall. Mater. Trans. B 40 (2009) 431–453.
[20] D. Gross, K. Nygren, G. Pataky, J. Kacher, H. Sehitoglu, I. Robertson, The evolved microstructure ahead of an arrested fatigue crack in Haynes 230, Acta Mater. 61 (2013) 5768–5778.
[21] R. Pippan, H. Weinhandl, Discrete dislocation modelling of near threshold fatigue crack propagation, Int. J. Fatigue 32 (2010) 1503–1510.
[22] A.J. Wilkinson, S.G. Roberts, P.B. Hirsch, Modelling the threshold conditions for propagation of stage I fatigue cracks, Acta Mater. 46 (1998) 379–390.
[23] P.B. Chowdhury, H. Sehitoglu, R.G. Rateick, H.J. Maier, Modeling fatigue crack growth resistance of nanocrystalline alloys, Acta Mater. 61 (2013) 2531–2547.
[24] P.B. Chowdhury, H. Sehitoglu, R.G. Rateick, Predicting fatigue resistance of nano-twinned materials: Part I-Role of cyclic slip irreversibility and Peierls stress, Int. J. Fatigue 68 (2014) 277–291.
[25] P.B. Chowdhury, H. Sehitoglu, R.G. Rateick, Predicting fatigue resistance of nano-twinned materials: Part II–Effective threshold stress intensity factor range, Int. J. Fatigue 68 (2014) 292–301.
[26] J.R. Rice, R. Thomson, Ductile versus brittle behaviour of crystals, Phil. Mag. 29 (1974) 73–97.
[27] J. Weertman, Rate of growth of fatigue cracks calculated from the theory of infinitesimal dislocations distributed on a plane, Int. J. Fract. Mech. 2 (1966) 460–467.
[28] J. Rice, The mechanics of crack tip deformation and extension by fatigue crack propagation, ASTM, ASTM STP (1966) 415.
[29] V. Deshpande, A. Needleman, E. Van der Giessen, A discrete dislocation analysis of near-threshold fatigue crack growth, Acta Mater. 49 (2001) 3189–3203.
[30] R.J. Asaro, Y. Kulkarni, Are rate sensitivity and strength effected by cross-slip in nano-twinned fcc metals, Scripta Mater. 58 (2008) 389–392.
[31] C. Deng, F. Sansoz, Fundamental differences in the plasticity of periodically twinned nanowires in Au, Ag, Al, Cu, Pb and Ni, Acta Mater. 57 (2009) 6090–6101.
[32] J. Kacher, B. Eftink, B. Cui, I. Robertson, Dislocation interactions with grain boundaries, Curr. Opin. Solid State Mater. Sci. 18 (2014) 227–243.
[33] S. Mahajan, G. Chin, Twin-slip, twin-twin and slip-twin interactions in Co-8 wt.% Fe alloy single crystals, Acta Metall. 21 (1973) 173–179.
[34] Z. Wu, Y. Zhang, D. Srolovitz, Dislocation–twin interaction mechanisms for ultrahigh strength and ductility in nanotwinned metals, Acta Mater. 57 (2009) 4508–4518.
[35] T. Zhu, H. Gao, Plastic deformation mechanism in nanotwinned metals: an insight from molecular dynamics and mechanistic modeling, Scripta Mater. 66 (2012) 843–848.
[36] T. Lee, I. Robertson, H. Birnbaum, AnIn Situ transmission electron microscope deformation study of the slip transfer mechanisms in metals, Metall. Trans. A 21 (1990) 2437–2447.
[37] M. Dewald, W. Curtin, Multiscale modeling of dislocation/grain-boundary interactions: III. 60 dislocations impinging on Σ3, Σ9 and Σ11 tilt boundaries in Al, Modell. Simul. Mater. Sci. Eng. 19 (2011) 055002.
[38] M. Dewald, W. Curtin, Multiscale modelling of dislocation/grain-boundary interactions: I. Edge dislocations impinging on Σ11 (1 1 3) tilt boundary in Al, Modell. Simul. Mater. Sci. Eng. 15 (2007) S193.
[39] Z.-H. Jin, P. Gumbsch, E. Ma, K. Albe, K. Lu, H. Hahn, et al., The interaction mechanism of screw dislocations with coherent twin boundaries in different face-centred cubic metals, Scripta Mater. 54 (2006) 1163–1168.
[40] P. Müllner, C. Solenthaler, On the effect of deformation twinning on defect densities, Mater. Sci. Eng., A 230 (1997) 107–115.
[41] M. Prasad, M. Reiterer, K. Kumar, Microstructure and mechanical behavior of an as-drawn MP35N alloy wire, Mater. Sci. Eng., A 610 (2014) 326–337.
[42] T. Zhu, J. Li, A. Samanta, H.G. Kim, S. Suresh, Interfacial plasticity governs strain rate sensitivity and ductility in nanostructured metals, Proc. Natl. Acad. Sci. 104 (2007) 3031–3036.
[43] B. Miller, J. Fenske, D. Su, C.-M. Li, L. Dougherty, I.M. Robertson, Grain boundary responses to local and applied stress: an in situ TEM deformation study, MRS proceedings, Cambridge Univ Press, 2006. p. 0976-EE02-01.
[44] J. Evans, Heterogeneous shear of a twin boundary in α-brass, Scr. Metall. 8 (1974) 1099–1103.
[45] Z.-H. Jin, P. Gumbsch, K. Albe, E. Ma, K. Lu, H. Gleiter, et al., Interactions between non-screw lattice dislocations and coherent twin boundaries in face-centered cubic metals, Acta Mater. 56 (2008) 1126–1135.
[46] H. Karnthaler, The study of glide on 001 planes in fcc metals deformed at room temperature, Philos. Mag. A 38 (1978) 141–156.
[47] J. Wang, H. Huang, Novel deformation mechanism of twinned nanowires, Appl. Phys. Lett. 88 (2006) 203112.
[48] P. Chowdhury, H. Sehitoglu, H. Maier, R. Rateick, Strength prediction in NiCo alloys – the role of composition and nanotwins, Int. J. Plast (2015).
[49] A. Pineau, Crossing grain boundaries in metals by slip bands, cleavage and fatigue cracks, Philos. Trans. Royal Soc. London A: Math., Phys. Eng. Sci. 373 (2015) 20140131.
[50] W. Schaef, M. Marx, H. Vehoff, A. Heckl, P. Randelzhofer, A 3-D view on the mechanisms of short fatigue cracks interacting with grain boundaries, Acta Mater. 59 (2011) 1849–1861.
[51] W.Z. Abuzaid, M.D. Sangid, J.D. Carroll, H. Sehitoglu, J. Lambros, Slip transfer and plastic strain accumulation across grain boundaries in Hastelloy X, J. Mech. Phys. Solids 60 (2012) 1201–1220.

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[52] V. Vitek, Intrinsic stacking faults in body-centred cubic crystals, Phil. Mag. 18 (1968) 773–786.
[53] P. Chowdhury, H. Sehitoglu, W. Abuzaid, H. Maier, Mechanical response of low stacking fault energy Co–Ni alloys–Continuum, mesoscopic and atomic level treatments, Int. J. Plast 71 (2015) 32–61.
[54] A. McEvily, R. Boettner, On fatigue crack propagation in FCC metals, Acta Metall. 11 (1963) 725–743.
[55] A.J. McEvily, W. Illg, The rate of fatigue-crack propagation in two aluminum alloys, National Advisory Committee for Aeronautics, 1958.
[56] L. Wang, J. Zhou, S. Zhang, H. Liu, S. Dong, Effect of dislocation–GB interactions on crack blunting in nanocrystalline materials, Mater. Sci. Eng., A 592 (2014) 128–135.
[57] J.R. Rice, Dislocation nucleation from a crack tip: an analysis based on the Peierls concept, J. Mech. Phys. Solids 40 (1992) 239–271.
[58] J. Rice, G. Beltz, Y. Sun, Peierls framework for dislocation nucleation from a crack tip, Topics in fracture and fatigue, Springer, 1992, pp. 1–58.
[59] E. Tadmor, S. Hai, A Peierls criterion for the onset of deformation twinning at a crack tip, J. Mech. Phys. Solids 51 (2003) 765–793.
[60] X. Zhou, R. Johnson, H. Wadley, Misfit-energy-increasing dislocations in vapor-deposited CoFe/NiFe multilayers, Phys. Rev. B 69 (2004) 144113.
[61] R. Peierls, The size of a dislocation, Proc. Phys. Soc. 52 (1940) 34.
[62] J.P. Hirth, J. Lothe. Theory of dislocations. 1982.
[63] K. Tanaka, Y. Nakai, M. Yamashita, Fatigue growth threshold of small cracks, Int. J. Fract. 17 (1981) 519–533.
[64] A. Navarro, E. De Los Rios, Short and long fatigue crack growth: a unified model, Philos. Mag. A 57 (1988) 15–36.
[65] S. Dong, J. Zhou, D. Hui, L. Wang, Fracture toughness of nanocrystalline metal matrix composites reinforced by aligned carbon nanotubes, J. Mater. Res. 1–10 (2015).
[66] W. Yu, W. Gerberich, On the controlling parameters for fatigue-crack threshold at low homologous temperatures, Scr. Metall. 17 (1983) 105–110.
[67] S. Taira, K. Tanaka, Y. Nakai, A model of crack-tip slip band blocked by grain boundary, Mech. Res. Commun. 5 (1978) 375–381.
[68] B. Joos, Q. Ren, M. Duesbery, Peierls-Nabarro model of dislocations in silicon with generalized stacking-fault restoring forces, Phys. Rev. B 50 (1994) 5890.
[69] G. Schoeck, The Peierls model: progress and limitations, Mater. Sci. Eng., A 400 (2005) 7–17.
[70] F. Nabarro, Dislocations in a simple cubic lattice, Proc. Phys. Soc. 59 (1947) 256.
[71] G. Gottstein, U. Kocks, Dynamic recrystallization and dynamic recovery in <111> single crystals of nickel and copper, Acta Metall. 31 (1983) 175–188.
[72] P. Haasen, Plastic deformation of nickel single crystals at low temperatures, Phil. Mag. 3 (1958) 384–418.
[73] M. Adams, A. Cottrell, CXXXI. Effect of temperature on the flow stress of work-hardened copper crystals, London, Edinburgh, Dublin Philos. Mag. J. Sci. 46 (1955) 1187–1193.
[74] T. Blewitt, Deformation of copper single crystals at 300 K and 78 K, Phys. Rev. 91 (1953) 1115.
[75] A. Cottrell, R. Stokes, Effects of temperature on the plastic properties of aluminium crystals, Proc. Royal Soc. London A: Math., Phys. Eng. Sci., Royal Soc., 1955, pp. 17–34.
[76] S. Howe, B. Liebmann, K. Lücke, High temperature deformation of aluminum single crystals, Acta Metall. 9 (1961) 625–631.
[77] M.D. Sangid, H.J. Maier, H. Sehitoglu, An energy-based microstructure model to account for fatigue scatter in polycrystals, J. Mech. Phys. Solids 59 (2011) 595–609.
[78] M.D. Sangid, T. Ezaz, H. Sehitoglu, I.M. Robertson, Energy of slip transmission and nucleation at grain boundaries, Acta Mater. 59 (2011) 283–296.
[79] D. Farkas, M. Willemann, B. Hyde, Atomistic mechanisms of fatigue in nanocrystalline metals, Phys. Rev. Lett. 94 (2005) 165502.
[80] G. Potirniche, M. Horstemeyer, P. Gullett, B. Jelinek, Atomistic modelling of fatigue crack growth and dislocation structuring in FCC crystals, Proc of the royal society of London a: mathematical, physical and engineering sciences, The Royal Society, 2006, pp. 3707–3731.
[81] K. Nishimura, N. Miyazaki, Molecular dynamics simulation of crack growth under cyclic loading, Comput. Mater. Sci. 31 (2004) 269–278.
[82] C.L. Rountree, R.K. Kalia, E. Lidorikis, A. Nakano, L. Van Brutzel, P. Vashishta, Atomistic aspects of crack propagation in brittle materials: multimillion atom molecular dynamics simulations, Annu. Rev. Mater. Res. 32 (2002) 377–400.
[83] V. Iacobellis, K. Behdinan, Bridging cell multiscale modeling of fatigue crack growth in fcc crystals, Int. J. Numer. Meth. Eng. (2015).
[84] G.J. Pataky, H. Sehitoglu, H.J. Maier, High temperature fatigue crack growth of Haynes 230, Mater. Charact. 75 (2013) 69–78.
[85] X. Wu, A. Koul, A. Krausz, A transgranular fatigue crack growth model based on restricted slip reversibility, Metall. Trans. A 24 (1993) 1373–1380.
[86] R. Pippan, Dislocation emission and fatigue crack growth threshold, Acta Metall. Mater. 39 (1991) 255–262.
[87] R. Pippan, The condition for the cyclic plastic deformation of the crack tip: the influence of dislocation obstacles, Int. J. Fract. 58 (1992) 305–318.
[88] P. Chowdhury, Fatigue crack growth (FCG) modeling in the presence of nano-obstacles, University of Illinois at Urbana-Champaign, 2011.
[89] B. Li, L. Rosa, Prediction models of intrinsic fatigue threshold in metal alloys examined by experimental data, Int. J. Fatigue (2015).
[90] P. Chowdhury, G. Ren, H. Sehitoglu, NiTi superelasticity via atomistic simulations, Philos. Mag. Lett. (2015).
[91] P. Chowdhury, L. Patriarca, G. Ren, H. Sehitoglu, Molecular dynamics modeling of NiTi superelasticity in presence of nanoprecipitates, Int. J. Plast. (2016).

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