Modeling fatigue crack growth resistance of nanocrystalline alloys

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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.

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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 toward 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 \( \Delta K_{th} \) and, most significantly, the
near-threshold crack growth rate $da/dN$. 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 $\tau_0$ (i.e. the difficulty of plastic flow advancing past the obstacle, manifested as an elevation of the unstable fault energy $\gamma_{\text{uf}}$). $\gamma_{\text{uf}}$ 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 $da/dN$ 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 $s_0$ 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)
The dislocation gliding mechanism depends on the dislocation core properties. Glissile motion occurs by alternately rearranging atomic distortion that proceeds via successive tearing and forming of atomic bonds surrounding the core structure [33]. The driving shear stress for such motion scales with the activation energy barriers for the translational motion onto a close-packed slip plane. The energetics of dislocation translation lie in the relative motions of the core atoms. Alteration of the dislocation gliding condition, as influenced by nano-obstacles and the respective energetics, necessitates a non-continuum modeling framework. In that regard, molecular dynamics (MD) allows the capture and quantification of the physics of slipping at the atomistic length scale. MD simulates the time evolution of atomic nuclei (considered as classical Newtonian particles) by integrating their equations of motion [34]. The metallic bonding is modeled through a homogeneously distributed electron cloud functional and a pairwise interaction potential. A semi-empirical embedded atom method (EAM) formalism, curve fitted with experimental and/or ab initio material properties, employs such modeling to accurately describe the bonding energy landscape [35]. Utilizing MD simulations with an EAM potential Ezaz et al. [31] quantified the energetics of dislocation glide upon interaction with twins under monotonic conditions. In the literature some researchers [36–38] have employed MD-EAM methods to study massive cyclical slip emissions leading to nanovoid coalescence as the crack advancing mechanism in the presence of GBs. However, the physics of slip irreversibility accumulation, as the underlying incentive for crack tip plasticity, has not yet been explored.

In our approach we employ atomistic simulations to reveal the nature of slip–twin interaction under cyclical conditions, and the underlying fault energy barriers. Such a perspective reveals the exact role of CTBs as irreversibility-inducing microstructural elements as well as effective barriers to cyclic slip. Quantification of the cyclical slip–twin reaction energetics allows the calculation of ideal shear stresses for to and fro glide, as modified by the presence of CTBs and/or residual dislocations. We incorporate these atomistically extracted material properties in fracture mechanics-based formulations to simulate FCG undergoing large scale slip activities. The mechanics simulations employ cyclical irreversibility as the principal driving force of crack advancement in the presence of nanotwins. The combination of two different length scale methodologies is important, in that the continuum descriptions of FCG utilize input from the governing atomistic physics. Hence we obtain an in-depth understanding of FCG as influenced by nanotwins. Such an insight highlights the role of some critical characteristic dimensions associated with these nano-obstacles (e.g. twin lamellar thickness and twin to crack tip spacing) on the FCG metrics.

2. Methods

To develop a FCG methodology we employed both atomistic slip-twin and fracture mechanics-based crack-tip
slip simulations. An open source software LAMMPS (large-scale atomic/molecular massively parallel simulator) [39] was used to perform the MD simulations. A semi-infinite discrete dislocation simulation set-up was then established using input from the MD results. The combination of these simulations provides a convenient conduit to explore some fundamental aspects of the mechanism of FCG.

For the MD simulations a nickel single crystal grain was constructed with the crystallographic orientation shown in the inset in Fig. 3. This grain contains a coherent twin of finite thickness. A stress concentrator (atom size void) placed in the matrix simulates a dislocation source. The whole system was energetically minimized, using the conjugate gradient (CG) algorithm [34]. This resulted in an energetically stable single nanotwinned grain. The CG algorithm iteratively solves atomic coordinates to reach the minimum energy of the system within a predefined convergence limit. An acceptance criterion adjusts the new atomic positions, conjugate to the previous ones that follow the direction of steepest descent on the potential energy curve. Moreover, enforcement of three-dimensional periodic boundary conditions on the supercell eliminates the effects of free surface energy, thereby simulating a system of bulk material. The supercell dimensions were configured such that the physical observables (e.g. temperature, pressure, kinetics and potential energy of the system) converged to system size independence. In view of the goals of the present work we conducted a number of MD simulations with varying source to twin distances as well as twin lamellar widths. Consequently, the supercell size was varied accordingly to give the optimally converged dimensions for each simulation, avoiding any artifacts of periodicity.

Cyclical shear was applied to the supercell under strain control conditions. A strain range of $e_{\text{max}} = 9.22\%$ (i.e. $R_e = 0.48$) was selected to facilitate slip nucleation from the void (slip source), and sufficient plastic flow to provide to and fro glissile motion across the twin. The MD simulations were run for a duration of several hundred picoseconds. Such a timescale is inherent in MD simulations, limited by the computational capability. Our investigation required the calculation of parameters such as the local plastic shear strain due to slip, the Burgers vectors thereof, and the energetics of slip–twin reactions. These parameters are unaffected by the high deformation rates arising from such a timescale. In order to conduct non-equilibrium MD simulations (i.e. evolution of the system under the imposed conditions) we employed an iso-baric–isothermal (NPT) ensemble along with a Nosé–Hoover thermostat algorithm. Hence, the total number of atoms $N$, the external pressure $P$, and the temperature $T$ (at 10 K) of the system were held constant. The dynamics of deformation proceeded utilizing the velocity Verlet algorithm as the time integrator. Atomistic snapshots at different time points were carefully analyzed using visual molecular dynamics (VMD) [40] and AtomEye configuration viewer [41]. These visualization tools, combined with in-house MATLAB programs, helped capture the details of slip–twin interactions (e.g. the conservation of Burgers vectors) and calculate fault energies, glide distance of slip, etc. Volume-averaged virial stress formulation, neglecting the kinetic energy contribution [42], was employed in order to quantitatively assess the stress–strain response of the system.

One essential part of our investigation was to calculate the energetics of complex cyclical slip–twin reactions, necessitating accurate descriptions of the atomic level energy landscape through EAM formulations [35]. A comparative study of EAM potentials available in the literature demonstrated that the Foiles and Hoyt potential [43] provides good agreement between the unstable fault energy $\gamma_{\text{inst}}$, the density functional theory (DFT) calculations (254 mJ m$^{-2}$), and the intrinsic stacking fault energy ($\gamma_{\text{int}}$) with the experimental finding (127 mJ m$^{-2}$). The interplanar potential energy profiling incorporating all of these parameters is termed the generalized stacking fault energy (GSFE) curve [44], as shown in Fig. 6. The GSFE represents the energy pathway to create the lattice distortion of a dislocation along the Burgers vector direction. A typical GSFE is calculated by sliding one crystalline half-space on top of another on the slip plane along the slip direction. We utilized the Foiles and Hoyt EAM potential to compute the modified GSFE, as influenced by local stresses during back and forth dislocation glide traversing the twin (to be discussed in detail later). For a more thorough description of the MD simulation procedures employed in the present work readers are referred to Ezaz et al. [31].

3. Results

3.1. Molecular dynamics simulations

Fig. 3 shows a typical MD-based cyclical shear stress–strain response of a nanotwinned grain with a dislocation

![Fig. 3. Cyclical stress–strain response of a nanotwinned grain with a dislocation source (not shown) in the matrix in the vicinity of the coherent twin boundary as obtained by MD simulations. The configuration above produces pure screw dislocations.](image-url)
source located in the matrix. Cyclical deformation is applied to the extent that it facilitates dislocation nucleation, and with a sufficient degree of slip to intersect the twin, located at a distance \(d\) from the source. The strain range for subsequent cyclical loading is set up such that to and fro dislocation motions occur across the width \(t\) of the twin. Separate MD simulations were carried out with varying finite twin lamellar widths and crack to twin spacings to study the influences of these dimensions. With a gradual increase in \(t\) or \(d\) the external loading needs to be increased in order for the slip to reach and traverse the entire width of the nanotwin. Consequently, a gradually greater number of dislocations nucleate with the increase in the applied load. The multitudes of dislocations undergo relatively more complex forms of interactions with the CTBs at larger \(t\) and/or \(d\). Nevertheless, we observed a generalized pattern of cyclical slip–twin interaction with simultaneous incorporation and transmission of slip for all cases of varying \(t\) and/or \(d\). Hence the fundamental similarities reside in the type of interaction and the introduction of irreversible slip activity in each cycle, irrespective of the number of incident dislocations. In the following section the cyclical slip–twin reaction involving only one incident dislocation (pure screw type) is described in detail for the case of smaller \(t\) and \(d\) (requiring a lower applied load).

As can be seen in Fig. 3, the stress–strain approaches a saturated response as the cyclical slip–twin interaction mechanism also achieves a recurrent steady-state. Since the MD simulations were performed on pristine crystals, and at high deformation rates, the stresses from the MD are high compared with the experimental stress–strain response. However, the dislocation reactions associated with the slip–twin interactions are unaffected, as verified by running simulations at different strain rates. Therefore, the cyclical stress–strain plots in Fig. 3 are interpreted only to obtain a quantitative estimation of the quasi-steady-state

![Fig. 4.](image-url)
response of the system under investigation. The next section describes a detailed study of the CTB–dislocation interactions to clarify the reaction type.

### 3.1.1. Cyclical slip–twin interactions

MD simulations revealed the exact nature of the steady-state cyclical slip–twin reactions. During forward loading, after elastic straining, a perfect screw dislocation of Burgers vector \( \frac{a}{2} [1 \bar{1} 0] \) nucleates from the source on the most favorable slip system with the maximum resolved shear stress. Immediately after emission the perfect dislocation dissociates into two Shockley partials (leading and trailing) separated by a ribbon of stacking fault (Eq. (1)).

\[
\frac{a}{2} [1 \bar{1} 0] \rightarrow \frac{a}{6} [2 \bar{1} 1] + \frac{a}{6} [1 \bar{2} \bar{1}] + \text{Stacking Fault}
\]  

Under continued application of forward shear loading the extended dislocation (with a leading and a trailing Shockley partial) glides towards the CTB (Fig. 4a). Being obstructed by the CTB, the two partials recombine and generate new screw dislocations at the site of incidence (Fig. 4b). The new dislocations similarly dissociate into Shockley partials. One of the new dislocations is incorporated into the CTB as twinning partials, and another (extended) is transmitted inside the twin (Fig. 4c). Eq. (2) summarizes this reaction. Transmitted partials \( \frac{a}{6} [2 \bar{1} 1] \) and \( \frac{a}{6} [1 \bar{1} 2] \) become \( \frac{a}{6} [2 \bar{1} 1] \) and \( \frac{a}{6} [1 \bar{2} \bar{1}] \), respectively.

\[
\frac{a}{6} [2 \bar{1} 1] \rightarrow \frac{a}{6} [2 \bar{1} 1] + \text{Stacking Fault}
\]
in the matrix frame. The total Burgers vector is then conserved on both sides of Eq. (2). Fig. 4d provides a double Thompson’s tetrahedron depiction of the forward slip–twin reaction.

With further unloading the twinning partials continue to glide in opposite directions, eventually causing twin migration by one atomic layer. The twin migration process may involve growth or shrinkage of the twin depending on the direction of motion of the participant twinning partials. The matrix Shockley partials continue gliding towards the source until a full dislocation (which also dissociates to become extended) of opposite sign nucleates from the source, meets with the returning one, and they annihilate each other. At the end of unloading another new negative dislocation (considering the original nucleated slip, at the beginning of forward loading, to be of positive type) nucleates and glides towards the twin, repeating the mechanism over subsequent cycles.

Table 1 summarizes the slip–twin reactions. Here \( b_s \), \( b_e \) and \( b_r \) refer to the screw, edge component, and residual dislocation on the CTB, respectively. In summary, the reaction process involves transmission of unobstructed slip past the CTB (designated outgoing), and incorporation of slip with \( b_r \) in the CTB. The full dislocations are of pure screw type (which dissociate into partials) for both the incident and outgoing systems. For all the active slip systems the resolved shear stress \( \tau_{ RSS} \) under global applied stress \( \tau \) is calculated using the formulation:

\[
\tau_{ RSS} = \sigma_{ij}m_i n_j
\]

In Eq. (4) \( \sigma_{ij} \) is the remote stress tensor, \( m_i \) the slip plane normal vector, and \( n_i \) the vector representing the slip direction. For our case the applied \( \sigma_{ij} \) is reduced to \( \tau_{13} \) (\( \tau \) in Fig. 3). As can be seen in Table 1, the magnitudes of the ratio of \( \tau_{ RSS} \) to \( \tau \), defined as the Schmid factor (SF), for the active slip systems are fairly high. The maximum SF is operative on the CTB, which facilitates the incorporation of glissile twinning partials. The next largest SF acting on the outgoing slip system inside the twin assists in the transmission of slip past the CTB. The analyses, as summarized in Table 1 and Fig. 4, concern forward flow of slip past the CTB. However, the reverse reaction is modified only in the form of enhanced resistance (due to the presence of twinning partials in close vicinity) at the CTB. The reverse incidence of slip upon the CTB results in similar interaction products from dislocations at the reaction site. For more complex cases involving a multitude of incident dislocations (at larger \( t \) and/or \( d \) with a higher applied load) the interaction type remains fundamentally identical, undergoing simultaneous incorporation and transmission of slip. The subsequent sections address quantification of the slip irreversibility and the origin of the discrepancy of forward vs. reverse slip resistance at the CTB.
3.1.2. Cylindrical slip irreversibilities

Fig. 5a shows a simple example of how irreversible plastic shear strain during cylindrical loading can be quantified, considering the case of a single incident dislocation (at smaller $t$ or $d$). Steady-state cylindrical slip–twin interaction involves the incidence of a dissociated full dislocation (scREW) on the CTB. The reaction results in the simultaneous incorporation and transmission of extended dislocations. The final locations of these dislocations are at positions c and e (partials) and d (extended full dislocation, shown as full for simplicity) at the end of forward loading. The partials at c and e contribute to migration of the twin by one atomic layer. During reverse flow the extended dislocation at position d is transmitted back into the crystal, again leaving new partials at c’ and e’, which repulse the partials at c and e. The returning crack-bound extended dislocation is annihilated by another incoming dislocation of opposite sign (negative) at location f. We calculated the ratio $p$ between the irreversible plastic shear strain $\gamma_{irr}$ and the total plastic shear strain $\gamma_{total}$ generated by dislocation glide over a cycle using Eq. (5). These $\gamma$ values represent shear strains due to dislocation glide as they appear in Eq. (5). Even though Fig. 5a shows the cyclical process involving only one incident dislocation, on gradually increasing $t$ and/or $d$ a number of dislocations will contribute to the overall irreversible phenomena in an identical manner. The parameter $p$ is then computed as a varying function of $t$ and $d$. Fig. 5b and c demonstrates the results.

$$p = \frac{\gamma_{irr}}{\gamma_{total}} = \frac{\gamma_{ce} + \gamma_{ce'} + \gamma_{at}}{\gamma_{ad} + \gamma_{db} + \gamma_{ce'} + \gamma_{bt}} \quad (5)$$

The trend for cyclical crack tip slip irreversibilities $p$, as calculated in Fig. 5b and c, tends to become independent of $t$ and $d$ at sufficiently large magnitudes. At lower values of $t$ and $d$ a relatively small number of dislocations are emitted from the source and traverse the entire thickness of the twin. Consequently, a shorter spacing between the source and the twin as well as thinner twins will expedite the return of source-bound positive slip, and at the same time preclude gliding of negative slip sufficiently farther away from the source. Thus the annihilation process (location $f$ in Fig. 5a) occurs in very close proximity to the source (as in the insets in Fig. 5b and c). As a result, the magnitude of $p$ is low in the small $t$ and/or $d$ regime, as calculated with Eq. (5). However, an increase in $t$ or $d$ necessitates a larger applied load in order for slip to occur and traverse the twin. This results in a gradually greater number of dislocation emissions. The involvement of multitudes of dislocations leads to an increase in the pile-up stress during both forward and reverse flow. This results in even greater blockage of returning positive dislocations, thereby permitting unobstructed negative slip to travel further away from the source. As a result, the annihilation process occurs at a greater distance from the source (as indicated in the insets). Due to the involvement of large-scale slip activity for even higher $t$ or $d$ the annihilation point eventually settles at a stable unvarying position, corresponding to the plateau region in Fig. 5b and c.

The underlying origin of glide irreversibilities as influenced by CTBs can be traced back to the discrepancies in the energy pathways for slip for forward and reverse transmission across CTBs. Such a phenomenon modifies the resistance of slip penetrating the CTBs under cyclical conditions, as further discussed below.

3.1.3. Energy barrier and ideal glide strength

The potential energy variation–displacement relationship of a pair of partial dislocations (an extended full dislocation separated by a stacking fault) in an otherwise perfect fcc crystal is described by the GSFE, as in Fig. 6. During glissile slip motion sliding of atomic planes occurs by overcoming the unstable fault energy $\gamma_{us}$ (inset in Fig. 6). The unmodified GSFE curve points to the resistance of dislocation glide scaling with $\gamma_{us}$, as imposed by the crystal. A Shockley partial dislocation glides on the (1 1 1) plane with the Burgers vector along the (1 1 2) direction. The modified GSFE takes the form of an increase in $\gamma_{us}$ due to the presence of the CTB (or any other local stress sources), as shown in Fig. 7a. In order to compare the relative resistance encountered during forward and reverse flow the modified $\gamma_{us}$ in the vicinity of a CTB is calculated (Fig. 7c).

With a view to estimating the resistance stress provided by a CTB to the approaching slip for back and forth transmission we calculated the modified GSFE in the vicinity of the CTB using a dynamic approach. Considering the dynamic nature of dislocation glide over time, computing the variation in the potential energy difference in some preselected atoms allows quantification of the modified GSFE (discussed in detail in Appendix A). The $\gamma_{us}$ values derived from these modified energy curves are plotted as a function of distance normal to the CTB in Fig. 7c. In Fig. 7b the dislocation at A is approaching the CTB but is still unaffected by the stresses resulting from the matrix–twin interfacial atomic mismatch. Thus $\gamma_{us}$ at A denotes the energy barrier that a dislocation has to overcome when it is gliding freely inside the crystal. The magnitude of $\gamma_{us}$ at A matches the peak in Fig. 6, which represents the energy barrier to unobstructed gliding, amounting to 254 mJ m$^{-2}$. The local stress generated due to atomic mismatch at and around the CTB elevates $\gamma_{us}$ once the approaching dislocation is in closer proximity. The maximum energy barrier that the incident dislocation needs to overcome is achieved when the slip interacts with the CTB, an intermediate step in formation of the final reaction products (Fig. 7b c point B). The elevated energy at point B corresponds to a $\gamma_{us}$ value as high as 340 mJ m$^{-2}$. Therefore the energy path A $\rightarrow$ B $\rightarrow$ C (red curve) describes the variation in $\gamma_{us}$ for transmitted dislocations during forward flow. In the course of reverse flow the returning dislocation encounters an even greater energy barrier due to the presence of the dissociated twinning.
Fig. 7. (a) Schematic demonstrating the expected increase in energy barrier ($\gamma_{us}$) due to the presence of a local stress source. The dark line depicts the planar fault energy for dislocation glide through a perfect crystal, while the green line represents the enhanced energy encountered in the presence of a CTB. The maximum slope of the (un)modified GSFE equals the ideal shear stress of the crystal $t_{\text{max}}$. Ezaz et al. [31] extensively explored the contribution of local stresses to the fault energetics of slip–twin interactions. (b) As a pair of Shockley partials approaches the CTB the energy barrier ($\gamma_{us}$) is elevated in the neighborhood of the twin–matrix interface. $\gamma_{us}$ is maximum at the CTB (position B). At C the $\gamma_{us}$ is the same as at A. Upon interaction with a CTB a pair of Shockley partials is left on the CTB, while another pair transmits into the twin. As the transmitted pair glides away from the interface $\gamma_{us}$ decreases to the level of a perfect lattice barrier. During the reverse transmission upon flipping of loading the returning dislocation encounters enhanced $\gamma_{us}$ due to the presence of the Shockley partials on the CTB (at point D). As the returning extended dislocation is transmitted back into the matrix it undergoes a similar multiplication, leaving another pair of twinning partials on the CTB. Schematic of load cycles in MD simulations (strain control) showing where A, B, C, D and A' occur. (c) Change in unstable energy $\gamma_{us}$ as a pair of partial dislocations approach a CTB during forward/reverse loading in the MD fatigue cycle. Path A → B → C provides an energy barrier against forward transmission (red curve), and C → D → A' against reverse transmission. The energy at D is greater than at B because of the presence of dissociated Shockley partials on the CTB during reverse loading. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)
partials on the CTB. Therefore the reverse energy barrier follows the path \( C \rightarrow D \rightarrow A' \) (blue curve). The \( \gamma_{us} \) maximum reaches a magnitude of 452 mJ m\(^{-2}\) at point D. The elevation of the reverse transmission energy barrier compared with the forward barrier can be attributed to the increase in local stress around the CTB due to the residual twinning partials. The GSFE for slip glide, as modified in the above mentioned manner, facilitates calculation of the ideal shear strength of the crystal \( \tau_{\text{max}} \). \( \tau_{\text{max}} \) is a function of \( \gamma_{us} \), and is calculated from the maximum slope of the modified or unmodified GSFE curve (Eq. (6)). Applying corrections for thermal activation and strain rate to the modified or unmodified GSFE curve (Eq. (6)). Apply-

corrections for thermal activation and strain rate to

calculate the reverse energy barrier compared with the forward barrier can be attributed to the

elevation of the reverse transmission energy barrier com-

ting with an increase in local stress around the CTB due to the residual

twinning partials. The GSFE for slip glide, as modified in

Above, we investigate continuum slip emissions from a

fatigue crack whose glide paths become irreversible upon cyclical loading. Atomistically computed \( \tau_n \) values are then utilized to characterize the continuum level dislocation glide, and subsequent fracture mechanics simulations.

3.2. Continuum dislocation simulations

We modeled a pre-existing mode III fatigue crack in the presence of a nanotwin. The crack emits a series of screw dislocations. These dislocations intersect the twin and, eventually, their cyclical glide paths become irreversible via annihilation. The slip glide resistance (due to lattice friction and penetrating twins) influences the equilibrium positions and the total glide path irreversibility. Cracks advance by accumulating plastic displacement at the tip, originating from the irreversibility of cyclical slip. For a given crack length \( (a) \), twin thickness \( (t) \) and twin position from the crack tip \( (d) \) and stress intensity levels \( (\Delta K_{\text{III}}) \) we can predict the corresponding values of \( da/dN. \) \( da/dN \) is expressed as a function of the equilibrium positions of discrete dislocations at a certain \( \Delta K_{\text{III}}. \)

3.2.1. Fracture mechanics calculations

In the continuum model we selected a mode III fatigue crack and the associated emission of pure screw dislocations (Fig. 8). The MD derived glide strengths for a screw dislocation were utilized. The continuum dislocations can overcome the glide resistances under the applied external load, and eventually assume equilibrium positions. At the equilibrium position a dislocation emitted from a crack tip experiences three forces: (1) resolved applied shear stress \( \tau_{\text{Applied}}; \) (2) image stress \( \tau_{\text{Image}}; \) (3) pile-up stress \( \tau_{\text{Pile-up}}. \) With the nucleation of new dislocations the local stress at the crack tip decreases due to enhanced image and pile-up stress. In order to compensate for this decrease the applied load has to be increased to facilitate further nucleation. Thus Eq. (8) summarizes the net shear stress \( \tau_n \) acting on the \( n \)th dislocation.

\[
\tau_n = \tau_{\text{Applied}} - \tau_{\text{Image}} - \tau_{\text{Pile-up}}
\]

\( \tau_n \) is formulated in Eq. (9).

\[
\tau_n = \frac{K_{\text{III}}}{\sqrt{2\pi x_n}} - \frac{\mu b}{4\pi x_n} \sum_{\sigma} \left( \frac{x_i}{x_n} \right) \frac{1}{x_i - x_n}
\]

Eq. (9) gives \( \tau_n \) as a function of \( K_{\text{III}} \). the applied global stress intensity factor for mode III loading, \( \mu \), the shear modulus, \( b \), the Burgers vector, and \( x_n \), the location of the \( n \)th dislocation along its glide path from the source (crack tip). \( \tau_n \) ought to be of sufficiently large magnitude in order for slip to overcome the unstable energy barrier \( (\gamma_{us}) \). Therefore with increasing global applied loading \( \tau_n \) needs to surpass and/or equal \( \tau_o \) to initiate glide. Thus Eq. (10) provides the conditions for gliding, which is further rearranged to formulate Eq. (11).

\[
\tau_n \geq \tau_o \quad K_{\text{III}} \frac{\sqrt{2\pi x_n}}{4\pi x_n} - \frac{\mu b}{2\pi x_n} \sum_{\sigma} \sqrt{\frac{x_i}{x_n}} \frac{1}{x_i - x_n} = 0
\]
Fig. 9) with no obstacle (twin) in the glide path. At a certain time point in the loading cycle the forward \(x^f_1\) and reverse \(x^r_1\) equilibrium positions of the dislocation are solved by setting the lattice friction stress equal to the applied resolved shear stress. In the forward half-cycle as the applied load is increased the dislocation continues to glide away until the maximum \(K_{III}\) is reached. Fig. 9 demonstrates the trajectory for the case of a single dislocation during forward/reverse loading. In forward loading a dislocation nucleates at a critical \(K_{III}\) value and then glides away to assume its final position (red curve). During reverse loading the dislocation does not immediately start to return towards the crack tip because of elastic strain recovery. As the shear stress in the reverse direction exceeds the lattice friction resistance it starts to glide towards the crack tip and eventually is annihilated by a newly nucleated negative dislocation. Continued reverse loading triggers the nucleation of another negative dislocation which repeats the mechanism over another cycle. This simplistic demonstration of the irreversibility of a discrete dislocation glide path over a fatigue cycle elucidates the fundamental procedure of the continuum-based simulations.

The introduction of nanoscale twins on the glide path of slip modifies the total irreversibility as well as slip obstruction by the crack. Eq. (12) provides an evaluation of the slip irreversibility parameter \(p\) (previously defined as the ratio between \(\gamma_{irr}\) and \(\gamma_{total}\)) as a function of the dislocation positions at equilibrium during forward and reverse flow (denoted by the superscripts \(f\) and \(r\), respectively).

\[
p = \frac{\gamma_{irr}}{\gamma_{total}} = \sum_{i=1}^{n} \frac{x^f_i}{2(x^f_i - x^r_i)}
\]  

(12)

Fig. 10 shows the evolution of \(p\) as evaluated with the specified values of \(t\) at constant \(d\), with a change in the applied stress intensity factor range. \(p\) increases non-linearly (square root trend) with \(\Delta K_{III}\), and eventually achieves a plateau. The computed tendency of \(p\) highlights the functional dependence of irreversible glide phenomena, and hence the crack tip plasticity, on the variation in twin thickness \(t\) on the nanoscale. This is consistent with the MD calculations elucidated earlier in Fig. 5b and c. In response to changes in the twin lamellar width the equilibrium positions of dislocations change accordingly. This would lead to different degrees of irreversibility in the overall dislocation glide paths, as implied through Eq. (12). These results points to a change in FCG rate as a function of \(t\) or \(d\). In order to further explore the \(t\) and/or \(d\) dependence of FCG a comparison of \(da/dN\) under such conditions was evaluated.
3.2.2. FCG simulations

A cyclical crack accumulates plastic displacement on an incremental basis. If there are \( n \) dislocations emitted from the crack tip the plastic displacement at the tip caused by each emission contributes to the overall crack extension. Based on the formalisms introduced earlier the rate of crack tip advancement per cycle can be formulated as:

\[
\frac{da}{dN} = \int_{0}^{x_{\text{max}}^{f}} du
\]

(13)

\[
\frac{da}{dN} = \frac{x_{\text{max}}^{f}}{2\mu} \sum_{i=1}^{n} (\tau_{n}^{f} - \Delta \tau_{n})
\]

(14)

In Eq. (13) \( x_{\text{max}}^{f} \) is the maximum distance away from the crack during forward loading traveled by the farthest dislocation, \( u \) is the crack tip displacement as a function of \( x_{j} \) and \( \mu \) is the shear modulus in the slip direction, \( \tau_{i}^{f} \) is the shear stress at the end of the forward half-cycle (a function of \( x_{j} \)), and \( \Delta \tau_{n} \) is associated with the distance \( x_{j} \) traveled by the returning crack bound dislocations (a function of \( x_{i}^{f} - x_{i}^{f} \)). Combination of Eqs. (9) and (14) leads to the \( da/dN \) formulation given in Eq. (15). In this formalism \( da/dN \) is essentially a function of the equilibrium dislocation positions. The solutions for these slip locations \( (x_{j}) \) at the maximum \( K_{\text{III}} \), as obtained from the equilibrium condition (Eq. (11)) during forward/reverse flow, provide input to the \( da/dN \) evaluation. Calculation of \( da/dN \) in this manner inherently incorporates the atomistically computed ideal glide stress as well as the twin penetration strength.

\[
\frac{da}{dN} = \frac{x_{\text{max}}^{f} \Delta K_{\text{III}}}{2\mu \sqrt{2\pi}} \sum_{i=1}^{n} \left( \frac{1}{\sqrt{x_{i}^{f}}} - \frac{1}{\sqrt{x_{i}^{f} - x_{i}^{f}}} \right)
\]

\[
- \frac{x_{\text{max}}^{f} h}{8\pi} \sum_{i=1}^{n} \left( \frac{1}{x_{i}^{f} - x_{i}^{f}} \right)
\]

\[
- \frac{x_{\text{max}}^{f} h}{4\pi} \sum_{i=1}^{n} \sum_{j=1}^{n} \left( \sqrt{\frac{x_{i}^{f}}{x_{j}^{f}}} \right) \frac{1}{x_{j}^{f} - x_{i}^{f}}
\]

\[
- \left( \frac{x_{i}^{f} - x_{j}^{f}}{x_{j}^{f} - x_{i}^{f}} \right) \left( \frac{1}{x_{j}^{f} - x_{i}^{f}} - \frac{1}{x_{j}^{f} - x_{i}^{f}} \right)
\]

(15)

We employed the \( da/dN \) formulations from Eq. (15) to quantitatively investigate the sensitivity of the slip blocking strength of nanotwins against FCG. Fig. 11 demonstrates that for a twin placed at a large distance \( d \) from the crack tip (of the order of 1000\( \times \) the Burgers vector) FCG becomes totally independent of the resistance of the interface to the interacting slip. Thus such a calculation provides information regarding the critical zone of influence of the CTB. As shown in Fig. 11, the critical interface influence size resides in the plateaux regions for which \( da/dN \) is independent of the slip-blocking strength at small \( d \) values. The CTB influence zone ranges across a few Burgers vector values, consistent with the MD findings (Fig. 7c). Determination of the neutral CTB influence size assists in the calculation of FCG as a function of \( t \) and \( d \).

Fig. 12a and b shows how the FCG metrics change with variations in \( t \) and \( d \), as predicted earlier in the evaluation of cyclical slip irreversibilities in Fig. 10. These plots of \( da/dN \) vs. the applied \( \Delta K_{\text{III}} \) reveal a \( t \) and \( d \) dependence of the rate of FCG as well as the threshold behavior. For smaller \( t \) and/or \( d \) FCG is significantly influenced by the nanotwin.
dimensions. Thinner twins as well as twins placed very close to the crack tip lead to enhanced FCG metrics.

4. Discussion

4.1. Cyclical slip–twin interactions and irreversibilities

Earlier works have pointed out the role of the local stress state and the type of dislocation (screw, edge or mixed) in dictating the nature of dislocation–CTB interactions [31,45]. In the present work we have examined the cyclical slip–twin interaction mechanism for fatigue crack tip-nucleated dislocations. Table 1 summarizes the cyclical slip–twin interaction mechanism for fatigue crack advancement through the nucleation and coalescence of nanovoids formed due to crack tip slip activity by MD. While these simulation studies addressed the FCG mechanism experimentally observed in especially the smaller sized (<30 nm) nanograined materials [47,48], cyclical irreversible slip activity as the underlying driving force of crack propagation was not particularly explored from a mechanistic perspective. We observed that the obstruction of slip and accumulation of crack tip displacements, as dictated by glide path irreversibility, were both influenced by the presence of CTBs. The calculation of glide path irreversibilities further illuminates an understanding of the mechanism of FCG in the presence of coherent twins, as presented in Fig. 5b and c.

The quantified cyclical slip irreversibility $p$ tends to become independent of $t$ and/or $d$ at sufficiently large magnitudes of these dimensions, as shown in Fig. 5b and c. We observed a decrease in $p$ to a value indicating almost completely reversible slip for the case of a crack tip (source) located in close proximity to nanotwins, and also for twins with diminishing lamellar spacings. This trend could be attributed to the limited availability of slip gliding space for the case of smaller $t$ or $d$, aided by the expedited return of dislocations upon reversal of loading. The reduced space allows a smaller degree of glissile motion by newly nucleated negative dislocations towards the CTB along the same slip system as positive slip during forward flow. This permits the returning crack-bound positive slip to undergo annihilation with negative dislocations in the close neighborhood of the source (crack tip).

The observed trends of quantified irreversible dislocation activity, as in Fig. 5, possess important implications regarding the mechanism of crack advancement in the presence of nano-obstacles. The fundamental mechanism of fatigue crack advancement is governed by the cyclical irreversibility of crack-nucleated dislocations during cycling. The nano-obstacles render the dislocation glide path irreversible by holding back the returning dislocations. Hence, if the obstacle (a coherent nanotwin in our case) promotes lowering of the cyclical slip irreversibility plastic displacement at the crack would be suppressed accordingly. Therefore, FCG is expected to be at a reduced rate, along with similar changes in the characteristic microstructural dimensions ($t$ and $d$) at lower magnitudes. The underlying reason for cyclical slip irreversibility can be traced back to energy barriers to slip transmission on the atomic length scale at matrix–twin interfaces during the forward and reverse fatigue half-cycles. The discrepancies in forward and reverse transmission energy trigger the irreversibility of dislocation gliding, resulting in the accumulation of local plastic displacement at the crack tip.

Calculation of the energy barriers ($\gamma_{\text{us}}$) in the vicinity of the CTB for the forward and reverse fatigue half-cycles explains the discrepancies between the forward and reverse transmission strengths, as illustrated in Fig. 7c. The energy pathways for the forward (red curve along A → B → C) and reverse (blue curve along C → D → A') transmission of slip across the CTB are markedly different. This enhanced energy barrier necessitates a greater resolved shear stress acting on the returning dislocations to force them back into the matrix, as they approach the CTB from within the twin. This, in turn, requires application of a higher global loading for such a reverse transmission of slip. As a result, the crack-bound dislocations are delayed at the CTB during the reverse half-cycle. This delay allows negative dislocations to nucleate from the crack and glide towards the CTB along the same slip system, meeting the reversing positive slip.

As observed, the principal mechanism of slip irreversibility over fatigue cycles is the impedance to gliding of returning dislocations by residual dislocations on the
CTB. The enhanced energy barrier during reverse flow owing to this residual slip on the CTB would pose a greater degree of obstruction to reversing dislocations. The present work quantifies the degree of glissile irreversibility as related to the characteristic microstructure dimensions, as well as captures the governing physics in terms of the underlying energetics. Even though the present study is limited to discussions of cases concerning only screw dislocations, similar physics are expected for edge and mixed dislocations. Pure edge or mixed dislocations leave residual dislocations on the CTB upon interacting with coherent cations, similar physics are expected for edge and mixed dislocations. Even though the present study is limited to discussions of cases concerning only screw dislocations, similar physics are expected for edge and mixed dislocations. Pure edge or mixed dislocations leave residual dislocations on the CTB upon interacting with coherent twins, as examined earlier in the literature [6,7,31,49]. Despite the varied nature of slip–twin reactions from case to case, the enhanced resistance encountered by reversing slip and their subsequent annihilation by dislocations of opposite sign would occur in a similar generalized pattern for mixed or pure edge cases. Hence the overall irreversible glide path pattern would essentially be identical with similar trends in FCG characteristics.

4.2. Role of microstructural dimensions on FCG

In the fracture mechanics simulations of a mode III fatigue crack emitting screw dislocations the cyclical slip irreversibility \( p \) is again evaluated as a function of the applied stress intensity factor. In Fig. 10 the functional dependence of \( p \) on \( \Delta K_{III} \) shows a square root trend. This could be attributed to the involvement of multitudes of dislocations that glide away to interact with the nanoscale obstacle (twin) at larger \( K_{III} \). The forces barring gliding of dislocations away from the source (originating from increasing pile-up and image stress) restrict dislocation movement to a greater extent at larger \( K_{III} \). Mughrabi [50] summarized the estimated cyclical slip irreversibilities, which were experimentally found to be almost negligible at low loading amplitudes (leading to a long fatigue life), and close to unity at larger loading amplitudes (resulting in a short fatigue life). For diminishing twin lamellae spacings the irreversibility also decreased, as depicted in Fig. 10. The mechanism lies in the lowered capability of thinner twins to hold back dislocations at larger applied \( K_{III} \), resulting in a low slip irreversibility.

Another important question regarding the transmission stress required for dislocations to penetrate these nanoscale obstacles is illustrated in Fig. 11. From the MD simulations we can estimate the critical twin–matrix interface zone size as normalized by the Burgers vector within which the CTB stress field would effectively elevate the energy barrier to transmission (Fig. 7c). The effective range of the interface influence zone size is in the range of a few multiples of the Burgers vector. To determine the role of the penetration strength of the nanotwins we looked at the evolution of \( da/dN \) at constant \( K_{III} \) with a varying degree of CTB influence zone (i.e. transmission strength of the twins). The results, shown in Fig. 11, indicate a neutral plateau in \( da/dN \) at low \( 2q/b \) for varying twin to crack spacings, where \( q \) is the distance from the twin-matrix interface. For twins located far enough from the crack the rate of FCG is independent of the influence of dislocation transmission stress. We chose a value of \( 2q/b \) in this neutral plateau for subsequent \( da/dN \) vs. \( \Delta K_{III} \) simulations in order to compare the role of \( t \) and/or \( d \) on the FCG properties.

The continuum simulation framework involving discrete dislocations provides quantitative evidence of a role of the microstructural dimensions \( t \) and \( d \) in FCG. Fig. 12a and b demonstrates how the change in any one of these microstructural characteristic lengths (with the other being kept constant) affects \( da/dN \). As can be seen, both the Paris and threshold regimes are influenced by such a variation in \( t \) or \( d \). For a decrease in either the width of the nanotwin lamella or the twin to crack tip spacing \( da/dN \) also decreases. Crack advancement in the threshold regime is minuscule by nature, and is characterized by cycle by cycle discrete plasticity. Our approach of modeling the crack tip plasticity accounts for individual dislocation contributions, thereby faithfully capturing the incremental crack growth for both massive and minute slip activities.

In summary, the critical microstructural characteristic lengths \( t \) and \( d \) associated with these obstacles play a pronounced role in FCG simulations. The correlation of FCG metrics with the change in these characteristic microstructural dimensions is governed by variations in the irreversibility and blockage of slip emitted from the crack tip interacting with an annealing nanotwin in the vicinity. FCG progresses via a combination of these two phenomena as influenced by nanotwins. If the CTB permits a reduced degree of cyclical slip reversibility the cyclical crack extension will act likewise. Therefore, FCG is expected to occur at varying rates corresponding to the changes in these characteristic microstructural dimensions \( t \) and \( d \). The insight obtained from such observations further clarifies the mechanism of cycle by cycle crack propagation. Slip irreversibility increases non-linearly as these characteristic lengths become greater, eventually reaching saturated levels. Similar trends in \( da/dN \) with respect to changes in spacing of the twin to the crack tip or the twin lamella thickness are observed in the continuum FCG simulations. Fig. 12a and b summarizes the variations in \( da/dN \) with these changes in the microstructural characteristic nanodimensions, thereby mapping the crack growth regimes. The trends in FCG in these calculations are consistent with earlier experimental findings in the literature as reported by Sangid et al. [21] and Singh et al. [5].
5. Conclusions

Utilizing MD and fracture mechanics simulations of discrete dislocation formulations we have studied the mechanism of FCG at the appropriate length scale by quantifying cyclical slip irreversibilities. Our goal was to isolate the role of nanotwins in the mechanism of FCG, as brought to our attention by recent experimental findings. The major contributions of this work can be summarized as follows.

1. The analysis presented in this study underscores the role of twin spacing and twin lamellar width on FCG. We note that the influence of these nanodimensions becomes more prominent when the twin spacing and twin width are typically less than 20 nm. The increase in FCG resistance is governed by the modified cyclical slip irreversibility and dislocation annihilation behavior upon slip–twin interaction. The FCG metrics, such as $da/dN$ and the threshold stress intensity range, are increased to a substantial extent on refinement of the nanotwin spacing and thickness. However, as these characteristic dimensions increase their role in FCG becomes less.

2. The investigation unfolded enhanced energy barriers for slip to glide across nanoscale CTBs owing to the presence of residual dislocations during reverse flow under cyclical conditions. Quantification of the mismatch in energy barriers to to and fro glide across twins provides a physical explanation for the irreversible glissile motion of slip. Such an insight extends our mechanistic understanding of previously observed experimental findings on FCG as influenced by nanoscale twins.

3. Considerable attention has been devoted to ensuring convergence of the unstable energy values when choosing fault dimensions of the order of the dislocation core. The sensitivity of the selected area of atoms to the unstable energy values was determined for dislocation advance in the matrix and near CTBs. In addition, the friction stress levels were scaled to account for the strain rate and temperature effects. As a result, the differential in friction stress upon forward and reverse loading was shown to play the most significant role in FCG.

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Appendix A

Since dislocation glide occurs via motion of the core through consecutive tearing and forming of atomic bonds around the core the sequential rows of atoms on the slip plane ahead of the oncoming dislocation alternately come within the influence of the mobile core. Therefore, by calculating the variation between the enhanced potential energy ($E$) of such atoms and the bulk perfect lattice energy ($E_{\text{perfect}}$) one would be able to compute the $\gamma$ surface (using Eq. (A1) after Vitek et al. [44]). We devised a novel technique of calculating the fault energies during dynamic slip motion.

\[
\gamma = \frac{E - E_{\text{perfect}}}{A}
\]  

(A1)

Ahead of an oncoming dislocation a group of atoms, designated tracing atoms (with an area on the slip plane $A = lw$ in Fig. A1), were carefully selected, where $l$ and $w$ are the distances parallel and normal to the dislocation line, respectively. The curves in Fig. A1 substantiate the length scale independence of modified/unmodified $\gamma_{us}$ on the range of the selected tracing area dimensions (normalized by the theoretical core width of a screw dislocation, $2\xi \approx d$ where $d$ is the interplanar distance ($d \approx 2.03$ Å for nickel) between (1 1 1) slip planes [51]).

A large $w$ value spreading beyond the influence of the core distortion encompasses lower energy bulk atoms in the calculation, therefore the normalized values are sufficiently small for convergence, as shown in Fig. A1. The value of $l$ was also selected to ensure convergence, as again shown in Fig. A1. The energy of the tracing atoms was confirmed to have a $\gamma_{us}$ value consistent with density functional theory. For the case of an extended dislocation, as the leading Shockley partial approaches the trailing atoms the value of $\gamma$ starts to increase, and achieves a maximum value $\gamma_{us}$ when the leading partial passes it. The departing leading partial leaves a stacking fault behind in its wake. At this point $\gamma$ assumes the value $\gamma_{\text{sf}}$. As the trailing partial translates the value of $\gamma$ in the tracing area again starts to
increase, eventually decreasing to the perfect lattice value. Then the value of \( \gamma \) returns to zero.

\( \gamma \) as a function of the reaction path coordinate computed in this study (away from the twin boundaries) is based on the geometry shown in Fig. A2a and produces the well-known baseline GSFE of the sliding half-block approach (Fig. A2b).

In order to calculate the modified GSFE due to local stress sources the tracing atoms are selected at varying proximities from the local stress source. Therefore, the stress source would contribute accordingly to the potential energy of the tracing atoms. Thus one can calculate the modified \( \gamma_{us} \) or the whole \( \gamma \) displacement plot as influenced by the stress source in that particular position. Such a technique is applied to obtain the variation of \( \gamma_{us} \) near the CTB during forward/reverse flow (Fig. 7c). The maximum slope calculated from such a modified whole \( \gamma \) displacement (as in Fig. 7a) provides \( \tau_{\text{max}} \) under the influence of local stress, which is then appropriately scaled to room temperature and the lower strain rate, as explained in Appendix B.

Appendix B

Plastic flow (i.e. dislocation glide) as a function of temperature is modeled by an Arrhenius-type equation as follows [52].

\[
\dot{\gamma} = \gamma_0 \exp \left( -\frac{E_a}{kT} \right) \tag{B1}
\]

where \( E_a \) is the activation energy barrier, \( T \) is the absolute temperature (Kelvin), \( k \) is the Boltzmann constant, and \( \gamma_0 \) is a constant associated with the rate of deformation. The derivative of \( E_a \) with respect to the glide resistant stress \( \tau_o \) (a function of temperature and strain rate) provides the kinetic signature of plastic deformation, which is defined as the activation volume \( V^* \). \( V^* \) scales with the physical area swept by the dislocations. For nanocrystalline materials or in confined volumes where there are limited dislocations sources it is of the order of several \( b^3 \), while for bulk materials its magnitude can be 1000\( b^3 \). Its magnitude can be determined experimentally or from MD simulations. From the MD simulations the difference in flow stresses (\( \Delta \sigma \)) for the nucleation of a single dislocation loop is calculated at two different strain rates (\( \dot{\gamma}_2 \) and \( \dot{\gamma}_1 \)) and a constant temperature, using Eq. (B2) [52]:

\[
V^* = -\frac{\partial E_a}{\partial \tau} = kT \frac{\partial \ln(\dot{\gamma})}{\partial \tau} = \frac{kT}{\Delta \sigma} \ln \left( \frac{\dot{\gamma}_2}{\dot{\gamma}_1} \right) \tag{B2}
\]

We note that \( E_a \) is a decreasing function of \( \tau_o \). Considering the linear \( \tau_o \) dependence of \( E_a [52] \) one can write

\[ E_a = E^* - V^* \tau_o \tag{B3} \]

Using a temperature normalization introduced by Zhu et al. [53],

\[
\tau_o = \frac{E^*}{V^*} \frac{kT}{\mu N v_o} \ln \left( \frac{kT N v_o}{\mu V^*} \right) \tag{B4}
\]

where \( E^* \) is the athermal activation energy barrier, \( N \) is the number of nucleation sites, \( v_o \) is the attempt frequency, and \( \mu \) is the shear modulus. The value of \( E^* \) is established from a knowledge of the critical stress at \( \sim 0 \) K and \( V^* \). Both quantities are determined from the MD simulations conducted in this study. Then the above equation allows the determination of \( \tau_o \) at different strain rates and temperatures. The constants utilized in our work are as follows: Boltzmann constant \( k = 1.3806503 \times 10^{-23} \) m\(^2\) kg s\(^{-2}\) K\(^{-1}\); athermal activation energy barrier \( E^* = 1.3 \) eV; activation volume \( V^* = 2.25 b^3 \); Burgers vector \( b = \frac{a}{2}[1 \ 1 \ 2] \), where lattice constant \( a = 3.52 \) Å; number of nucleation sites \( N = 100 \); attempt frequency \( v_o = 3.14 \times 10^{11} \) Hz; shear
modulus $\mu = 76$ GPa; temperature $T = 300$ K (room temperature); shear strain rate $\dot{\gamma} = 1 \times 10^{-4}$ s$^{-1}$. Because the MD calculations are conducted at 10 K and at high strain rates it was deemed necessary to scale the results for lower strain rates and room temperature. We note that this is still a topic of current research; the modifications made above and illustrated in Table B1 represent the current state of knowledge. Future refinements in this area will not, however, change the conclusions reached in this work.

The intrinsic (unmodified) $\gamma_{\text{us}}$ in Table B1 corresponds to the unstable stacking fault energy of pure Ni. The modified $\gamma_{\text{us}}$ levels in Table B1 are for a dislocation within the twin boundary zone, as explained in the text. The corresponding critical stress levels are encountered during forward/reverse transmission, as shown in Fig. 7c. The $\tau_{\text{max}}$ values are obtained from the slope of the $\gamma$ displacement curves from the simulations. The third column is obtained from Eq. (B4).

### References