FATIGUE CRACK GROWTH (FCG) MODELING IN THE PRESENCE OF NANO-OBSTACLES

BY
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THESIS
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Abstract

A combination of molecular dynamics and dislocation dynamics simulations is performed to model fatigue crack growth (FCG) in a nano-twinned nickel single crystal. Molecular dynamics simulations are employed to investigate the irreversible interaction of crack-tip emitted dislocations with nano-twins in the vicinity of the crack upon cyclic loading. A method is developed to quantify the irreversibility of slip, and calculate it as a function of the twin lamella thickness and crack-tip to twin lamella spacing. Subsequently, atomistically calculated slip irreversibility is utilized in dislocation dynamics crack growth simulations to understand the role of thickness of the nano-twins as well as the crack-tip to twin spacing on da/dN.

In molecular dynamics simulations, in order to study the cyclic slip-twin interactions, the nano-twinned single grain specimen is set up such that it favors two separate cases comprising pure screw and pure edge dislocation nucleation from the crack-tip. Both screw and edge dislocations demonstrate a cyclic steady-state interaction mechanism with the nano-twin under strain control loading. The da/dN formulations, based on discrete dislocation dynamics, are derived for the cases ranging from single to multiple screw or edge dislocations emission from the crack-tip over cycles. The molecular dynamics slip irreversibility is incorporated into the dislocation dynamics based da/dN calculations. An implementation of these formulations demonstrates that both for the cases of decreasing nano- twin thickness or lowering of crack-tip to twin spacing, da/dN also decreases complying with some recent experimental findings in literature.
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Chapter 1: Introduction

1.1 Fatigue Characteristics

Fatigue is the single largest service failures (approximately 90%) in metals. Under fatigue loading, failure of engineering materials and components occurs at load levels far below that for static fracture (Suresh, 1998), (Hertzberg, 1996). Aircrafts, ships and ground vehicles components such as axles, transmission parts, turbine and compressor blades, and suspension systems are exposed to cyclic mechanical loads as well as temperature changes. During the service lifetime, the engineering components might undergo different modes of load fluctuations, such as – mechanical fatigue, creep fatigue, thermo-mechanical fatigue, corrosion fatigue, sliding and rolling contact fatigue, fretting fatigue etc.

The reason why materials fail under cyclic loads, substantially smaller in magnitude than the safe static limiting load, is that there are some permanent changes in material microstructure that occur in the form of accumulation of plastic deformation, even though very incremental on a cycle by cycle basis. These irreversible changes manifest themselves as potential sources of damage. The series of events that lead to final catastrophic failure under fatigue loading are: (i) irreversible microstructural changes culminating in high stress concentration sites such as PSBs that facilitate crack nucleation, (Mughrabi, 1978), (Essmann et al., 1981) (ii) microscopic crack formation at high stress concentration sites such as twin and grain boundaries, (Kim and Laird, 1978) (Boettner et al., 1964) (iii) growth and/or coalescence of these micro-cracks into macro-cracks that start propagating under repeated load reversals (Pearson, 1975), (Morris et al., 1981) and (iv) final failure after substantial degree of stable macro-crack advancement to an unstable
extent that causes complete fracture of the engineering component (Mughrabi, 2009). A number of microstructural, mechanical and environmental variables dictate the conditions for micro-crack nucleation and its subsequent stable propagation as a macro-crack to final failure.

The total fatigue lifetime ($N_f$) of the component for safe operation is the sum of the number of cycles of load reversals to initiate a crack ($N_i$) and the number of cycles to propagate the crack ($N_p$) in a stable fashion to some final tolerable size beyond which it advances rapidly to catastrophic failure.

$$N_f = N_i + N_p$$

Relative proportions to the total life of $N_i$ and $N_p$ depend on the material and load levels. With relatively high loads that produce some plastic strain during each cycle, fatigue lives are relatively short and fall under the category of low-cycle fatigue (approximately up to $10^4$ to $10^5$ cycles) whereas lower stress levels resulting in elastic deformation at the macro-scale, end up as high-cycle fatigue. At low stress levels (i.e., for high cycle fatigue), a large fraction of the fatigue life is spent on crack initiation or growth of a micro-crack over a finite cluster of grains. With increasing stress level, (i.e. for low cycle fatigue regime), the crack propagation at the macro-level dominates, and there is a large literature in characterizing this type of crack growth. Over decades, engineers and materials scientists have developed numerous empirical and semi-empirical models to forecast the safe operating conditions and lifetime of the service components in engineering applications under different influencing factors, and hence improve fatigue properties of metals and alloys. These factors incorporate stress concentrators, temperature, environment, nature of loading and material microstructure. However, with the advent of new simulation tools such as molecular dynamics and dislocation dynamics, one can advance both the
crack initiation and crack growth modeling fields. The present thesis is focused on the crack growth modeling.

1.2 Fatigue Mechanism

In view of improving fatigue properties, the ideal design goals in fabricating metals and alloys would be to optimize the microstructural variables for enhanced resistance to both crack initiation and crack propagation. Crack initiation and propagation involve different physical mechanisms, and respond differently to certain changes in microstructural variables, for instance, grain size in polycrystalline materials (Suh and Kitagawa, 1987). In order to understand the effects of microstructural influencing factors such as grain size, and hence engineer desired fatigue characteristics in metals and alloys for specific applications, it is imperative to have a proper insight into both the mechanisms and their governing parameters.

Cracks nucleate from microscopic or macroscopic stress concentration sites such as grain or twin boundaries, inclusions, surface roughness, microstructural and compositional inhomogeneities etc. The physics behind the nucleation of cracks is the accumulation of small plastic strain at these sites on each cycle caused by irreversible to-and-fro motions of glissile dislocations leading to localization of slip and the formation of micro-cracks that subsequently grow into advancing macro-cracks (Mughrabi, 2009). In other words, the irreversible bulk dislocation activities manifest themselves in one form or another at the surface or grain interfaces, and contribute to the gradual evolution of high stress concentration sites such as Persistent Slip Bands (PSB) leading to micro-crack nucleation.
Once a micro-crack is nucleated, either it starts advancing with incremental growth over cycles or coalesces with other growing micro-cracks ahead of it to eventually form a macro-crack (Pearson, 1975), (Morris et al., 1981). The stable macro-crack begins propagating after a critical threshold value of applied stress intensity range ($\Delta K_{th}$) is reached. The initial macro-crack growth rate is small, and characterized by single shear along primary slip system resulting in a tortuous crack path at low $\Delta K$ levels, and with near-tip plastic zone smaller than individual grain dimension - stage I crack growth (Forsyth 1963) (Figure 1.1).

Figure 1.1 Direct stress stage I and stage II FCG (Forsyth, 1963).
Subsequently, at higher $\Delta K$ levels, the crack growth increases marked by simultaneous and alternating emissions of dislocations from crack-tip along two slip systems, with near-tip plastic zone encompassing many grains, leading to a planar crack path – stage II crack growth. The underlying mechanism of the FCG is the discrete nature of crack-tip plasticity in the form of dislocation emission and annihilation. This process leads to an irreversible cyclic dislocation dynamics by which the crack advances in a stable fashion. This occurs until the crack reaches an unstable size resulting in catastrophic failure. More elaboration on stage I and stage II is presented in chapter 2.

Studies on nano-crystalline metals and alloys by (Hanlon et al., 2003), (Hanlon et al., 2005), (Padilla and Boyce, 2009) etc. revealed some interesting insight into the role of grain refinement on both crack initiation and propagation life. They showed that grain refinement
ranging from micro- to ultrafine- to nano-scale sizes, which gradually enhances material strength and hardness under static loading to a substantial extent, also improves cyclic crack initiation properties, manifested in terms of an increased endurance limit and higher fatigue lifetime, but with a considerable reduction in the resistance of cyclic crack growth. These works point out the beneficial effects of grain size refinement under stress-controlled fatigue implying a greater resistance to fatigue crack initiation. On the contrary, crack growth results for the nano-crystalline materials such as electrodeposited fully dense nickel specimens (Hanlon et al., 2003) indicated reduced level of $\Delta K_{th}$ and markedly increased crack growth rate with the greater refinement of grain size. At the same time, recent studies by (Sangid et al., 2011) and (Singh et al., 2011) suggested considerable crack growth resistance in the presence of nano-grains and nano-twins. In terms of modeling efforts in fatigue crack growth, there have been few studies that built the foundation to the stress intensity range dependence. The thesis plans to build on some of these early models to bring further insight into FCG in the presence of obstacles at the nano-scale.

1.3 Research Motivation

Grain refinement to nano-scale sizes gives rise to substantial strengthening due to the obstruction of dislocation motion at grain boundaries but inflicts reduced ductility due to limited capability of smaller grains to accommodate plastic strain with diminishing grain size (Kumar et al., 2003). These nano-crystalline materials also exhibit enhanced fatigue endurance limit indicating greater resistance to crack initiation processes. Introduction of initially coherent mechanically and thermally stable nano-scale twins in ultra-fine grained copper (Lu et al., 2005) under monotonic loading is shown to impart similar strengthening effects but with the retention
of substantial ductility. This behavior is attributed to the fact that, unlike grain boundaries along which dislocations cannot glide, coherent twin boundaries can facilitate significant degree of glissile motion of dislocations along the interface, thereby promoting enhanced ductility (Lu et al., 2009).

Recent studies on the fatigue response of electro-deposited nano-twinned pure copper by (Singh et al., 2011) and nickel-cobalt alloys by (Sangid et al., 2011) established with substantial evidence that these nano-twinned materials provide enhanced damage tolerance in terms of increased fracture toughness, threshold stress intensity range and reduced FCG rate compared to conventional nano-crystalline materials. Furthermore, Transmission Electron Microscopic (TEM) analysis (Figure 1.3(a)) of post-fatigue specimens revealed substantial degree of dislocation activities such as pile-ups at twin and grain boundaries (GB) in the nano-twinned Nickel-cobalt alloys (Sangid et al., 2011), which implies to the existence of a primarily dislocation-mediated plastic deformation mechanism with the presence of twins and GBs. (Singh et al., 2011) demonstrated a decrease in the FCG rate in nano-twinned specimens with decreasing twin lamella thickness. These works indicate, in particular, that the observed noticeable improvement in the FCG resistance with the presence of nano-twins at fixed grain size might have originated from the dislocation-twin interactions present in the vicinity of the advancing crack. Further investigations on the dislocation length scale ought to be carried out to understand and isolate the contributing factors for such phenomena in details.

1.4 Research Goals

The above-mentioned findings clearly demand a need to further investigate the role of the presence of twins in nano-crystalline materials as well as their lamella thickness and/or any
Figure 1.3 Schematics showing the features of the present study. (a) A post-fatigue TEM image of a Ni-1.62%Co (wt) alloy specimen showing the presence of dislocation pile-ups at nano-twins indicating a slip-twin or grain boundary interaction based FCG mechanism. (b) To establish mechanism(s) for the advancement of crack in the vicinity of an annealing twin, and (c) to quantify the effects of varying twin lamella spacing (t) or crack-tip to twin distance on FCG rate.
other microstructural characteristic lengths that might play a role in the FCG rate. To develop a clear understanding of the FCG in the nano-twinned materials, it is imperative to probe into the detailed mechanism(s) of the dislocation emission from the advancing crack interacting with the nano-sized annealing twins present in the vicinity, and how incremental crack extension occurs in the presence of the irreversibility of the dislocation-twin interactions over each cycle. In that regard, molecular dynamics (MD) simulations provide a convenient conduit at the dislocation length scale to study these mechanisms. Through the MD simulations, cyclic irreversible slip phenomena are studied as a function of the microstructural characteristic lengths such as twin lamella thickness and crack to twin spacing. A systematic method is developed to quantify slip irreversibility utilizing appropriate formulations from literature. Subsequently, atomistically-calculated irreversibilities are incorporated into a discrete dislocation dynamics FCG model to extract quantitative information of the effects of annealing twin lamella spacing and crack to twin distance on da/dN.
2.1 Fatigue of Nano-crystalline Metals and Alloys

In micro-crystalline metals and alloys (grain size typically ranging from 1 μm to larger), grain refinement to ultrafine (100 to 1000 nm) to nano-scale (smaller than 100 nm) leads to higher strength and superior resistance to corrosion and wear and tear up to certain critical grain size. The strengthening behavior, typically up to 10 nm grain size, could be rationalized by the so-called Hall-Petch mechanism. The higher fraction of grain boundary volume in smaller grain materials impedes plastic deformation mechanisms with a higher degree of slip-GB interactions. The ultrahigh strength owing to grain refinement, although at a substantial expense of ductility, originates from the effective blockage of dislocation motion by GBs. The grain size effects fatigue response of metals and alloys as well (Lu et al., 2004).

Works by (Hanlon et al., 2003), (Hanlon et al., 2005), (Boyce and Padilla, 2011) and (Padilla and Boyce, 2009) showed the role of grain size on the fatigue crack initiation and propagation response. Reduction of grain size, resulting in high strength, also causes an increase in fatigue endurance limit (Hanlon et al., 2003) during stress-controlled cyclic loading of initially smooth-surfaced laboratory specimens, which indicates an enhanced resistance to crack initiation. (Boyce and Padilla, 2011) and (Padilla and Boyce, 2009) demonstrated that, in nano-crystalline pure nickel and alloys, crack nucleation is suppressed because nano-crystalline grains are not large enough to accommodate Persistent Slip Bands (PSB) which facilitate micro-crack nucleation in pure course-grained materials. However, reduction in grain size has been proposed to lead to deleterious effects on damage tolerance. Stable crack propagation experiments on nickel specimens with different grades of grain sizes, as reported by (Hanlon et al., 2003)
confirmed that the resistance to the crack advancement is deteriorated in finer grained specimens even though they demonstrate a better initiation properties in terms of enhanced endurance limit in high cycle fatigue experiments. These works on micro-, ultrafine- and nano-crystalline nickel revealed that finer grained specimens show reduced threshold stress intensity range, $\Delta K_{th}$, as well as increased $da/dN$. This observation is not supported by other studies as we discuss below.

(Singh et al., 2011) and (Sangid et al., 2011) revealed some intriguing observations regarding the resistance to the fatigue crack growth (FCG) in nano-crystalline metals and alloys. (Singh et al., 2011) examined the FCG behavior of initially nano-twinned ultra-fine grained pre-cracked copper specimens with different twin lamella spacing or density. The grain size was maintained constant in their study. Their works strongly suggested that, along with a desirable combination of strength and ductility, introducing twin in fixed grain sized materials to a gradually greater density also improves damage tolerance characteristics such as fracture toughness, threshold stress intensity factor range ($\Delta K_{th}$), and most interestingly the subcritical FCG rate. Works by (Sangid et al., 2011) on electro-deposited nano-crystalline nickel-cobalt alloys, with high density of nano-twins in the grains, further corroborated the existence of the superior FCG resistance compared to conventional nano-crystalline metals and alloys without nano-twins. TEM images of as-received and post-fatigue nickel-cobalt alloy specimens (Figure 1.3(a)) confirmed both the prevalence of twins as well as an enhanced degree of dislocation pile-ups at grain and twin boundaries, indicating a dislocation-mediated plasticity as the primary deformation mechanism.
The observation of the superior resistance to the FCG of nano-twinned face-centered cubic (fcc) metals and alloys in the abovementioned studies demands a better understanding of the mechanisms involved in advancing a crack under cyclic loading in ductile fcc materials with the presence of annealing twin boundaries, where the crack propagation mechanism would be affected by the high fraction of twin volume. There has been a considerable number of carefully crafted FCG models based on continuum mechanics (Wu et al., 1993) as well as discrete dislocation crack-tip plasticity (Yokobori et al., 1975), (Yokobori and Yoshida, 1974), (Pippan, 1989), (Pippan, 1991), (Pippan, 1992), (Neumann, 1969) that attempt to capture the physics of crack propagation and hence predict the failure mechanism. In the following section, an overview of the FCG models is presented.

2.2 FCG Overview

In ductile solids, the FCG could be understood as two prominent stages of propagation mechanisms, namely, stage I and stage II after (Forsyth, 1963) (Figure 1.1). At low ΔK, cracks initiate along the extruded persistent slip bands (PSB), and start propagating along the slip plane of the maximum shear stress (Figure 1.1) under mode I (opening) and mode II (sliding). The near-tip plastic zone size in stage I is smaller than the grain dimension, and crack surface profile is highly tortuous. Stage I active FCG remains almost undetected until it transitions to stage II at higher ΔK. Instead of traveling along a crystallographic slip plane, stage II FCG follows a general planar path controlled by the direction of the maximum tensile stress (Figure 1.1) under mode I. The near-tip plastic zone is large enough to incorporate many grains in stage II, and the crack advances in an almost planar path perpendicular to the maximum tensile stress direction.
The fracture surface profile for stage II is marked by distinctively fine striations in many engineering metals and alloys. At very high $\Delta K$, formation of micro-voids ahead of the advancing crack and their coalescence with the crack-tip results in very fast FCG. For ductile single crystal metals, (Neumann, 1969) proposed an alternating duplex slip model for stage II FCG explained in Figure 2.1.

Figure 2.1 Stage II FCG model (Neumann, 1969). Points in stress-time schematic on the right correspond to the crack growth schematics on the left. (k) shows the crack at the maximum tensile stress after 10 cycles, and (l) is the following compression phase.
In Figure 2.1, when the applied tensile load approaches \( \mathbf{a} \), a series of dislocations emit along slip system 1 which eventually work-hardens causing slip system 2 with easier glide conditions to get activated by the time applied tensile load reaches \( \mathbf{b} \) (maximum tension). Upon reversing to maximum compression at \( \mathbf{c} \), all the dislocations along 2 return to their source in a completely reversible fashion, thereby eliminating the collective slip step created in the forward half cycle along system 2. But dislocations along system 1 experience irreversible changes in glide conditions, imposed by work hardening mechanisms or any other microstructural influence, and do not return to their source, thereby causing retention of net slip step extension along system 1. At \( \mathbf{c} \) (maximum compression), the new crack surfaces along 1, created due to the residual slip step at the crack-tip, merely touch each other which detach themselves upon tensile loading in the subsequent cycles. Similarly, from \( \mathbf{c} \) to \( \mathbf{d} \), dislocations first nucleate and glide along 2, and after work hardening of 2, they slip along 3. Upon unloading to \( \mathbf{e} \), system 2 becomes irreversible for dislocations to return while 3 being completely reversible, thereby causing net crack extension along system 2. Figure 2.1(k) shows the crack at the maximum tensile stress after 10 cycles, and Figure 2.1(l) is the following compression phase. Thus, on each fatigue cycle, two slip systems get activated alternately during forward loading with one undergoing irreversibility of returning dislocations during unloading causing the crack to advance along the irreversible slip system. The final crack path profile is shown is Figure 2.1(l) with a red line. This model is experimentally verified in copper single crystals (Neumann, 1969).

Quantitatively, the power law of Paris relates the applied loading to the stable FCG which was further modified to suit crack closure effects through the works by (Elber, 1970).

\[
\frac{da}{dN} = C \Delta K_{\text{eff}}^m
\]
Different models have been proposed to rationalize the existence of threshold stress intensity range along with different governing mechanisms of the stable FCG. (McEvily Jr and Boettner, 1963) provided insight into the role of the crystallographic orientation and the stacking fault energy of material, and hence cross slip tendency on the FCG. Pippan (1989, 1991 and 1992), (Riemelmoser et al., 1997) used a discrete dislocation dynamics based model for a mode III propagating crack to provide a rationale into the existence of the threshold stress intensity range below which no crack growth occurs with and without the presence of slip obstacle in the vicinity of an advancing crack.

(Schijve et al., 2004), (Schijve, 1974), (Schijve, 1981) analyzed the fatigue crack growth along shear planes that are inclined at 45° to the tensile stress axis at high applied loads. Also, the FCG modeling by (Rice, 1967), (Weertman, 1973), (McClintock, 1963), (McClintock and Irwin, 1965) provided rigorous continuum analysis of the crack-tip plasticity that leads to the cyclic crack extension. Recently, (Yang et al., 2008) reported experimental observation of nano-void coalescence leading to FCG. (Farkas et al., 2005) conducted atomistic simulations to demonstrate the role of nano-void coalescence on FCG. (Potirniche et al., 2006) and (Horstemeyer et al., 2010) carried out atomistic simulations to model FCG in a polycrystalline material as a function of CTOD. (Deshpande et al., 2001) modeled FCG based on discrete dislocation plasticity of the crack-tip through finite element simulations. The Table 2.1 presents a brief account of the key FCG models.
Table 2.1 Summary of the key FCG models.

<table>
<thead>
<tr>
<th>Crack Growth Models – Investigator(s)</th>
<th>Mechanism</th>
<th>Crack Growth Model</th>
<th>da/dN proportionality</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>(Neumann, 1969) (Neumann, 1974)</td>
<td>Alternate shearing on two slip planes</td>
<td>Crystallographic slip characteristics</td>
<td>$\propto h$</td>
<td>explains planar crack growth in stage II and striation formation</td>
</tr>
<tr>
<td>(McEvily Jr. and Boettner, 1963) (McEvily Jr. and Illg, 1958)</td>
<td>Cross-lip of screw dislocations in favorably oriented grains</td>
<td>Crystallographic slip characteristics</td>
<td>$\propto K_N S_{NET}$</td>
<td>explains stacking fault energy and crystal orientation dependence on FCG</td>
</tr>
<tr>
<td>(Schijve, 1974) (Schijve, 1981) (Schijve et al., 2004)</td>
<td>Cracking along single or double shear planes at 45° to normal load</td>
<td>Continuum based Fracture mechanics</td>
<td>$\propto (\Delta K_{eff})^m$</td>
<td>explains crack-front orientation incompatibility at high $\Delta K$</td>
</tr>
<tr>
<td>(Rice, 1967) (Weertman, 1973) (Weertman, 1966)</td>
<td>Crack-tip displacement range over a cycle</td>
<td>Continuum based crack-tip plasticity</td>
<td>$\propto \int_{0}^{p} \Delta u$</td>
<td>relates macroscopic strengthening effects to FCG rate</td>
</tr>
<tr>
<td>(McClintock, 1963) (McClintock and Irwin, 1965)</td>
<td>Cyclic strain accumulation in growing near-tip plastic zone</td>
<td>Continuum based crack-tip plasticity</td>
<td>$\propto \int_{0}^{p} (\Delta \gamma)^2$</td>
<td>provides quantitative and conceptual basis for tensile FCG of ductile metals</td>
</tr>
<tr>
<td>(Pippan, 1989) (Pippan, 1991) (Pippan, 1992) (Riemelmoser et al., 1997)</td>
<td>Annihilation of cyclically emitted dislocations</td>
<td>Discrete dislocation crack-tip plasticity</td>
<td>$\propto$ CTOD</td>
<td>predicts lower and upper limit for $\Delta K_{th}$</td>
</tr>
</tbody>
</table>

$h$ = slip band thickness, $\Delta u$ = displacement range, $\Delta \gamma$ = strain range, $r_p$ = cyclic plastic zone size, $\Delta K_{eff}$ = effective stress intensity range, $S_{NET}$ = maximum stress in terms of remaining net sectional area, $K_N$ = modified stress concentration factor
From a careful overview of the FCG models, the discrete nature of the crack-tip plasticity in the form of nucleation of dislocations and their glissile motion is found to constitute the underlying mechanism of the crack growth. Net crack growth over a cycle occurs as a result of the displacement imparted by the nucleation of dislocations in the forward part of the fatigue loading which are not recovered in the reverse part of the loading. The following section discusses in details how the concept of cyclic slip irreversibility has been used in different models to explain fatigue crack initiation as well as propagation.

2.3 Cyclic Slip Irreversibility

The sub-structural microscopic cause of fatigue damage evolution is due to the accumulation of plastic strain over load reversal cycles. The plastic strain accumulation occurs when forward and reversed gliding of dislocations become irreversible in the process. In the period of the to-and-fro motions of dislocations during cyclic load reversals, there exist several microstructural phenomena because of which dislocations do not return to their initial positions, thereby resulting in local permanent plastic strain accumulation. Some of these phenomena, as summarized by (Suresh, 1998), are – (i) cross-slip of screw dislocations and their subsequent annihilation by interacting with other dislocations, (ii) interaction with microstructural defects such as grain and twin boundaries, (iii) oxidation of surface slip steps etc., and any other microstructural changes that make dislocations in any part the cyclic loading not return to their initial sources. This irreversible process of slip at the microscopic scale constitutes the underlying mechanisms of the fatigue damage evolution.
Figure 2.2 Surface roughening by irreversible random slip in PSBs (Mughrabi, Differt, Essmann 1986).

(a) SEM image of a PSB on a copper single crystal emerging as an extrusion with surface roughness.

(b) Schematic of surface profile of a PSB showing both matrix and PSB dislocation arrangements. Encircled sites are possible crack nucleation sites with high stress concentrations.

(c) Model of dislocation glide in PSBs (i) section perpendicular to screw dislocations (ii) top view of the glide plane. Two screw dislocations nucleate from the source S and annihilate by cross slip at A and B respectively. The dislocation moving to the right reverses its glide at C.

(d) Irreversibility, p as a function of total local plastic strain amplitude $\gamma_{pl}$ (re-created from original). $y_s$ is annihilation distance, $c_s$ is fraction of $\gamma_{pl}$ contributed by screw dislocations, $b$ is the burgers vector.

$$\frac{2y_s c_s \gamma_{pl}}{b}$$
The irreversible dislocation glide is shown as the fundamental mechanism how cracks nucleate (Essmann, 1982) and propagate (Neumann, 1969). Micro-cracks nucleate when gradual irreversible slip activities in the bulk of the material culminate in the formation of Persistent Slip Bands (PSB) (Essmann, 1982) that either emerge to the surface in the form of extrusions/intrusions or penetrate through or interact with grain boundaries, inclusions and other microstructural barriers, thereby eventually creating high stress concentration sites at some of these barriers.

(Differt et al., 1986) first quantified the degree of irreversibility of dislocations gliding in a PSB in an attempt to estimate the surface roughness of extrusions and intrusions in single crystal copper (Figure 2.2). They defined a cyclic slip irreversibility parameter \( p \) as the ratio between the irreversible shear strain \( \gamma_{irr} \) and the cumulative total local plastic shear strain \( \gamma_{pl} \). In a PSB, there exists a dynamic equilibrium of screw dislocation nucleation and annihilation upon cross-slip, leading to the cyclic accumulation of plastic strain. They utilized the parameter \( p \) in order to obtain an expression of surface roughness of the extrusions and intrusions. Their model essentially incorporated a quantification of the sub-surface irreversible dislocation activities inside the PSB into the evolution of surface roughness. A number of other studies utilized similar quantified slip irreversibility parameters to capture the physics of the crack initiation, as summarized by (Shyam and Milligan, 2005). In addition to crack initiation, irreversible dislocation dynamics governs the advancement of cracks as well.

During the propagation of crack, the crack tip emits dislocations that interact with microstructural barriers in the vicinity and undergo one of the irreversibility-inducing
mechanisms (Suresh 1998) that renders the glide process from and to the crack-tip irreversible, resulting in a net crack growth increment. The degree of the slip irreversibility at the crack-tip dictates the crack growth per cycle. In other words, if slip in a grain ahead of a crack tip is completely reversible, no net crack growth would occur, therefore, with increasing slip irreversibility the net plastic displacement at the crack-tip also increases. The higher net displacements result in a higher crack growth rate.

The discrete nature of the permanent plastic strain accumulation is proved to be a fundamental phenomenon that, if quantified appropriately, can capture the gradual damage evolution mechanism(s). Since crack growth scales with the irreversibility of discrete plasticity at atomic length scales, it is also possible to have an insightful understanding of the relationship between the mechanical driving force (i.e. applied loading) and crack growth rate. (Mughrabi, 2009) summarizes the results where the estimated cyclic slip irreversibilities ($p$) were found almost negligible at low loading amplitudes (leading to high fatigue life), and close to unity at larger loading amplitudes (resulting in low fatigue life).

Through molecular dynamics simulations, it is possible to investigate the discrete nature of plasticity at the crack-tip in terms of dislocations emission at an atomic length scale as well as the interaction of slip with any microstructural barriers present in the neighborhood of the advancing crack such as coherent twins, incoherent grain boundaries etc. which are capable of rendering the gliding of the emitted dislocations irreversible. In the present study, we attempt to utilize the aforementioned concept of parameter, $p$, to quantify the degree of irreversibility of the crack-tip initiated local slip activities ahead of a propagating crack in the vicinity of a nanoscale
coherent twin. Then, the atomistically calculated $p$ is incorporated to the incremental propagation of the crack per cycle $(da/dN)$, thereby providing an quantitative insight into the mechanism of dislocation mediated fatigue crack advancement in the presence of nano-twins.

2.4 Slip-twin Interaction

Slip irreversibility ahead of a crack tip imposed by nano-scale coherent twins is expected to be a function of the factors such as the nature of dislocation-twin interactions, the twin lamella thickness in the light of the following findings. There are different types of slip-twin interactions possible in fcc metals (Mahajan and Chin, 1973), (Hartley and Blachon, 1978). These interactions have been observed experimentally as well as studied through atomistic simulations (Ezaz et al., 2011).

Presence of initially coherent nanoscale twins in grains can result in considerable strength and ductility (Lu et al., 2009) enhancement. Strengthening occurs due to the coherent twin boundaries (CTB) providing substantial energy barrier for incoming slip transmission across the twin lamella thickness, resulting from residual dislocations, depending on resolved shear stresses on the CTB and interacting slip systems (Ezaz et al., 2011). Enhanced ductility is a result of considerable degree of plastic strain accommodation in the form of dislocation gliding along the CTB as they gradually lose coherency by absorbing slip (Christian and Mahajan, 1995), (Lu et al., 2009), (Zhu et al., 2007). (Kumar et al., 2003) also found that both strength and ductility for these nano-twinned materials demonstrate a Hall-Petch type dependence on the twin lamella spacing. In other words, with decreasing twin lamella spacing, strength as well as ductility increases.
Whether the CTB would serve as an effective barrier to incoming slip for a particular case, depends on the type of dislocation (pure edge, pure screw or mixed) and resolved shear stress on the incoming slip systems, on CTB, and on outgoing slip systems as confirmed by experimental and simulation observations (Wu et al., 2009). That the CTBs can completely block the incident slip, partially block and allow transmission across the twin or completely absorb the slip on CTB (Ezaz et al., 2011), (Zhu et al., 2007) governs the tailoring of superior strength and ductility observed experimentally. In the present study, slip-twin interactions for pure edge and screw dislocations are studied with a detailed burgers vector analysis to capture a comprehensive picture of the irreversible twin-slip interactions over cycles.
Chapter 3: Methodology

3.1 Introduction to Atomistic Simulations

Atomistic modeling falls into two categories – Classical Statistical Mechanics and Quantum Mechanics (Tadmor and Miller, 2011). Quantum Mechanics is the mathematical description of the time evolution of a physical system via wave functions, considering wave-particle duality of matter and energy. Classical Statistical Mechanics correlates microscopic motion of individual atoms of matter to macroscopically observable properties such as temperature, pressure, entropy, free energy etc.

3.2 Overview on Atomistic Modeling of Materials

In quantum mechanical modeling of material, physical observables are obtained by applying mathematical operations on wave functions (Tadmor and Miller, 2011). Mathematically, a wave function is a function from a space that maps the possible states of the system into complex numbers. Wave functions, under certain physical boundary conditions, are found through solving for approximate solutions to exact Schrödinger equations. These models do not require any assumptions about potentials; rather they need only electronic and geometric information. They can be coupled with statistical mechanical models, and also be used to model chemical reactions. In quantum mechanical models, both system size and time steps are small, and there is a trade-off between accuracy and efficiency.

But in classical statistical mechanical modeling, electronic states are not usually accounted for, with accuracy limited by potentials. It is used for calculating equilibrium and dynamic properties, from a system of atoms, such as bulk properties of materials (eg. elastic
constants, free energies, molecular diffusivities, evolution of lattice defects etc.). Its system sizes are limited to $10^3$ to $10^7$ atoms and nano-second timescale, and chemical reactions are not possible to model. There are two approaches of classical statistical mechanics - Molecular Dynamics and Monte Carlo.

Figure 3.1 (a) Schematic showing the length scale of studying materials behavior (from Darrell Socie 2009) and (b) length and time scale of performing molecular dynamics simulations compared to quantum and continuum mechanics.
Monte Carlo is a stochastic technique based on using random numbers and probability statistics to investigate problems instead of searching for deterministic solutions (Frenkel and Smit, 2001). Solving equations which describe the interactions among a fairly small number of atoms is easy to perform but solving the same equations for thousands of atoms is computationally very expensive and sometimes infeasible. With Monte Carlo approach, a large system can be sampled in a number of random configurations, and that data can be used to describe the system as a whole.

Molecular dynamics is the simulation of time evolution of atomic nuclei (considered as classical Newtonian particles) by integrating their equations of motions (Frenkel and Smit, 2001). Time-dependent effective force field acting on atomic nuclei is calculated by taking gradient of an empirical potential energy field binding the atomic nuclei, as a replacement of interatomic bond energy created through electron cloud overlapping. This is the approach we utilize in our study.

The present research requires modeling crystallographic defects such as dislocations, matrix-twin interface (also known as twin boundaries) etc. In that regard, molecular dynamics simulations provide the most appropriate and effective tool to capture the physics in that length scale, and extract useful material properties and/or dynamic physical response of interest.

3.3 Molecular Dynamics

In MD simulations, the objectives are computational implementations of particle dynamics averaged over time and phase, based on statistical mechanics with the aim of extracting properties of interest of the system concerned. These simulations are directed towards
obtaining an atomistic trajectory of the physics under investigation to reveal the possible mechanism(s) that could be tied with the macroscopic behavior.

MD simulations can be carried out in several ways in terms of the time evolution of different system variables (Frenkel and Smit, 2001) – i.) Micro-canonical or NVE ensemble (constant number of atoms, volume and energy), ii.) Canonical or NVT ensemble (constant number of atoms, volume and temperature), iii.) Isobaric-isothermal or NPT ensemble (constant number of atoms, pressure and temperature), and iv.) Grand Canonical or TVμ ensemble (constant temperature, volume and chemical potential).

The following flow chart illustrates the steps of a typical MD simulation.

Figure 3.2 Flow chart for molecular dynamics simulation process after (Tadmor and Miller, 2011).

Step 0 – Initialize: This step declares the definition of the initial structure of material (eg. fcc, bcc, polymers, liquid etc.) and sets the size of the simulation supercell and the
coordinates of the atoms, the boundary conditions (e.g. periodic or non-periodic) and the atomic velocity coupled with the initially-set temperature profile.

Step 1 – Atomistic Model: It computes the potential and kinetic energy of the system defined from the interatomic potential (e.g. Lennard-Jones, EAM, MEAM etc.), which contains the inter-atomic bonding information, and evaluates the forces acting on individual atoms from the gradient of the total energy landscape based on the current positions and velocities. Finally this step calculates the temperature tied with the kinetic energy of the system using a suitable thermostat algorithm (e.g. Anderson, Nose-Hoover etc.).

Step 2 – Integrate: It updates atomic coordinates, velocities and supercell physical dimensions with the increment of simulation time using time integration algorithms such as Velocity Verlet, Quenched Dynamics etc.

Step 3 – Output Results: It provides useful properties and/or variables from the simulation for later analysis and visualization such as lattice distortions, time-averaged temperature, stress etc.

Steps 1, 2 and 3 constitute the principal integration loop. This loop continues until the minimum energy configuration under the desired thermodynamic conditions to be simulated is met, and thus the system evolves over time.

The validity of MD results is largely dependent on how the interatomic interactions are described throughout the simulations. To model material behavior through MD, it is imperative that the properties and/or physics of material under scrutiny match as closely as possible to reality. As for instance, in order to be able to study material deformation, the governing physics
of deformation in atomic scale, incorporating the complex electronic interaction causing tearing of interatomic bonding, movement of atomic nuclei through overlapping electron clouds, formation of defects as opposed to perfect lattice etc. should be taken into account as rigorously as possible. In view of all the above-mentioned rationale, EAM potential provides the required bonding energy landscape for MD simulations in view of our investigation objectives in the present work.

3.4 EAM Potential

Schrodinger’s equation would provide the most exact solution of many-electron phenomena of material deformation but at the expense of, and sometimes going beyond the limit of the computational capacity (Tadmor and Miller, 2011). In order to facilitate efficiency in terms of computational cost, Density functional Theory (DFT), Tight Binding (TB) etc. have been developed with a greater extent of approximations respectively (Tadmor and Miller, 2011) but, nevertheless, they still remain computationally expensive to a substantial degree for modeling deformation phenomena of materials. So, much more approximate approaches to model these behaviors, as opposed to quantum mechanical methods, have been devised which consist of fitting empirically obtained material parameters to appropriate functional forms so as to model accurate interatomic interactions.

Among these descriptions of interatomic interactions, one particular approach, namely Embedded Atom Method (EAM), was of special interest in view of the research objective of the present work. An EAM description of material bonding takes into account the relation between the interatomic bond energy and coordination, surface energetics etc. which renders EAM to be very effective in modeling certain aspects of metallic material behavior, especially, for face
centered cubic (fcc) crystal in terms of capturing bulk deformation phenomena such as dislocation dynamics, fracture properties, fault energetics etc. It has been proved to be effective in capturing non-directional metallic bonding character and atomic coordination effects such as accounting for a missing atom in a lattice or vacancy formation (Tadmor and Miller, 2011). So, EAM potential could be effectively employed for the purpose of investigating the plastic deformation mechanisms of fcc crystal such as the glide of dislocations.

In view of the nature of bonding of metallic materials, where the environment of all the atomic nuclei is a homogeneously distributed electron cloud, an EAM potential models this special electronic bonding of metals by considering both pair-wise interaction energy and the energy required for each atom to be embedded in a local electron cloud at a certain position in the lattice, contributed by all the other atoms of the system. This electron density at the site of each atom is approximated by a simple linear superposition of electron cloud contributions of all neighboring atoms. So, the energy of each atom could be thought of as being originated from two sources: i.) interatomic attractive/repulsive energy by the neighboring atom (defined by a pair potential function), and ii.) the energy required to place one atom in an electron gas environment.

In order to describe the two-atom interaction energy, a simple pair potential function could be used such as Lennard-Jones, Morse potential etc (Tadmor and Miller, 2011). To account for the embedding energy, a special energy functional is required to be formulated which would be a function of electron density contribution to a certain lattice site from all the neighboring atoms within a certain cut-off radius. These considerations lead to the following typical form of an EAM potential energy expression:
Where, $\varphi_{\alpha\beta}$ is a pair potential, and $U_\alpha$ is the energy associated with placing an atom in an electron cloud given by the density function, $\rho^\alpha$. This density function is a linear superposition of another function, $g_\beta$, which, itself, is a function of interatomic distances, $r^{\alpha\beta}$. $g_\beta$ stands for a spherical distribution of electron density around an individual atom $\beta$, and accounts for the sum of squares of overlap integrals between electronic orbitals centered on atoms $\alpha$ and $\beta$. In principle, in order to develop a pair-functional potential such as EAM, one needs to design a unique embedding function, $U_\alpha$, density function $g_\beta$, and a pair potential to account for the pair interactions, $\varphi_{\alpha\beta}$ (Figure 3.3).

Figure 3.3 A pictorial description of EAM potential for fcc metals. (a) Pair-wise interaction between atoms is approximated by a simple ‘pair potential’ function $\varphi_{\alpha\beta}$, (b) energy for overlapping electron cloud at a certain atom site is approximated by an energy functional of electron density $U_\alpha$. 

$$E = \frac{1}{2} \sum_{\alpha, \beta} \varphi_{\alpha\beta}(r^{\alpha\beta}) + \sum_{\alpha} U_\alpha(\rho^\alpha)$$
In the MD simulations of the present work, EAM potential developed by (Foiles and Hoyt, 2006) for pure nickel is used since it provides a better agreement with the experimental and DFT-calculated results of Generalized Stacking Fault Energy (GSFE) (Vitek, 1968) compared to other EAM potentials available in literature (Foiles et al., 1986), (Mishin et al., 1999) (Figure 3.4). The interatomic interactions used here are developed based on a Morse potential along with the electron density function as follows,

\[
f(r) = E_o(e^{-2b(r-r_o)} - 2e^{-b(r-r_o)})
\]
\[
\rho(r) = \rho_o r^n(e^{-ar} + 2n+3 e^{-2ar})
\]

Where, \(E_o = 1.39664 \text{ eV}, r_o = 2.14146 \text{ Å}, b = 1.22848 \text{ Å}^{-1}, \rho_o = 1, n = 8, \text{ and } a = 3.58321 \text{ Å}^{-1}\)

![Comparison of Generalized Stacking Fault Energy (GSFE) for pure nickel from different EAM potentials. Foiles et al. (2006) gives good agreement of energy barrier, \(\gamma_{us}\) with DFT (276.5 mJ/m\(^2\)) and intrinsic stacking fault energy (\(\gamma_{isf}\)) with experiment (127mJ/m\(^2\)).](image-url)
The cut-off radius for pair-wise interaction and electron density contribution to a
particular atom site is taken to be 4.85Å. The vacancy formation energy and the melting point
predicted by this potential is 1.76 eV and 1565K respectively. Experimentally determined
intrinsic stacking fault energy, 127mJ/m², is fitted in this potential. The results in the Figure 3.4
shows that intrinsic stacking fault energy prediction from this potential, in molecular statics
relaxation, is very close to the experimental value.

3.5 Virial Stress

In order to be able to extract continuum measures from underlying atomistic systems, it is
imperative to understand microscopic definition of corresponding continuum fields, particularly,
the Cauchy stress tensor in view of our problem. Cauchy stress formulation emerges from the
concept of the traction acting across internal surfaces of a solid; therefore, stresses could be
defined at the atomic level in a similar fashion in terms of the forces acting along the bonds,
calculated from the potential. To look into the cyclic stress-strain response of the nano-twinned
grain in the current simulations, the volume-averaged virial stress formulation is employed
(Tadmor and Miller, 2011), the most general form of which is as follows:

\[
\sigma_{ij} = \frac{1}{V} \left( -\sum_{\alpha} \frac{p_i^\alpha p_j^\alpha}{m^\alpha} + \frac{1}{2} \sum_{\alpha, \beta, \alpha' \beta'} \varphi_{\alpha' \beta'} \frac{r_i^{\alpha} r_j^{\beta}}{r^{\alpha' \beta}} \right)
\]

Stress elements, \(\sigma_{ij}\) is a function of volume (V), momentum (p), mass (m), interatomic distances
(r) of the atoms and pair potential (\(\varphi\)). The kinetic energy contribution of the atoms to the virial
stress tensor is neglected to obtain a more accurate description of continuum Cauchy stresses
(Zhou, 2003). Throughout the present work, Virial definition of stress for simulations is used when necessary.

3.6 Description of LAMMPS

MD simulations in the current research are carried out with the LAMMPS developed in Sandia National Laboratories (Plimpton, 1995), (http://lammps.sandia.gov). It stands for Large-scale Atomic/Molecular Massively Parallel Simulator. It is an open source molecular dynamics code written in C++. It incorporates all the fundamental and updated algorithms such as Velocity Verlet, Conjugate Gradient, Nose-Hoover, Virial stress formulation etc., and hence provides a good handle on the material properties investigation.

3.7 Simulation Procedure

In the molecular dynamics simulations, a nickel single crystal supercell is created, and then a coherent nano-twin is introduced into the supercell. The whole structure is energetically minimized using Molecular Statics (MS) relaxation method. MS relaxation provides information about a crystal at minimum energy configuration. An energy minimization of a system of atoms is carried out by iteratively adjusting atom coordinates with an appropriate algorithm. Conjugate gradient algorithm is used to relax the twinned single crystal simulation supercell by iteratively solving for the minimum energy configuration for the atomic positions within a predefined convergence limit. This algorithm uses a random rearrangement of atoms with an acceptance criterion and determines specific positional rearrangements of atoms, conjugate to the previous rearrangements that follow the direction of steepest descent on the potential energy curve. Conjugate Gradient algorithm is selected for addressing our problem at hand because of its computational efficiency in terms of fast convergence to some predefined criteria of force and/or total energy of the system.
A void is introduced into the matrix to simulate a dislocation source (crack-tip). Cyclic loading is applied on the simulation supercell under strain control condition with periodic boundary conditions existent in all orthogonal directions. The periodic boundary condition ensures the presence of no free surface along the boundary of the simulation cell, thereby simulating bulk material. As cyclic straining is applied on the system, atomistic snapshots at different time-steps are carefully analyzed to capture the evolution of the microstructure. The simulations are run at $10^9$/s strain-rate from $\varepsilon_{\text{min}} = -4.46\%$ to $\varepsilon_{\text{max}} = 9.22\%$ ($R_e = -0.48$), employing NPT algorithm to perform non-equilibrium molecular dynamics (NEMD).

Figure 3.5 A typical simulation supercell used in the molecular dynamics simulations with a nano-twin and a void as a dislocation source to simulate the crack-tip.
Chapter 4: Results and Discussions

4.1 Cyclic Straining of a Nano-twinned Grain

A single nano-twinned grain is constructed with the crystal orientation as shown in the Figure 4.1 for MD simulations. In order to simulate bulk material without any surface, periodic boundary condition is employed in all x, y and z directions. The twin is constructed as [111] type. An atomistically sharp crack-tip is present in the vicinity of the twin. Shear loads in two different directions are applied on the nano-twinned grain under strain control condition with fixed plastic strain amplitude as shown in the Figure 4.1. The cyclic stress-strain behavior is recorded for both cases as shown in the Figure 4.2. Stress from the MD simulations was calculated according to the Virial definition of Cauchy stress neglecting the kinetic energy contribution (Zhou, 2003).

![Figure 4.1](image_url) The nano-twinned grain under two different modes of shear loading.
Figure 4.2 Cyclic stress-strain hysteresis curves for case 1 and 2.
Figure 4.2 shows the cyclic stress-strain response of both cases under strain control. Since MD simulations are performed on pristine crystals, and at high deformation rates, the stresses from MD are high compared to experimental material stress-strain response. However, the dislocation reactions associated with slip-twin interactions are expected to be similar. Therefore, the cyclic stress-strain plots in the present works are interpreted only to obtain the quantitative estimation of the quasi-steady state response of the system under investigation.

The reason for applying these two particular shear loadings is to impart maximum and zero resolved shear stress on the coherent twin boundaries (CTB). Since slip-twin interactions are largely dependent on the resolved shear stress (RSS) on the CTB as well as on the incoming and outgoing slip systems, applying shear in these two particular directions would help provide the two extremities of RSS on CTB and hence facilitate the study of slip-twin interactions for two extreme cases (Table 4.1). Four cycles of loading are applied to both cases in order to be able to obtain a steady state of the cyclic stress-strain response (Figure 4.2).

The stress-strain plots demonstrate that the material reaches the steady state cyclic response after the first cycle, and throughout the subsequent cycling the steady state response prevails.

4.2 Steady State Response at Dislocation Level

Atomistic visualization softwares such as Visual Molecular Dynamics (VMD) (Humphrey et al., 1996), (http://www.ks.uiuc.edu/Research/vmd), and AtomEye (Li, 2003), (http://li.mit.edu/Archive/Graphics/A/) are used to probe into the snapshots of the microstructure
evolution during the simulations of the fatigue cycling. These snapshots reveal dislocation nucleation and their interactions with the annealing twin present in the vicinity of the dislocation source (crack-tip). During the cycles of load reversal, dislocations nucleate and glide on their slip planes, and when the load is reversed, after elastic recovery, dislocations start moving in the opposite directions at the point of yielding in reverse plastic flow. Throughout each cycle, to-and-fro glide of dislocations emitted from the crack-tip occurred across the twin, and their complex interactions with the twin are studied. Special MATLAB codes are developed to determine and analyze the conservation of the burgers vectors of all the interacting dislocations at the CTB.

Geometry of crack-tip is found to be a principal factor in determining whether the type of dislocations emitted would be of mixed, pure edge or pure screw type. For case 1, the geometry of the dislocation source is engineered to emit pure screw dislocations from the crack-tip, which subsequently glide away towards the twin to interact. Similarly, for case 2, pure edge dislocations emit from the crack-tip and continue gliding to react with the CTB. Figure 4.3 and 4.4 describe the steady state dislocation-twin interactions for screw and edge dislocations from case 1 and case 2 respectively. Interactions of pure edge or screw dislocations with coherent twin boundaries have also been studied through atomistic simulations by (Jin et al., 2008), (Zhu et al., 2007), (Jin et al., 2006). Observations in our simulations comply with these findings in literature.

Both for the edge and screw dislocations, with increasing twin lamella spacing and/or crack-tip to the CTB distance, the steady state reaction mechanism involves more than one dislocation that undergo a more complicated form of slip-twin interactions. Nevertheless, the
type of slip-twin interactions with the changes of these microstructural characteristic lengths could be generalized into a common pattern. In the following sections, the most typical examples of these mechanisms, after the steady-state cyclic response is achieved, are discussed in details both for screw and edge dislocations.

### 4.2.1 Case 1 (Screw Dislocation)

In Figure 4.3, during the forward half of the cycle after elastic straining (at point A), a perfect pure screw dislocation of the burgers vector, $\frac{a}{2}[1\bar{1}0]$ emits from the crack-tip. Immediately after the emission, the full screw dislocation dissociates into two Shockley partials separated by a ribbon of stacking fault (Copley and Kear, 1968) (Figure 4.3(a)).

\[
\frac{a}{2}[110] = \frac{a}{6}[211] + \frac{a}{6}[121] + \text{Stacking Fault}
\]

<table>
<thead>
<tr>
<th>Full (matrix)</th>
<th>leading (matrix)</th>
<th>trailing (matrix)</th>
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<td>Full (matrix)</td>
<td>leading (matrix)</td>
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Under the application of the external load, the leading and the trailing Shockley partials glide towards the CTB, and being baffled by the CTB, the two partials re-combine and cause multiplication generating new screw dislocations at the site of incidence. Both the new screw dislocations dissociate into Shockley partials (Figure 4.3(b)). One of the new screw dislocations stays on the CTB and another transmits inside the twin.

\[
\frac{a}{6}[211] + \frac{a}{6}[121] = \frac{a}{6}[121] + \frac{a}{6}[112] + \frac{a}{6}[211]_{\text{T}} + \frac{a}{6}[121]_{\text{T}}
\]

<table>
<thead>
<tr>
<th>leading (matrix)</th>
<th>trailing (matrix)</th>
<th>twinning (CTB)</th>
<th>twinning (CTB)</th>
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<tr>
<td>leading (matrix)</td>
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<td>(CTB)</td>
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Till the end of the loading cycle, the twinning partials on the CTB keep gliding to the opposite directions to each other, gradually increasing their separation distance in order to minimize the elastic strain energy. This kind of interaction is also observed by (Zhu et al., 2007), (Jin et al., 2006). The transmitted partials inside the twin keep gliding until they reach the upper twin boundary or the load is reversed. Because of the gliding of the twinning partials, the twin boundary migrates by one atomic layer (Figure 4.3(b)).

Upon the reversal of the load (unloading), the previously transmitted leading and trailing partials (inside the twin) now flip their motion after the elastic strain recovery. The returning partials interact with the CTB and undergo similar multiplication, thereby creating two new twinning partials gliding on the CTB and two dissociated Shockley partials into the matrix (Figure 4.3(c)).

\[
\frac{a}{6}[211]_{\text{twin}} + \frac{a}{6}[121]_{\text{twin}} = \frac{a}{6}[211] + \frac{a}{6}[121] + \frac{a}{6}[\overline{1}21] + \frac{a}{6}[\overline{1}12]
\]

leading twinning leading trailing
(twin) (twin) (CTB) (CTB) (matrix) (matrix)

With further unloading, the twinning partials again continue positioning themselves in greater separation distance, eventually causing twin migration by one atomic layer. The matrix partials continue gliding towards the crack-tip until a new full dislocation (also dissociated) of opposite sign nucleates from the crack-tip, and meets with the returning ones on the way, and they annihilate each other. At the end of the unloading, a new negative dislocation (at the beginning of the loading, first nucleation is of positive type) nucleates and continues gliding towards the twin, repeating the same mechanism over the subsequent cycles (Figure 4.3(d)).
Case 1

Screw Dislocation

(a) Nucleation and dissociation of a full screw dislocation into leading and trailing Shockley partials (red)

(b) Leading and trailing partials hit CTB and multiply into two more full screw dislocations subsequently dissociating into partials on CTB (black) and inside twin (green)

(c) Twinning partials (black) from forward load cause one layer of twin migration (not shown). Returning Shockley partials (green) multiply into more twinning partials (purple) and matrix Shockley partials (red) which get annihilated by newly nucleating incoming partials (red) of opposite sign

(d) Twinning partials on CTB (purple) continue gliding in opposite directions resulting in twin migration again. Another negative pair of Shockley partials (red) nucleate from crack-tip.

Figure 4.3 Steady state slip-twin interactions (screw).
4.2.2 Case 2 (Edge Dislocation)

In Figure 4.4, a most typical case of the steady state slip-twin interactions for edge dislocations (incident) is described. Upon loading, a leading Shockley partial dislocation nucleates followed by a trailing partial, and continues gliding towards the CTB (Figure 4.4(a)). Once the leading partial reacts with the CTB, it creates another leading partial transmitting inside the twin and a sessile Frank partial dislocation at CTB (Figure 4.4(b)) (Ezaz et al., 2011).

\[
\frac{a}{6}[121] = \frac{a}{6}[121]_T + \frac{2a}{9}[111]
\]

The Frank partial dislocation dissociates into two more Shockley partials. One of these two Shockley partials transmits into the twin, and becomes the trailing partial for the previously transmitted leading partial, separated by a ribbon of stacking fault. The other Shockley partial glides back into the matrix, and interacts with the incoming trailing Shockley partial which is still continuing its glide towards the CTB, and then they annihilate.

\[
\frac{2a}{9}[111] = \frac{a}{6}[211] + \frac{a}{6}[211]_T
\]

\[
\frac{a}{6}[211] + \frac{a}{6}[211] = 0
\]
Upon unloading, if the transmitting dislocations inside the twin do not reach the other CTB, after the elastic strain recovery, they flip their directions of motion in reverse plastic flow, and start returning towards the firstly encountered CTB. Reversal of edge dislocation motions, after interacting with grain boundaries, upon reversing load, is also observed experimentally by (Mughrabi, 2010). When the returning leading partial from inside the twin hits the CTB, a twinning partial and a stair rod dislocation nucleate.

$$\frac{a}{6}[2\ 1\ 1]_T = \frac{a}{6}[1\ 1\ 2]_T + \frac{a}{6}[3\ 0\ 1]_T$$

leading twinning stair rod
(twin) (CTB) (CTB)

Meanwhile, the returning trailing partial catches up with this stair rod, and two more stair rod dislocations on the CTB and one Shockley partial into the matrix nucleate.

$$\frac{a}{6}[3\ 0\ 1]_T + \frac{a}{6}[1\ 2\ 1]_T = \frac{a}{6}[2\ 1\ 1] + \frac{a}{6}[0\ 1\ 3] + \frac{a}{3}[1\ 0\ 0]$$

stair rod trailing leading stair rod stair rod
(twin) (twin) (matrix) (CTB) (CTB)

The stair rod dislocations are unstable and eventually break down into one twinning partial on the CTB and another Shockley partial into the matrix (Figure 4.4 (c)).

$$\frac{a}{6}[0\ 1\ 3] + \frac{a}{3}[1\ 0\ 0] = \frac{a}{6}[1\ 1\ 2]_T + \frac{a}{6}[1\ 2\ 1]$$

stair rod stair rod twinning trailing
(CTB) (CTB) (CTB) (matrix)
Figure 4.4 Steady state slip-twin interaction (edge).

(a) Nucleation of pure edge leading and trailing Shockley partials (red)

(b) Incident partials interact with CTB and create unstable sessile residual dislocation (black) and one pair of glissile Shockley partials transmitting inside twin (purple)

(c) Returning Shockley partials from inside the twin (not shown) interact with residual left on CTB and create another set of sessile unstable dislocations (blue)

(d) Unstable sessile dislocations dissociate into new stable sessile dislocation (blue), twinning partial (purple) and returning glissile Shockley partials into matrix (red) which subsequently get annihilated with another newly nucleated negative pair of partials from crack-tip (red)
Two twinning partials (one nucleated through the incidence of returning leading partial and another from the dissociation of the stair rod dislocations) annihilate each other. The matrix Shockley partial dislocations also get annihilated by another newly nucleated negative dislocation (dissociated into partials) from the crack-tip.

\[ \frac{a}{6}[112]_T + \frac{a}{6}[112]_T = 0 \text{ (annihilation)} \]
\[ \text{twinning (CTB)} + \text{twinning (CTB)} \]

\[ \frac{a}{6}[211] + \frac{a}{6}[121] + \frac{a}{6}[121] + \frac{a}{6}[211] = 0 \text{ (annihilation)} \]
\[ \text{leading (matrix)} + \text{trailing (matrix)} + \text{leading (matrix)} + \text{trailing (matrix)} \]

Annihilation of twinning partials is found to be a special case when twin lamella spacing and/or the crack-tip to twin distance is large. In other cases (smaller crack-tip to twin distance or twin lamella spacing), the interaction mechanism is slightly modified with the retention of twinning partials on the CTB instead of annihilation. But same fundamental mechanism of annihilation occurs for the returning dislocations towards the crack-tip upon unloading, thereby leading to an overall irreversible dislocation dynamics.

At the end of the unloading cycle, after the first nucleation of negative dislocation that eventually annihilates the returning dislocation, a new pair of negative partial dislocations nucleate and continue gliding towards the CTB (not shown in Figure 4.4). The whole mechanism
is repeated over the next cycle with only a change of signs of burgers vectors in the abovementioned mechanism.

4.3 Summary of Slip-twin interactions Observed

For case 1 and case 2, under applied loading $\sigma_{ij}$, resolved shear stresses (RSS) on the slip systems with normal vector $m_i$ and slip direction $n_j$ have been analyzed using the following formulation.

$$\tau_{\text{RSS}} = \sigma_{ij}m_i n_j$$

For Case 1, incident dislocation is of pure screw type whose interaction with the CTB leads to multiplication of more screw dislocations some of which transmit inside the twin, and some glide on the CTB (preferentially) since the RSS on CTB is high. For Case 2, pure edge dislocations nucleate and upon interacting with the twin, transmit inside the twin leaving sessile residual dislocations on the CTB with no glissile dislocation on CTB due to zero RSS, although during unloading there are some incorporation of twinning partials on CTB because of high local stress imposed by residual sessile dislocations (Figure 4.4(d)).

Table 4.1 Resolved shear stress and burgers vectors for case 1 and 2.

<table>
<thead>
<tr>
<th>Case</th>
<th>RSS (incident)</th>
<th>RSS (CTB)</th>
<th>RSS (Outgoing)</th>
<th>Slip-twin Reaction</th>
<th>Incident b (matrix)</th>
<th>Outgoing b</th>
<th>Residual b_r (CTB)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>b_s</td>
<td>b_e</td>
<td></td>
<td></td>
<td>$\frac{a}{2}[110]$</td>
<td>$\frac{a}{2}[110]_T$</td>
<td>$\frac{a}{2}[011]$</td>
</tr>
<tr>
<td>1</td>
<td>0.778</td>
<td>1</td>
<td>0.778</td>
<td>Multiplication</td>
<td>0</td>
<td>$\frac{a}{2}[121]$</td>
<td>$\frac{a}{6}[121]_T$</td>
</tr>
<tr>
<td>2</td>
<td>0.816</td>
<td>0</td>
<td>0.816</td>
<td>Transmission</td>
<td>0</td>
<td>$\frac{a}{6}[121]$</td>
<td>$\frac{2a}{9}[111]$</td>
</tr>
</tbody>
</table>
4.4 Calculation of Slip Irreversibility

Irreversibility of dislocation-twin interactions per fatigue cycle is calculated using the parameter introduced by (Differt et al., 1986) discussed in details in Chapter 2.

\[ p = \frac{\gamma_{irr}}{\gamma_{total}} \]

Figure 4.5 An example of calculation of slip irreversibility based on the slip-twin interactions observed.

As an example of a typical case, with slip transmission in the forward half of the cycle, and incorporation along with annihilation in the reverse half cycle as in the Figure 4.5, the following type of formulations could be derived to quantify the degree of total irreversible dislocation activities under fatigue cycle.

\[ p = \frac{\gamma_{irr}^p}{\gamma_{total}} = \frac{\gamma_{AE}^p + \gamma_{BD}^p}{\gamma_{AB}^p + \gamma_{BC}^p + \gamma_{BD}^p} = \frac{x_{AE} + x_{BD}}{x_{AB} + x_{BC} + x_{BD}} \]  \hspace{1cm} (1) \]

Strain caused by dislocations at the crack-tip is calculated as follows.
Plastic strain due to the gliding of one dislocation is,

\[ \gamma = \frac{b}{h} = \frac{bA}{htx_1} = \frac{btx_1}{V} \]

For more than one dislocations (two, for example),

\[ \gamma = \frac{btx_1}{V} + \frac{btx_2}{V} = \frac{bt}{V} \sum \frac{x_i}{V} = \left( \frac{2t}{V} \right) b \left( \sum \frac{x_i}{2} \right) \]

\[ \therefore \gamma = \rho b x \]  \hspace{1cm} (2)

where, \( b = \) burgers vector, \( \rho = \) dislocation density, \( x = \) length traveled by a dislocation,

\( A = \) area swept by dislocations, \( t = \) thickness in/out of plane,

Using the similar formulations as (1), slip irreversibility is calculated both for edge and screw dislocation cases as a function of the twin lamella spacing and the crack-tip to twin spacing. The results are shown in the Figure 4.7 and 4.8.
In Figure 4.7, as the twin spacing is increased with constant crack-tip to twin spacing d, slip irreversibility, p also increases non-linearly. For very small twin spacing, the dislocation annihilation takes place very close to the crack-tip, thereby minimizing the contribution of the term $x_{AE}$ to p in equation (1), with the incorporation length being almost unchanged. Therefore, p is small for small twin spacing. With increase in lamella spacing, the annihilation occurs further away from the crack-tip, and at some point with further increase in t, annihilation of returning dislocations occurs very close to the upper twin boundary (Figure 4.7) with increased $x_{AE}$ contribution to the parameter p. Incorporation length for different t stays almost unchanged. While calculating p for smaller t, all the dislocations in forward part of the cycle are allowed to traverse across the entire twin spacing and interact with the upper twin boundary and transmit back into the matrix on the other side of the twin. The p values reach a plateau at higher t as more than one dislocation nucleate while the firstly-nucleated dislocation continues traversing the entire thickness t and reach the other side of the twin.

Similar affects are observed if t is kept unchanged while d is increased gradually (Figure 4.8). For larger d, the location of annihilation point of returning dislocations with the newly nucleated incident dislocations moves further away from the crack-tip, to eventually settle at the lower CTB. At higher d, more than one dislocation nucleates and the length $x_{AE}$ becomes larger. Irreversibility due to screw dislocations is found to be greater than the edge because of the larger incorporation length on the CTB during the cyclic forward and reverse motion of the screw dislocations.

Atomistically calculated slip irreversibilities are subsequently fed into a dislocation dynamics based $da/dN$ formulations to simulate various spacing of crack-tip to twin as well as twin lamella, and understand their effects on the FCG.
Figure 4.7 Slip irreversibility calculated in molecular dynamics simulations as a function of the twin lamella spacing (t).
Figure 4.8 Slip irreversibility calculated in molecular dynamics simulations as a function of the crack-tip to twin spacing (d).
4.5 Dislocation Dynamics da/dN Formulations

In order to derive da/dN formulations based on the discrete dislocation assumption, we use the force balance acting on dislocations nucleated from the crack-tip and located some distance away from it at the equilibrium positions under the application of applied load at any instance of the cyclic loading. The dislocation nucleation criterion is based on the (Rice and Thomson, 1974) formulations. According to this approach, at its equilibrium position, after gliding away from the crack-tip, a certain dislocation experiences three forces – i) applied loading, ii) force due to the image stress and iii) pile-up force originating from the attractive or repulsive forces of other dislocations present in the vicinity.

The force balance formulations, based on Pippan (1989, 1991, 1992), are utilized in the present work to derive da/dN formulations, and subsequently atomistically calculated slip irreversibilities are incorporated therein.

![Figure 4.9](image.png)

Figure 4.9 Crack growth upon slip emission from the crack-tip interacting with an obstacle (annealing twin) present in the vicinity.

Over each cycle, the crack-tip opens and closes with an incremental growth. For a general loading mode case, da/dN in terms of the crack-tip displacement could be written as,
\[
\frac{da}{dN} = \frac{\cos\theta}{x_{\text{max}}} \int_0^{x_{\text{max}}} \Delta u \, dx
\]
\[
\frac{da}{dN} = (u_f - u_r) \cos\theta
\]

where, \(x_{\text{max}}\) = maximum length away from crack-tip traveled by a dislocation

\(\theta = \) angle between crack propagation and slip emission direction (\(0^\circ\) for mode II or III)

\(u_f = \) total displacement along the dislocation emission direction in forward loading

\(u_r = \) total displacement recovered by returning dislocations in reverse loading

The crack-tip displacement is related to the shear stress acting on the dislocation emitted, \(\tau\).

\[
\tau = 2\mu \frac{du}{dx}
\]
\[
\therefore \ du = \frac{\tau}{2\mu} \, dx
\]

Total displacement of the crack-tip in the slip direction could be obtained by integrating \(du\) over the maximum length away from the crack-tip traveled by dislocations. If there are \(n\) number of dislocations emitted from the crack-tip, steps left behind by each dislocation would contribute to the overall crack-tip displacement in the direction of the slip emission.

\[
u_f = \frac{1}{2\mu} \int_b^{x_{\text{max}}} \tau_{\text{max}} \, dx = \frac{x_{\text{f max}}}{2\mu} \sum_{i=1}^{n} \tau_{n}^{\text{max}}
\]

\[
u_r = \frac{1}{2\mu} \int_b^{x_{\text{max}}} \Delta\tau_{\text{min}} \, dx = \frac{x_{\text{f max}}}{2\mu} \sum_{i=1}^{n} \Delta\tau_{n}^{\text{min}}
\]

where, \(b = \) burgers vector of a dislocation
\[ \mu = \text{shear modulus} \]

\[ \tau_n = \text{shear stress acting on } n^{th} \text{ dislocation} \]

Therefore, for the \( n^{th} \) dislocation, the balance of the abovementioned three kinds of forces gives,

\[ \tau_{n}^{\text{max}} = \frac{K_{1}^{\text{max}}}{\sqrt{2\pi x_n^f}} - \frac{A}{2 x_n^f} - A \sum_{i \neq n} \left( \frac{x_i^f}{x_n^f} \right)^{1/2} \frac{1}{x_i^f - x_n^f} \tag{7} \]

\[ \Delta \tau_{n}^{\text{min}} = \frac{K_{1}^{\text{min}}}{\sqrt{2\pi (x_n^f - x_i^r)}} - \frac{A}{2 (x_n^f - x_i^r)} - A \sum_{i \neq n} \left( \frac{x_i^f - x_i^r}{x_n^f - x_n^r} \right)^{1/2} \frac{1}{(x_i^f - x_i^r) - (x_n^f - x_n^r)} \tag{8} \]

where, \( K = \text{stress intensity factor} \)

For screw, \( A = \frac{\mu b}{2\pi} \)

For edge, \( A = \frac{\mu b}{2\pi(1 - \nu)} \)

In the shear stress formulations above, equation (7 & 8), the first term comes from applied loading, and the second term from the image stress acting against the glide of the dislocations away from the crack-tip. The last term accounts for the pile-up stress acting on a particular dislocation due to the rest (Pippan 1989, 1991, 1992).

So, under mode II or III, the crack extension per cycle, \( da/dN \), becomes,

\[ \frac{da}{dN} = \frac{x_{\text{max}}}{2\mu} \sum_{i=1}^{n} \tau_{n}^{\text{max}} - \Delta \tau_{n}^{\text{min}} \tag{9} \]
\[
\frac{da}{dN} = \frac{x_{\text{max}}^f \Delta K}{2\mu \sqrt{2\pi}} \sum_{i=1}^{n} \left( \frac{1}{\sqrt{x_i^f}} - \frac{1}{\sqrt{x_i^f - x_i^r}} \right) - \frac{x_{\text{max}}^f A}{4\mu} \sum_{i=1}^{n} \left( \frac{1}{x_i^f} - \frac{1}{x_i^f - x_i^r} \right)
\]

\[
- \frac{x_{\text{max}}^f A}{2\mu} \sum_{i=1}^{n} \sum_{j \neq i} \left( \frac{x_j^f}{x_i^f} \right)^{1/2} \frac{1}{x_j^f - x_i^f} - \left( \frac{x_j^r}{x_i^f - x_i^r} \right)^{1/2} \frac{1}{(x_j^f - x_j^r) - (x_i^f - x_i^r)} \right)
\]

4.6 Dislocation Dynamics \( \frac{da}{dN} \) Simulations

Based on the dislocation dynamics formulations by Pippan (1989, 1991, 1992), \( x_n^f \) are calculated utilizing the fact that at equilibrium positions, the total shear stress acting on dislocations, as in equation (7), is equal to the lattice friction resistance to dislocation gliding. The expression for the lattice friction is used after Pippan (1989, 1991, 1992). In these simulations, as the applied loading is kept increased, updated postions of the present dislocations as well as that of newly nucleated dislocations are calculated. Figure 4.10(b) and 4.11(b) demonstrate the trajectories for cases of a single dislocation and multiple dislocations respectively during the forward loading for a mode III crack.

Once the \( x_n^f \) are known for forward loading, \( x_n^r \) (for reversed loading) are solved using the atomistically calculated slip irreversibility parameter, \( p \), to impose the affects of different twin lamella thicknesses and twin to crack-tip distance.

\[
p = \sum_{i=1}^{n} \frac{x_i^f}{2x_i^f - x_i^r}
\]  

(11)
Figure 4.10 (cont. on next page)
Figure 4.10 A single dislocation demonstration of trajectory during da/dN calculations (a) A mode III crack emits a positive screw dislocation in the forward loading, and a negative dislocation in the reverse loading, which annihilate the returning positive dislocation. (b) Trajectory of the dislocation is shown for the forward load. (c) During reverse loading, after elastic relaxation, it starts returning, and gets annihilated by a newly nucleated negative dislocation.

Figure 4.10 shows a single dislocation demonstration of slip irreversibility under a mode III crack in the dislocation dynamics simulations. In forward loading, a screw dislocation nucleates and glides away from the crack-tip, and eventually takes its equilibrium position at the maximum applied stress intensity factor. The distance of the dislocation from the crack, \( x_1^f \), versus applied load, \( K_{\text{III}} \), is shown. When the load is reversed, the dislocation does not start returning towards the crack immediately because of the elastic unloading. At reverse yielding, it
starts gliding towards the crack, and at the same time a new negative dislocation is emitted which annihilates the returning dislocation on the way at $x_1^r$. Red denotes the crack to dislocation distance during forward loading, and blue represents reverse loading.

(a)

(b)

Figure 4.11 (cont. on next page)
Figure 4.11 A multiple dislocation demonstration of dislocation trajectory during da/dN calculations using dislocation dynamics simulations. (a) A mode III crack emits n number of positive screw dislocations in forward loading, and negative dislocations in reverse loading which annihilate returning positive dislocations (dislocations are shown at maximum applied load in the schematic). (b) Trajectory of dislocations is shown from the point of nucleation to the maximum forward load. (c) During reverse loading, some of the dislocations start returning to the crack and get annihilated by new negative dislocations, and the rest undergo elastic relaxation.

Similarly, for multiple dislocations emission during the forward half of the fatigue cycle, when the load is reversed, some of the returning dislocations get annihilated on their way back to the crack-tip by negative dislocations coming from the crack-tip in reverse yielding. The trajectories of dislocations nucleated in the forward and reverse loading are shown in Figure...
4.11. The abovementioned $da/dN$ formulations from equation (10) are then implemented at different $\Delta K$ solving for $x_n^r$ from equation (11). In equation (11), $p$ is previously obtained from MD simulations (Figure 4.7 and 4.8). $da/dN$ versus $\Delta K$ are calculated for increasing twin lamella thickness at constant crack-tip to twin distance (Figure 4.12), and similarly for increasing crack-tip to twin distance at constant twin lamella spacing (Figure 4.13).

Figure 4.12 and 4.13 in the following pages, demonstrate how the change in any one of these microstructural characteristic lengths (while the other being constant) affects $da/dN$. For decrease either in the spacing of nano-twin lamella or the twin to the crack-tip, $da/dN$ also decreases.

The correlation of $da/dN$ with the change in these characteristic microstructural dimensions is governed by the change in irreversibility of the crack-tip emitted dislocations interacting with the annealing nano-twin in the vicinity. The trend of the slip irreversibilities, as calculated from MD simulations, as a function of these dimensions is depicted in the Figure 4.7 and 4.8. Slip irreversibility ($p$) increases non-linearly with positive slopes as these characteristic lengths become larger. Eventually, $p$ is found to become independent of these lengths with the slope reaching zero. Further increase of lengths does not change slip irreversibilities. Similar trends in $da/dN$ with respect to the change in the spacing of the twin to the crack-tip or the twin lamella thickness are observed in the dislocation dynamics FCG simulations. Figure 4.12 and 4.13 shows the variations in $da/dN$ as per the change in these microstructural characteristic lengths where $da/dN$ versus $\Delta K_{\text{III}}$ curves, as plotted, represent the Paris regime (stable crack growth regime).
Figure 4.12 \( \frac{da}{dN} \) versus \( \Delta K_{\text{III}} \) demonstrating the influence of twin thickness on FCG at a constant crack-tip to twin spacing of 50Å.
Figure 4.13 $da/dN$ versus $\Delta K_{\text{III}}$ demonstrating the influence of crack-tip to twin distance on FCG at a constant twin lamella spacing of 50 Å.
Chapter 5: Conclusions

5.1 Summary

The role of annealing twins on the FCG of nano-crystalline materials has been studied using molecular dynamics and dislocation dynamics simulations. Recent experimental results on FCG of electro-deposited Ni-Co alloys indicate beneficial effects of the presence of nano-twins. TEM images of post-fatigue specimens reveal that a dislocation mediated plastic deformation mechanism is prevalent at that length scale (Sangid et al., 2011). The high resistance to FCG due to the nano-twins observed is also supported by some current findings in literature in electro-deposited nano-twinned copper by (Singh et al., 2011). In the present study, the isolated role of twin lamella thickness and the location of the nano-twins with respect to the propagating crack on FCG is investigated. This study clearly identifies and isolates these effects along with developing a method of quantifying irreversibility of crack-tip emitted dislocations interacting with any nano-obstacles present in the vicinity of the crack-tip, thereby capturing the governing physics at the appropriate length scale.

Through MD simulations we developed a method to quantify the irreversible dislocation glide process leading to the cyclic crack extension with the presence of nano-obstacles. Molecular dynamics simulations inherently involve time scale effects such as high strain rate, but calculation of slip irreversibility in the current approach does not retain any of the artificial effects arising from the high strain rate phenomenon. The slip irreversibility computed with our approach is a function of local plastic strain generated by the gliding distance of the dislocations in forward and reverse loading. The distances traveled by dislocations depend on the type
interactions with annealing twins, location of the twin with respect to the crack-tip and the twin lamella thickness. These factors are not strain-rate dependent.

The dislocation dynamics simulations based on the atomistically calculated slip irreversibility demonstrates that with decreasing twin lamella thickness or crack-tip to twin spacing, \( \frac{da}{dN} \) also decreases. Since the slip irreversibility reaches a plateau at larger twin thickness or distance to crack, \( \frac{da}{dN} \) follow the same trend as per our findings.

5.2 Future Works

Currently, our model compared \( \frac{da}{dN} \) as a function of twin lamella width or crack to twin spacing. This model can also shed light on the threshold behavior based on a discrete dislocation mechanism, thereby isolating the effects of the aforementioned characteristic microstructural lengths on threshold for FCG with the presence of any other nano-obstacles. Furthermore, this model could be extended to investigate \( \frac{da}{dN} \) for different microstructure of Ni-Co alloys, thereby providing a conduit to understand the role of different grain sizes as well.
References


