ABSTRACT

WU, QIFENG. Predictions of Microstructurally Induced Failure Nucleation and Propagation in High Strength Martensitic Steel Alloys. (Under the direction of Professor Mohammed A. Zikry).

A dislocation-density based crystal plasticity formulation, which accounts for martensitic microstructures, variant morphologies, orientation relationships (ORs), retained austenite, carbide precipitates, dislocation-density evolution, and dislocation-density grain boundary (GB) interactions, has been developed to investigate large inelastic deformation and failure modes, such as quasi-static and dynamic crack nucleation and growth and diffusion assisted hydrogen embrittlement in high strength martensitic steels.

A dislocation-density GB interaction scheme for dislocation transmission and impedance across martensitic block and packet boundaries has also been developed, and it was incorporated into the dislocation-density based crystal plasticity formulation. This dislocation-density GB interaction scheme was then coupled with a fracture approach to investigate the effects of GB on crack nucleation. The failure criteria are based on resolving stresses onto microstructural fracture planes, such as the cleavage planes of \{100\} and the hydrogen assisted microstructural fracture planes of \{110\} in lath martensitic steels. This microstructurally based fracture method utilizes an overlapping finite-element method where failure surfaces are nucleated and propagated as a function of preferred failure planes and orientations, dislocation-density evolution, and martensitic block orientations. For hydrogen diffusion assisted fracture, a pressure dependent form of Fick’s Second Law diffusion equation was coupled to the crystal plasticity formulation and the non-linear finite element framework to investigate the effects of martensitic block/packet boundaries and carbide precipitates on hydrogen diffusion and embrittlement, and to understand and predict how
hydrogen diffusion affects dislocation-density evolution and subsequent martensitic embrittlement. Stresses along the three cleavage planes and the six hydrogen embrittlement fracture planes were monitored to characterize the competition mechanism between cleavage fracture and hydrogen diffusion assisted fracture along preferential crystallographic planes.

Dislocation-density evolution and accumulation ahead of the crack front had a dominant effect on crack propagation, and large dislocation-density generation ahead of crack front blunted crack and inhibited crack propagation, which significantly increased fracture toughness. GBs and blocks with large misorientations resulted in dislocation-density pile-ups, high local stresses, and this resulted in crack nucleation. Hydrogen diffusion was shown to suppress dislocation density emission, which led to martensitic embrittlement and subsequent fracture at low nominal strains.

Retained austenite resulted in lower interfacial stresses and larger plastic deformations, and also resulted in dislocation-density accumulation around crack fronts for quasi-static and dynamic fracture. This decreased overall strength and increased the toughness of martensitic steels due to enhanced slip activity along austensite-martensite interfaces. Carbide precipitates resulted in higher local stresses and lower plastic deformations. Due to the impedance of dislocation-densities, precipitate interfaces were shown to be the sites of crack nucleation. Size refinement of martensitic blocks and packets increased the frequency of crack deflection at block and packet interfaces, which would increase overall fracture toughness. For the diffusion assisted hydrogen embrittlement cases, GBs and blocks with large misorientations and carbide precipitates impeded dislocation-densities, led to high local tensile pressure and hydrogen accumulation, which locally embrittled martensitic blocks and resulted in crack nucleation. Stress accumulations ahead of
crack front resulted in large pressure gradient and hydrogen accumulation, and this led to a significant reduction of the critical fracture stress and accelerated crack growth.

These validated predictions indicate that the collective and interrelated effects of the orientation and size of martensitic blocks and packets, variants and GBs, the distribution of retained austenite and carbide precipitates can be fundamentally optimized at the microstructural scale for failure resistance for quasi-static, dynamic, and hydrogen diffusion assisted crack nucleation and propagation.
Predictions of Microstructurally Induced Failure Nucleation and Propagation in High Strength Martensitic Steel Alloys

by
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DEDICATION

This work is dedicated to my parents, my wife and sister for your endless love, support and understanding.
Qifeng Wu was born and raised in Nanchong, Sichuan, China. He attended Huazhong University of Science and Technology, China for his undergraduate studies in Naval Architecture and Ocean Engineering. He received a bachelor degree in Naval Architecture and Ocean Engineering in June of 2009. After graduation, he attended North Carolina State University (NCSU) for his graduate studies in Mechanical Engineering, and earned a Master of Science degree in Mechanical Engineering in May of 2011. In the summer of 2011, he continued his studies in PhD program in Mechanical Engineering at NCSU under advisor Professor Mohammed A. Zikry. The research related to this dissertation has generated the following research papers:


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CHAPTER 1: Introduction

1.1 Overview

Lath martensitic steels, due to their high strength, toughness, and fracture resistance are ideal material choices for critical engineering structures and components. These inherent properties are mainly a result of martensitic steel’s unique lath microstructure, and its orientation relationships (ORs) with parent austenite grain (Morito et al., 2003; Morito et al., 2006). Furthermore, the strength and toughness of lath martensitic steel are strongly related to block morphology, which is a group of laths with low angle misorientations, and a packet morphology, which is a collection of blocks with the same habit plane (Krauss, 1999; Swarr and Krauss, 1976), and block and packet sizes are proportional to the parent austenite grain size (Morito et al., 2005). Experimental observations have also shown that martensitic packet sizes are related to the size of cleavage facets, due to large misorientations of \{100\} cleavage planes at packet boundaries, and this affects the fracture toughness of martensitic steel (Wang et al., 2008).

Refinement of the block and packet size can reduce the coherence length on the \{110\} and \{112\} slip planes, and on the \{100\} cleavage planes. This decrease of the coherence length on slip planes can improve the strength by impeding dislocation motion, while the decrease of the coherence length on cleavage planes can improve fracture toughness by deflecting crack propagation at block and packet boundaries (Morris, 2011; Guo et al., 2004; C. Wang et al., 2007). While block and packet refinement can improve strength, it can also result in significant loss in ductility (Song et al., 2006; Tsuji et al., 2002).
In martensitic steels, ductility and toughness can be improved through retained austenite. Generally, small amounts of retained austenite are frequently observed in martensitic steel depending on the carbon content and heat treatment conditions (Park et al., 2004; Thomas, 1978). Retained austenite is mainly located at martensitic inter-lath boundaries and block/packet boundaries (Song et al., 2010; Morito et al., 2011; Ma et al., 2012). These block-like or pockets of retained austenite can improve ductility and toughness, but decrease the strength of martensitic steel (Nakagawa and Miyazaki, 1999; Moor et al., 2008). In addition, the transformation of retained austenite to martensite in the regions close to fracture surfaces has been observed in martensitic steel (Bilmes et al., 2001; Song et al., 2010). These transformations can induce plastic zones, absorb strain energy, and effectively improve fracture toughness.

The strength of steels can be increased through introduction of precipitates (Xu et al., 2011; Ghosh et al., 2005; Zhou et al., 2013), since these fine precipitates can impede dislocation movement. The strength improvement is related to the size, volume fraction, distribution, and crystal structure of precipitates (Shen and Hansen, 1997; Chen et al., 2014; Lu et al., 2012). Besides improving the strength, the hard precipitates usually reduce ductility and fracture toughness of steels (Chen et al., 2002; Simmons, 1995). Experimental observations have shown that the hard precipitates can act as the sites of crack nucleation (Yin et al., 2007; Zhang et al., 2001; Du et al., 2012).

In martensitic steels, various precipitates including $\text{M}_2\text{C}_6$, $\text{M}_6\text{C}$, $\text{M}_7\text{C}_3$, MX and $\text{M}_2\text{X}$ are frequently observed, where $\text{M}$ represents a metallic element, and $\text{X}$ is carbon or nitrogen atoms (Ping et al., 2005; Ma et al., 2012; Krauss, 1999). A primary precipitate is the carbide
precipitate $M_{23}C_6$, where $M$ is mainly Cr and can be replaced with Fe, Mo, Ni (Song et al., 2010; Maruyama et al., 2001). The $M_{23}C_6$ carbide precipitates mainly locate at martensitic block and packet boundaries, and parent austenite grain boundaries (Kipelova et al., 2013; Taneike et al., 2004). The $M_{23}C_6$ carbide precipitates have face centered cubic crystal structure, and have cube-to-cube ORs with parent austenite grain (Shtansky et al., 2000; Kaneko et al., 2011). Since they tend to coarsen easily due to solubility of iron and chromium, the $M_{23}C_6$ carbide precipitates have a large size of 0.1 – 0.3 µm with a volume fraction of around 2% (Abe, 2008). These large hard $M_{23}C_6$ carbide precipitates at martensitic block/packet boundaries can act as the sites of crack nucleation (Krauss, 2001), which significantly affect the fracture toughness of martensitic steels.

The fracture toughness of martensitic steels can be significantly affected by environmental factors. Hydrogen embrittlement is a process by which metals and alloys become brittle and fracture due to introduction of hydrogen, which is a result of combined mechanisms that can involve electrochemistry, diffusion, microstructures, fracture mechanisms and external loading (Lynch, 2012; Olden, Thaulow, Johnsen, et al., 2008). Hydrogen embrittlement is a three-step process: (1) the introduction of hydrogen into metals, through electrochemical charging or gaseous absorption; (2) the transportation of hydrogen atoms through metal lattice; (3) the embrittlement of metals, hydrogen assisted crack nucleation and growth (Serebrinsky et al., 2004; Eliaz et al., 2002). Several embrittlement mechanisms have been proposed, which includes hydride formation and fracture (Lufrano et al., 1996), hydrogen enhanced decohesion (HEDE) (Oriani and Josephic, 1977; Oriani and
Josephic, 1974), and hydrogen enhanced local plasticity (HELP) (Birnbaum and Sofronis, 1994; Martin et al., 2011).

High strength martensitic steels are extremely susceptible to hydrogen embrittlement, even at very low hydrogen concentrations (Ramamurthy and Atrens, 2013; Nagao et al., 2012; Lee and Gangloff, 2007; Lee et al., 2010). The effects of hydrogen concentration on embrittlement in martensitic steels have been investigated using quasi-static and creep tests, which indicate that hydrogen can decrease tensile strength in a power law manner (Wang et al., 2007; Wang et al., 2005; Kim et al., 2009). Microstructural features, such as grain size, carbide precipitates, and retained austenite, can affect the susceptibility of martensitic steels to hydrogen diffusion and embrittlement (Fuchigami et al., 2006; Kim et al., 1986; Craig and Krauss, 1980). Hydrogen diffusion assisted microstructural fracture in lath martensitic steel occurs on \{110\} glide planes (Shibata et al., 2012; Kim and Morris, 1983), which is different from the cleavage planes of \{100\} (Morris, 2011; Guo et al., 2004).

Different numerical approaches have been used to predict hydrogen diffusion and embrittlement. Finite element models for hydrogen diffusion have been used to investigate the effects of hydrostatic stress on hydrogen distribution ahead of a stationary crack tip (Sofronis and McMeeking, 1989; Krom et al., 1999; Taha and Sofronis, 2001). Hydrogen assisted crack growth in high strength steels was investigated by the use of a hydrogen dependent cohesive zone model (Serebrinsky et al., 2004) and it was coupled to a stress-assisted hydrogen diffusion model, but this approach does not account for the crystalline structure and the inherent anisotropy of martensitic steels. Rimoli and Ortiz (2010) coupled cohesive zone model and grain boundary diffusion to crystal plasticity to investigate
intergranular hydrogen diffusion and embrittlement. However, the critical martensitic characteristics, such as ORs, variant morphologies, parent austenite orientations, initial dislocation densities, retained austenite, carbide precipitates, and crack growth along specific crystallographic planes are not accounted for in these investigations.

All of these investigations indicate that the combined effects of the morphology and crystallography of martensitic blocks and packets, retained austenite, carbide precipitates, and hydrogen diffusion, have a significant influence on the strength, ductility, and fracture toughness, through the dislocation evolution at both the interfaces and the packet and block boundaries, and the complex crack nucleation and propagation.

1.2 General Research Objectives and Approach

The objective of the present work, therefore, is to develop an integrated framework that incorporates microstructural features of martensitic steels, retained austenite and carbide precipitates, such that failure at different scales can be investigated. An essential aspect of the approach is the modeling of crack nucleation and growth along specific crystallographic planes, incompatible interfaces of martensite (b.c.c.) and retained austenite (f.c.c.), and boundaries of martensitic blocks. A fracture method based on the overlap element method of Wu and Zikry (2014) and Hansbo and Hansbo (2004) has been developed to generate failure surfaces as a function of microstructural characteristics, dislocation-density evolution, and martensitic block orientations.

A multiple-slip dislocation-density based crystal plasticity constitutive formulation (Zikry and Kao, 1996; Shanthraj and Zikry, 2011; Ziaei and Zikry, 2014) is used to obtain a detailed understanding and accurate characterization of interrelated material mechanisms,
which occur over different scales in crystalline materials. The formulation is based on the
framework recently developed by Shanthraj and Zikry (2011) for f.c.c. and b.c.c. crystalline
structures. The dislocation-density evolution equations are coupled through the interaction of
forest densities, which account for the formation and annihilation of junctions. The evolution
equations are coupled to a multiple-slip crystal plasticity formulation, and specialized finite-
 element techniques (Zikry, 1994) are used to characterize the dominant dislocation-density
interaction mechanisms. A dislocation-density GB interaction scheme that is representative
of the resistance to dislocation transmission across block and packet boundaries has been
developed, and it is incorporated into a multiple-slip dislocation-density based crystalline
plasticity formulation. The formulation accounts for variant morphologies and ORs that are
uniquely inherent to lath martensitic microstructures. This framework is then used to
characterize the dominant microstructural mechanisms that control crack nucleation and
growth at large inelastic deformation and dynamic loading condition.

1.3 Dissertation Organization

This dissertation is outlined as follows: Chapter 2 presents the dislocation-density-
based crystal plasticity formulation, the derivation of the dislocation-density GB interaction,
the stress assisted hydrogen diffusion model, and the representation of martensitic
microstructure. Chapter 3 presents the microstructure-based failure criterion, the numerical
implementation of overlapping element method for fracture, and the computational
techniques for dislocation-density-based crystal plasticity. Chapter 4 covers the investigation
into the heterogeneous effects of retained austenite on the behavior of martensitic high
strength steels. Chapter 5 contains the results on microstructural crack nucleation and
propagation in high strength martensitic steels with distributions of retained austenite.

Chapter 6 outlines the results on the effects of $M_23C_6$ carbide precipitates and block size on microstructural dynamic fracture in martensitic steels. Chapter 7 presents the results on diffusion assisted hydrogen embrittlement failure in high strength martensitic steels. Chapter 8 contains the results on the effects of misorientations on intergranular and transgranular fracture in bicrystal martensitic steels. Finally, in Chapter 9 recommendations for future research are given.
CHAPTER 2: Microstructure Modeling and Representation

2.1 Multiple Slip Crystal Plasticity Formulation

The constitutive formulation for rate-dependent multiple-slip crystalline plasticity, coupled to evolutionary equations for the dislocation densities, will be outlined below (Zikry and Kao, 1996; Shanthraj and Zikry, 2011).

The velocity gradient tensor, \( L_{ij} \), is calculated from the deformation gradient as

\[
L_{ij} = \dot{F}_{ij} F_{ij}^{-1}.
\]  

(2.1)

It is assumed that the velocity gradient can be additively decomposed into elastic and plastic parts, \( L^e_{ij} \) and \( L^p_{ij} \). These will be further decomposed into the symmetric deformation rate tensors, \( D^e_{ij} \) and \( D^p_{ij} \), and antisymmetric spin tensors, \( W^e_{ij} \) and \( W^p_{ij} \), as

\[
D_{ij} = D^e_{ij} + D^p_{ij}, \quad W_{ij} = W^e_{ij} + W^p_{ij}.
\]  

(2.2)

The plastic parts are related to the crystallographic slip rates as

\[
D^{p}_{ij} = P^{(\alpha)}_{ij} \gamma^{(\alpha)}, \quad W^{p}_{ij} = \omega^{(\alpha)}_{ij} \gamma^{(\alpha)},
\]  

(2.3)

where \( \alpha \) is summed over all slip-systems, and \( P^{(\alpha)}_{ij} \) and \( \omega^{(\alpha)}_{ij} \) are the symmetric and antisymmetric parts of the Schmid tensor, defined in terms of the slip planes and directions as

\[
P^{(\alpha)}_{ij} = \frac{1}{2} \left( s^{(\alpha)}_i n^{(\alpha)}_j + s^{(\alpha)}_j n^{(\alpha)}_i \right) \quad \text{and} \quad \omega^{(\alpha)}_{ij} = \frac{1}{2} \left( s^{(\alpha)}_i n^{(\alpha)}_j - s^{(\alpha)}_j n^{(\alpha)}_i \right).
\]

(2.4)

As a measure of plastic strain, the effective plastic shear slip is calculated from the plastic deformation rate tensor as
\[
\gamma_{\text{eff}} = \frac{2}{3} \int \sqrt{D_{ij} D_{ij}} \, dt.
\]  

(2.5)

The stress is updated using the Jaumann stress rate corotational with the lattice, \( \sigma_{ij}^{\Delta, e} \), as

\[
\sigma_{ij}^{\Delta, e} = C_{ijkl} D_{kl}.
\]  

(2.6)

where \( C_{ijkl} \) is the fourth-order isotropic elastic modulus tensor defined by

\[
C_{ijkl} = \mu (\delta_{ik} \delta_{jl} + \delta_{jk} \delta_{il}) + \lambda \delta_{ij} \delta_{kl}
\]  

(2.7)

The Jaumann stress rate is related to the material stress rate, \( \dot{\sigma}_{ij} \), in the reference coordinate system as

\[
\dot{\sigma}_{ij} = \sigma_{ij}^{\Delta, e} + W_{ik} \sigma_{kj} + W_{jk} \sigma_{ki}.
\]  

(2.8)

Power law hardening is assumed, relating the slip rates on the various slip systems to the resolved shear stress as

\[
\dot{\gamma}_{\alpha}^{(a)} = \dot{\gamma}_{\text{ref}}^{(a)} \left( \frac{\tau_{\alpha}^{(a)}}{\tau_{\text{ref}}^{\alpha}} \right)^{-1/m} \text{ no sum on } \alpha,
\]  

(2.9)

where \( \dot{\gamma}_{\text{ref}}^{(a)} \) is the reference shear strain-rate which corresponds to a reference shear stress, \( \tau_{\text{ref}}^{\alpha} \), and \( m \) is the strain-rate sensitivity parameter,

\[
m = \frac{\partial \ln \tau_{\alpha}^{(a)}}{\partial \ln \dot{\gamma}_{\alpha}^{(a)}}.
\]  

(2.10)

The reference shear stress includes forest hardening associated with the immobile dislocation density, which accounts for the interaction between slip systems through the
coefficient, $a_{ij}$, and thermal softening through the negative thermal softening exponent, $\zeta$, and reference temperature $T_r$ (293 K) (Franciosi et al., 1980).

$$r_{ref}^\alpha = (r_s^\alpha + \mu b \sum_{j=1,ass} a_{ij} \rho_{im}^j \left( \frac{T}{T_r} \right)^\zeta)$$

For high strain-rate investigations under the assumption of adiabatic heating, the temperature is updated using

$$\dot{T} = \frac{\chi}{\rho c_p} \sigma_{ij} \sigma_{ij}' D_{ij}^p,$$

where $\chi$ is the fraction of plastic work converted to heat, $\rho$ is the mass density, $c_p$ is the specific heat of the material, and $\sigma_{ij}'$ is the deviatoric stress.

### 2.2 Dislocation-Density Evolution

It will be assumed that the total dislocation density can be decomposed additively into mobile and immobile components.

$$\rho^{(\alpha)} = \rho_{im}^{(\alpha)} + \rho_m^{(\alpha)}$$

During an increment of slip, mobile dislocations may be generated, immobile dislocations may be annihilated, or junctions may be formed or destroyed coupling the mobile and immobile dislocation densities, leading to the coupled differential equations governing dislocation density evolution,

$$\dot{\rho}_m^{(\alpha)} = \dot{\rho}_{\text{generation}}^{(\alpha)} - \dot{\rho}_{\text{interaction} -}^{(\alpha)}$$

$$\dot{\rho}_{im}^{(\alpha)} = \dot{\rho}_{\text{interaction} +}^{(\alpha)} - \dot{\rho}_{\text{annihilation}}^{(\alpha)}.$$
The dislocation density evolution follows the formulation of Shanthraj and Zikry (2011). Dislocation density generation is related to the distance, $y_{\text{back}}$, traversed by a dislocation emitted from a source with density, $\rho_{\text{source}}$, both related to the spacing of immobile forest obstacles, i.e., Frank Read mechanism. The average velocity of mobile dislocations, $v^{(\alpha)}$, is used to determine the generation rate as

$$\dot{\rho}_{\text{generation}} = \rho_{\text{source}}^{(\alpha)} \frac{v^{(\alpha)}}{y_{\text{back}}}.$$  \hfill (2.16)

The Orowan equation, $\dot{\gamma}^{(\alpha)} = \rho_{m}^{(\alpha)} b^{(\alpha)} v^{(\alpha)}$, allows the generation rate to be recast as

$$\dot{\rho}_{\text{generation}} = \frac{\phi \sum_{\beta} \sqrt{\rho_{im}^{(\beta)}}}{b^{(\alpha)}} \left( \frac{\rho_{im}^{(\alpha)}}{\rho_{m}^{(\alpha)}} \right) \dot{\gamma}^{(\alpha)},$$  \hfill (2.17)

where $\phi$ is a geometric parameter and $b^{(\alpha)}$ is the magnitude of the Burger’s vector on slip system $\alpha$.

Dislocation density interaction involves the immobilization of mobile dislocation segments due to junction formation that occurs when dislocation densities on different slip systems interact. The frequencies of interaction between mobile dislocation densities on slip system $\alpha$ and mobile and immobile dislocations on slip system $\beta$ are defined as $\rho_{m}^{(\alpha)} \rho_{m}^{(\beta)} v^{(\alpha\beta)}$ and $\rho_{m}^{(\alpha)} \rho_{im}^{(\beta)} v^{(\alpha)}$, where the relative velocity between the slip systems, $v^{(\alpha\beta)}$, is defined using the Orowan equation as

$$v^{(\alpha\beta)} = \frac{\dot{\gamma}^{(\alpha)}}{\rho_{m}^{(\alpha)} b^{(\alpha)}} + \frac{\dot{\gamma}^{(\beta)}}{\rho_{m}^{(\beta)} b^{(\beta)}}.$$  \hfill (2.18)
The length of the formed junction is assumed to be proportional to the spacing of immobile dislocations as

$$l_c = \frac{1}{\sum_\beta \sqrt{\rho_{im}^{(\beta)}}},$$

(2.19)

and only a fraction of these junctions, $f_0$, are stable. The rates of immobilization of dislocation densities on slip system $\alpha$ due to mobile and immobile dislocations on slip system $\beta$ are therefore $f_0 \rho_m^{(\alpha)} l_c v^{(\alpha \beta)}$ and $f_0 \rho_{im}^{(\alpha)} l_c v^{(\alpha)}$, respectively. The rate of immobilization of mobile dislocation densities on slip system $\alpha$ is therefore

$$\rho_{\text{interaction}^-}^{(\alpha)} = f_0 \sum_\beta \left( \rho_m^{(\beta)} l_c \frac{v^{(\alpha \beta)}}{b^{(\alpha)}} + \rho_m^{(\alpha)} l_c \frac{v^{(\beta)}}{b^{(\beta)}} \right) + f_0 \sum_\beta \rho_{im}^{(\beta)} l_c \frac{v^{(\alpha)}}{b^{(\alpha)}}$$

(2.20)

The addition of immobile dislocation densities due to interactions also takes into account the possibility of dislocation interaction forming immobile junctions. Frank’s rule is used to determine energetically favorable interactions for immobile junction formation. A dislocation density interaction tensor for junction formation on slip system $\alpha$ due to interaction of slip systems $\beta$ and $\gamma$ is defined as

$$n_{\alpha \beta \gamma}^{\rho \rho} = \begin{cases} 1 & \text{if } \mu b^{(\alpha)} < \mu b^{(\beta)} + \mu b^{(\gamma)} \text{ and } b^{(\alpha)} = b^{(\beta)} + b^{(\gamma)} \\ 0 & \text{otherwise} \end{cases}.$$

(2.21)

The rates of junction formation on slip system $\alpha$ are then defined as

$$n_{\alpha \beta \gamma}^{\rho \rho} f_0 \rho_m^{(\beta)} \rho_m^{(\gamma)} l_c v^{(\beta \gamma)} \text{ and } n_{\alpha \gamma}^{\rho \rho} f_0 \rho_m^{(\gamma)} l_c \left( \rho_m^{(\beta)} v^{(\beta)} + \rho_{im}^{(\beta)} v^{(\gamma)} \right)$$

(2.22)

for mobile/mobile and mobile/immobile interactions. The total addition of immobile dislocation densities due to interactions then becomes
\[ p_{\text{interaction}}^{(\alpha)} = f_0 \sum_{\beta \neq \gamma} \left( \rho_m^{(\beta)} l_c \frac{\gamma^{(\gamma)}}{b^{(\gamma)}} + \rho_m^{(\gamma)} l_c \frac{\gamma^{(\beta)}}{b^{(\beta)}} \right) + f_0 \sum_{\beta \neq \gamma} \left( \rho_m^{(\beta)} l_c \frac{\gamma^{(\gamma)}}{b^{(\gamma)}} + \rho_m^{(\gamma)} l_c \frac{\gamma^{(\beta)}}{b^{(\beta)}} \right). \]  

(2.23)

To obtain the interaction tensor, \( n_{\alpha \beta} \), the total number of interactions between slip systems has to be considered. In f.c.c. crystals, using the family of \(<110>\{111\> slip systems, the total interactions can be reduced to six basic interaction types based on the symmetry of the crystal structure (Kubin et al., 2008b). These interactions are: the self interaction, between the same slip system; the co-linear interaction, between slip systems with parallel Burgers vectors; the co-planar interaction, between co-planar slip systems; the interaction between slip systems forming Lomer locks; the glissile junction, between non-co-planar slip systems; and the interaction between slip systems forming Hirth locks. The interaction tensor can be obtained by considering the product of each interaction type. To explicitly account for the storage of locks, the mobile and immobile dislocation densities on the 12 slip systems in f.c.c. crystals are appended with 6 immobile dislocation densities pertaining to the storage of Lomer locks on the \{100\} planes. This leads to a total of 12 x 12 mobile-mobile interactions and 12 x 18 mobile-immobile interactions. Similarly, in b.c.c. crystals, using the \(<111>\{110\> and \(<111>\{112\> families of slip systems, the total interactions are reduced to 3 interaction types. These interaction types are: the self and co-linear interaction between the same slip system and slip systems with parallel Burger’s vector; the interaction between slip systems to form binary junctions having \(<100\> Burger’s vectors; and the interaction between slip systems and binary junctions to form ternary junctions having \(<111\> Burger’s vectors. To explicitly account for the storage of junctions, the mobile and immobile dislocation densities on the 24 slip systems in b.c.c. crystals are appended with 19 immobile dislocation densities.
pertaining to the storage of <100> binary junctions on various crystallographic planes. This leads to a total of 24 x 24 mobile-mobile interactions and 24 x 43 mobile-immobile interactions. Thus, the formation of ternary junctions (Bulatov, 2006; Madec et al., 2008), can be explicitly accounted for through the interaction of dislocation locks and binary junctions with mobile dislocation densities.

Dislocation density annihilation due to recovery is modeled using an Arrhenius relationship as

\[ \dot{\rho}_{\text{annihilation}}^{(\alpha)} = \nu^{(\alpha)} e^{-\frac{H}{kT}}, \]  

(2.24)

where the frequency of which immobile dislocations are intersected by mobile dislocations on other slip systems is related to the attempt frequency, \( \nu^{(\alpha)} \), as

\[ \nu^{(\alpha)} = f_0 \sum_{\beta} \rho_{im}^{(\alpha)} \frac{\dot{\gamma}^{(\beta)}}{b^{(\beta)}}. \]  

(2.25)

The activation enthalpy, \( H \), is related to the immobile dislocation density and saturation density, \( \rho_s \), as

\[ H = H_0 \left( 1 - \frac{\rho_{im}^{(\alpha)}}{\rho_s} \right). \]  

(2.26)

The annihilation rate of dislocation densities on slip system \( \alpha \) becomes

\[ \dot{\rho}_{\text{annihilation}}^{(\alpha)} = \left( f_0 \sum_{\beta} \rho_{im}^{(\alpha)} \frac{\dot{\gamma}^{(\beta)}}{b^{(\beta)}} \right) e^{-\frac{H_0}{kT} \left( 1 - \frac{\rho_{im}^{(\alpha)}}{\rho_s} \right)}. \]  

(2.27)
The generation, interaction, and annihilation rates are then substituted into equations 2.14 and 2.15 to obtain a coupled nonlinear set of evolutionary equations for the dislocation densities. The evolutionary equations can be expressed as

\[
\frac{d\rho_m^\alpha}{dt} = \dot{\gamma}^{\alpha}\left(\frac{g_{\text{source}}^\alpha}{b^2} - \frac{g_{\text{interaction}}^\alpha - g_{\text{immobilized}}^\alpha}{b}\sqrt{\rho_m^\alpha}\right)
\]  

(2.28)

\[
\frac{d\rho_{\text{im}}^\alpha}{dt} = \dot{\gamma}^{\alpha}\left(g_{\text{interaction}}^\alpha + \frac{g_{\text{immobilized}}^\alpha}{b}\sqrt{\rho_m^\alpha} + g_{\text{recov}}^\alpha - g_{\text{source}}^\alpha\right)
\]

(2.29)

to delineate the dislocation activities such as generation, interaction, immobilization, and annihilation (Zikry and Kao, 1996; Shanthraj and Zikry, 2011). The coefficients, not known a priori, are summarized in Table 2.1. The dislocation activity is coupled to the stress response through the Taylor relationship (Eq. 2.11).

### 2.3 Dislocation-Density GB Interaction Scheme

In this section, a dislocation-density GB interaction scheme is presented. The martensitic block boundary can be considered as similar to a grain boundary (GB) interface. For dislocation-density transmission through the boundary, an incoming slip system usually does not completely coincide with an outgoing slip system, and residual dislocations can remain within the boundary due to the conservation of lattice defect vector (Shanthraj and Zikry, 2013; Sangid et al., 2011; Shi and Zikry, 2009; Lee et al., 1990). The energy required to produce the residual dislocation at the boundary is considered as the energy barrier for thermally activated dislocation transmission (Ma et al., 2006; Roters et al., 2010). The constitutive relation (Eq. 2.9) has been modified at the boundary through the introduction of a GB transmission factor (GBTF) based on the energy barrier as
\[
\dot{\gamma}^{(\alpha)} = \gamma_{ref}^{(\alpha)} \left[ \frac{\tau^{(\alpha)}}{\tau_{ref}} \right] \left[ \frac{\tau^{(\alpha)}}{\tau_{ref}} \right]^{-\frac{1}{m-1}} \text{GBTF}^{(\alpha)}, \tag{2.30}
\]

where \( \text{GBTF}^{(\alpha)} = e^{\left( \frac{U_{GB}^{(\alpha)}}{kT} \right)} \). It can range from 0 to 1, 0 corresponds to full blockage and 1 corresponds to full transmission.

The line tension model for the activation of a Frank-Read source in the presence of a GB developed in Koning et al. (2002) can then be used to obtain the energy required for dislocation transmission. The energy barrier caused by GB residual dislocation, for incoming and outgoing slip systems \( \alpha \) and \( \beta \), is given by

\[
U_{GB}^{(\alpha\beta)} = \kappa G \Delta b_{ef}^2 \Delta_2,
\tag{2.31}
\]

where \( \kappa \) is approximately equal to 0.5, \( G \) is the shear modulus, \( \Delta b_{ef} \) is the magnitude of the effective residual Burger’s vector, which is a function of the misorientation of the slip planes and the magnitude of the true residual Burger’s vector. \( \Delta_2 \) is the length of residual dislocation, and it is a function of the resolved shear stress for the outgoing slip system \( \beta \) in grain 2 (Figure 2.1). Details for calculation of \( \Delta b_{ef} \) and \( \Delta_2 \) are given in Shanthraj and Zikry (2013) and Koning et al. (2002). Dislocation-density transmission is considered on the most energetically favorable outgoing slip system by taking the lowest value of the energy, on all active outgoing slip systems, as

\[
U_{GB}^{(\alpha)} = \min_{\beta} U_{GB}^{(\alpha\beta)},
\tag{2.32}
\]
2.4 Thermo-Mechanical Coupling

For dynamic loading condition, the adiabatic heating generation caused by plastic work is given as

$$q_{\text{mechanical}} = \chi \sigma'_{ij} D^p_{ij}$$  \hspace{1cm} (2.33)

where $\chi$ is the fraction of plastic work transformed to heat energy, and $\sigma'_{ij}$ is the deviatoric stress. Plastic work acts as heat sources, and thermal evolution is decomposed as adiabatic part and heat conduction part, which is given as

$$\rho c_p \dot{T} = \lambda \nabla^2 T + q_{\text{mechanical}}$$  \hspace{1cm} (2.34)

where $\rho$ is the mass density, $c_p$ is the specific heat capacity, and $\lambda$ is the thermal conduction coefficient. The discretized finite element heat conduction equation is given as (LaBarbera and Zikry, 2013)

$$[C][\dot{T}] + [K][T] = [R_T]$$  \hspace{1cm} (2.35)

where $[C]$ is the matrix of rate of change of temperature proportional coefficients, $[K]$ is the matrix of temperature proportional coefficients, $[R_T]$ is the vector of nodal input heat sources for plastic work.

2.5 Stress Assisted Hydrogen Diffusion

For hydrogen diffusion and embrittlement, hydrogen atoms in the metal lattice are assumed to initiate as points defects, which can cause dilatational distortion, and interact with the stress field through the pressure $p = Tr(\sigma)/3$ (Serebrinsky et al., 2004). The pressure is positive for tensile stresses. The stress-assisted hydrogen diffusion equation can be given by (Dadfarnia et al., 2014; Olden, Thaulow, Johnsen, et al., 2008; Serebrinsky et al., 2004)
\[
\frac{\partial C}{\partial t} = D \nabla^2 C - \nabla \cdot \left( \frac{D V_H C \nabla p}{RT} \right)
\]

(2.36)

where \( C \) is the hydrogen concentration, \( D \) is the hydrogen diffusion coefficient, \( V_H \) is the partial molar volume of hydrogen in steels, and equal to \( 2.0 \times 10^{-6} \) m\(^3\)/mol (Sofronis and McMeeking, 1989), \( R \) is the universal gas constant, \( T \) is the absolute temperature.

### 2.6 Martensitic Microstructural Representation

Following Hatem and Zikry (2010), the martensitic lath structure is related to the global coordinates through the parent austenite grain orientation and variant orientations.

Commonly accepted ORs for lath martensitic steels are Kurdjumov-Sachs (KS) and Nishiyama-Wassermann (NW) ORs. KS ORs are based on a \( \gamma \) austenite transformation to \( \alpha' \) martensitic transformation as \((111)_{\gamma} // (011)_{\alpha'}\), \((\bar{1}01)_{\gamma} // (\bar{1}1\bar{1})_{\alpha'}\). The NW OR is a KS OR with a 5.12° rotation around the \([011]_{\gamma}\) direction. The 24 variants obtained from a KS OR are tabulated in Table 2.2.

To relate the martensitic local grain orientation to the global orientation, three transformations are needed. The first transformation, \([T]_1\), relates an observed OR to a theoretical OR, such as KS and NW ORs. The second transformation, \([T]_2\), relates a martensite OR to the parent austenite grain orientation. The third transformation, \([T]_3\), relates the parent austenite grain orientation to the global coordinates. These transformations are given by \([X]_{\text{Global}} = [T]_3 [T]_2 [T]_1 * [X]_{\alpha}\).

To characterize martensitic microstructure, we will follow the characterization scheme of Morito et al. (2003), which has been used by Hatem and Zikry (2009). We designate a block as a group of laths with approximately the same values of low angle
misorientations, and a packet as a collection of blocks with the same habit plane. Using this methodology, we can investigate the effects of variant distribution on crack nucleation and propagation in martensitic microstructures.
2.7 Tables and Figures

Table 2.1: g coefficients in Eqs. 2.28 and 2.29

<table>
<thead>
<tr>
<th>g Coefficients</th>
<th>Expression</th>
</tr>
</thead>
<tbody>
<tr>
<td>$g_{sour}^{\alpha}$</td>
<td>$b^\alpha q f\sum_{\beta}\sqrt{\rho_{im}^{\beta}}$</td>
</tr>
<tr>
<td>$g_{sinter-}^{\alpha}$</td>
<td>$l_c f_0 \sum_{\beta}\sqrt{a_{\alpha\beta}} \left[ \frac{\rho_{m}^{\beta}}{\rho_{im}^{\alpha\beta}} + \frac{\dot{\gamma}<em>m^{\beta}}{\dot{\gamma}</em>{im}^{\alpha\beta}} \right]$</td>
</tr>
<tr>
<td>$g_{simmob-}^{\alpha}$</td>
<td>$\frac{l_c f_0}{\dot{\gamma}<em>{im}^{\alpha\beta}} \sum</em>{\beta}\sqrt{a_{\alpha\beta}} \rho_{im}^{\beta}$</td>
</tr>
<tr>
<td>$g_{sinter+}^{\alpha}$</td>
<td>$\frac{l_c f_0}{\dot{\gamma}<em>{im}^{\alpha\beta}} \sum</em>{\beta}\sqrt{a_{\alpha\beta}} \rho_{m}^{\beta} \left[ \frac{\rho_{m}^{\beta} \dot{\gamma}<em>{im}^{\alpha\beta}}{b^{\beta}} + \frac{\rho</em>{m}^{\beta} \dot{\gamma}_{m}^{\alpha}}{b^{\gamma}} \right]$</td>
</tr>
<tr>
<td>$g_{simmob+}^{\alpha}$</td>
<td>$\frac{l_c f_0}{\dot{\gamma}<em>{im}^{\alpha\beta}} \sum</em>{\beta}\sqrt{a_{\alpha\beta}} \rho_{im}^{\beta} \dot{\gamma}_{im}^{\alpha\beta}$</td>
</tr>
<tr>
<td>$g_{recov}^{\alpha}$</td>
<td>$l_c f_0 \left( \sum_{\beta}\sqrt{a_{\alpha\beta}} \dot{\gamma}<em>m^{\beta} \right) e^{\frac{-H_0 (1 - \frac{\rho</em>{im}^{\alpha\beta}}{\rho_m^{\alpha\beta}})}{kt}}$</td>
</tr>
</tbody>
</table>
Table 2.2: The 24 variants corresponding to the K-S OR

<table>
<thead>
<tr>
<th>Variant no.</th>
<th>Parallel planes</th>
<th>Parallel directions</th>
<th>Variant no.</th>
<th>Parallel planes</th>
<th>Parallel directions</th>
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<td>1</td>
<td>(111)$_{\gamma}$</td>
<td>/[011]$_{\gamma}$</td>
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<td>(111)$_{\gamma}$</td>
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Figure 2.1 Dislocation configuration of a Frank-Read source in the vicinity of a GB.
CHAPTER 3: Fracture Approach and Numerical Method

3.1 Microstructure-Based Failure Criterion

The inherent fracture mode in martensitic steel is cleavage on \{100\}_{\alpha}' planes in the microstructure (Guo et al., 2004). To formulate this into a microstructural failure criterion, the orientation of the cleavage planes for each variant in the global coordinate system is obtained by applying the series of transformations outlined in Chapter 2.6.

\[
n_{\text{cleave}} = [T][T]^T[n_{\text{cleave},\alpha'}],
\]

(3.1)

The global orientation of the cleavage planes in the current configuration is then obtained by updating at every time-step, due to the lattice rotations of \( \hat{n}_{\text{cleave}} = W^*n_{\text{cleave}} \). The normal component of the traction acting on each cleavage plane has a direct influence on fracture along that plane. The maximum, over all the \{100\}_{\alpha}' cleavage planes, of the normal component of the traction on these planes is, therefore, monitored and compared with critical fracture stress \( \sigma_{\text{frac}} \) to determine failure. The failure criterion can be given by

\[
t_{\text{cleave}} > \sigma_{\text{frac}},
\]

(3.2)

where \( t_{\text{cleave}} = \max_{\{100\}_{\alpha} \text{ planes}} \left\{ n_{\text{cleave}}^T \left[ \sigma \right] n_{\text{cleave}} \right\} \).

Due to the heterogeneities caused by the microstructure, such as the orientation of martensitic blocks, retained austenite pockets, and dislocation-GB interactions, multiple cracking can occur. For each crack, a small circular region with a radius of \( r \) ahead of crack front is defined. The determination of the radius \( r \) is based on trial and error. The failure
criterion is evaluated only for the element ahead of the crack front in the circular region and the elements outside of the circular region (see, for example, Meer and Sluys, 2009).

3.2 Failure Criterion for Hydrogen Embrittlement

The failure criterion for hydrogen embrittlement is similar to that of cleavage fracture outlined in Chapter 3.1, but the inherent hydrogen diffusion assisted fracture mode in martensitic steel occurs on \( \{110\}_{\alpha'} \) planes (Shibata et al., 2012; Kim and Morris, 1983). To formulate this into a microstructural failure criterion, the orientation of the fracture planes for each variant in the global coordinate system is obtained by applying the series of transformations outlined in Chapter 2.6.

\[
n_{\text{fracture}} = [T]_3 [T]_2 [T]_1 n_{\text{fracture,\alpha'}}
\]  

(3.3)

The global orientation of the fracture planes in the current configuration is also obtained by updating at every time-step, due to the lattice rotations of \( \dot{n}_{\text{fracture}} = W^* n_{\text{fracture}} \).

The maximum, over all the \( \{110\}_{\alpha'} \) fracture planes, of the normal component of the traction on these planes is, therefore, monitored and compared with critical fracture stress \( \sigma_c \) on the \( \{110\}_{\alpha'} \) fracture planes to determine failure. The failure criterion for hydrogen embrittlement can be given by

\[
t_{\text{fracture}} > \sigma_c,
\]  

(3.4)

where \( t_{\text{fracture}} = \max_{\{110\} \text{ planes}} \left< n_{\text{fracture}}^T [\sigma] n_{\text{fracture}} \right> \).

The presence of hydrogen decreases the critical fracture stress, and the quantitative relationship of power law from experiments (M. Wang et al., 2007; Wang et al., 2005; Kim
et al., 2009), between the critical fracture stress and hydrogen concentration, is, therefore, applied on the \{110\} fracture planes as follows,

\[ \sigma_c = \sigma_{c0} C^{-0.14} \]  

(3.5)

where \(\sigma_{c0}\) is the initial critical fracture stress on \{110\} planes at a hydrogen concentration of 1 ppm, \(C\) is the hydrogen concentration. Reduction of critical fracture stress (RCFS), which represents embrittlement of martensite, is defined as

\[ RCFS = \frac{\sigma_{c0} - \sigma_c}{\sigma_{c0}} \]  

(3.6)

### 3.3 Failure Criterion for Intergranular Fracture

Intergranular cracks propagate along grain boundary (GB), which strongly depend on misorientations and impurities at GBs. Experiments have shown that the normal component of traction on GB planes has a direct influence on intergranular fracture (Pouillier et al., 2012). Therefore, the normal component of traction on GB plane is monitored and compared with a critical GB fracture stress \(\sigma_{GB}\) to determine intergranular failure. The failure criterion for intergranular fracture can be given by

\[ t_{GB} > \sigma_{GB} \]  

(3.7)

where \(t_{GB} = n_{GB}^T \{\sigma\} n_{GB}\), \(n_{GB}\) is the normal vector of GB plane.

### 3.4 Numerical Implementation of Overlapping Element Method

When the failure criterion is attained in one element, the elastic energy stored in the element will be released, and the elastic energy release rate should be related to plastic work under large plastic deformation. Numerical instability can be encountered, because the
resolved shear stresses, slip rates, and dislocation densities can vary widely, due to decreases in stiffness caused by introducing crack surfaces. To address these numerical issues, the stresses are unloaded after the failure criterion is attained as

\[ \sigma_{n+1} = \sigma_n \times \alpha^N, \]  

where \( N \) is the number of unloading steps after failure, and \( \alpha \) is the decay factor, which is a function of elastic energy \( Q_e \) and plastic work \( Q_p \), and can be written as

\[ \alpha = e^{-\frac{Q}{\beta Q_e}}, \]  

where \( \beta \) is a constant. After the stresses have been unloaded, overlapping elements are introduced to represent failure surface. For the limiting case with \( Q_e \gg Q_p \), which means little plastic work or brittle failure, the decay factor \( \alpha \) goes to zero, and the unloading process can be completed in one time step.

We follow the approach of Wu and Zikry (2014) and Hansbo and Hansbo (2004), and consider one element crossed by a crack defined implicitly \( f(X) = 0 \), dividing the element domain into two subdomains with areas \( A_{e1} \) and \( A_{e2} \) (Figure 3.1). The direction of crack propagation would be along the most favorable fracture plane (Morris, 2011; Wang et al., 2008). The 3D fracture model is implemented in a 2D setting by projecting the 3D crack path onto the 2D plane. Adding phantom nodes on top of the existing nodes, the original cracked element is replaced by two overlapping elements. The two overlapping elements do not share nodes, and therefore can have independent displacement fields. For each overlapping element, only the subdomain with area \( A_{e1} \) or \( A_{e2} \) (Figure 3.1), corresponding to one of the two subdomains for the original cracked element, is considered as active. For a 4-node
quadrilateral element with one-point integration and hourglass control, the internal nodal force vector of the cracked element is given by (Song et al., 2006)

\[ f_e^{\text{int}} = f_{e1}^{\text{int}} + f_{e2}^{\text{int}}, \]  

(3.10)

where \( f_{e1}^{\text{int}} \) and \( f_{e2}^{\text{int}} \) are the internal nodal force vectors of the overlapping elements, and are given by

\[ f_{(e1/e2)}^{\text{int}} = \frac{A_{(e1/e2)}}{A_0} \int [B^T \alpha_{(e1/e2)}] dV_e, \]  

(3.11)

In summary, the procedure for implementation of the overlapping element method is as follows:

1. Monitor failure criterion for the necessary elements, at each time step after equilibrium (Eqs. 3.2 and 3.4).
2. If the failure criterion is satisfied, physically unload stresses to a lower level in the following time steps (Eqs. 3.8 and 3.9).
3. Add phantom nodes after stress unloading is completed, and introduce overlapping elements (Figure 3.1).
4. Update new residual force and stiffness for overlapping elements (Eqs. 3.10 and 3.11), assemble new global residual force and stiffness, and solve for the new geometry.

3.5 Computational Techniques for Crystal Plasticity

The total deformation rate tensor, \( D_{ij} \), and the plastic deformation rate tensor, \( D_{ij}^p \), are needed to update the material stress state. The method used here is the one developed by Zikry (1994) for rate-dependent crystalline plasticity formulations, and only a brief outline
will be presented here. For quasi-static deformations, an implicit FE method with BFGS iteration is used to obtain the total deformation rate tensor, $D_{ij}$. To overcome numerical instabilities associated with stiffness, a hybrid explicit-implicit method is used to obtain the plastic deformation rate tensor, $D_{ij}^p$. This hybrid numerical scheme is also used to update the evolutionary equations for the mobile and immobile densities. For dynamic deformations, a lumped mass, one point integration, trapezoidal rule, and a stiffness based hourglass control are used. Details for this dynamic approach are given in Zikry (1994) and Shanthraj and Zikry (2011).
3.6 Tables and Figures

Figure 3.1 Decomposition of a cracked element with two overlapping elements.
CHAPTER 4: The Heterogeneous Effects of Retained Austenite on The Behavior of Martensitic High Strength Steels

In this chapter, the effects of pockets of retained austenite on the behavior of martensitic steels have been investigated. A dislocation-density based crystalline plasticity and specialized finite-element formulation were used to investigate how f.c.c. austenite pockets interact with b.c.c. martensitic laths. The formulation accounts for variant morphologies, orientation relationships, and retained austenite that are uniquely inherent to lath martensitic microstructures. Quasi-static and dynamic analyses were undertaken to investigate how the effects of the orientations of parent austenite grains and different crystallographic interfaces affect shear strain localization, strength, and toughness.

4.1 The Model

The multiple-slip dislocation-density-based crystal plasticity formulation is coupled to the specialized FE method to investigate the large strain behavior of martensitic steel with distributions of retained austenite. To model the microstructure of the martensite, we used a combination of blocks and packets. This approach is based on the approach developed by Hatem and Zikry (2009). Blocks are collections of laths with low misorientation, and packets are collections of blocks that have the same habit plane. In this study, 40 martensitic blocks are distributed randomly with 14 packets from one parent austenite grain, and the variant of martensite blocks were obtained based on the orientation relationships between the parent austenite grain and martensite blocks. The variant arrangements were obtained from experimental EBSD observations by Morito et al. (2003). It is assumed that the retained
austenite has a volume fraction of 5% (Thomas 1978), and that the pockets of retained austenite are randomly distributed inside the martensite blocks, or between the blocks and the packets (Figure 4.1). It is assumed that the retained austenite pockets has the same grain orientation as the parent austenite grain. The material properties (Table 4.1) that are used are representative of low-carbon martensitic steel and austenitic stainless steel (Byun et al. 2004).

The parent austenite grain is oriented based on the loading plane of (0 0 1)γ and a loading direction of [0 1 0]γ. The Kurdjumov-Sachs (K-S) OR is adopted as the martensite OR, and {111}γ is assumed as the habit plane. A convergent plane strain FE mesh of 4893 elements was used with a specimen size of 3.2 mm × 6.4 mm, and a displacement load is applied for a quasi-static nominal strain rate with symmetric boundary conditions applied on the left and bottom edges.

To validate the modeling approach, comparisons were made with experiments conducted by Shibata (2012) on low carbon martensitic steel for a quasi-static tensile strain rate of 8.3 x 10^{-6} s^{-1}. For this comparison, it is assumed that the material is 100% martensite. The nominal stress strain curves for the numerical and the experimental results are shown in Figure 4.2. The maximum difference between the experimental and the numerical stress values is approximately 10%. This small differences further validates the model. However, it should be noted the experimental results soften at approximately 4%, and the model shows instability at approximately 6%. This difference can be due to heterogeneities, such as second phase particles, which are not accounted for in the proposed model.
4.2 Results and Discussion

4.2.1 Retained Austenite-Martensite Interaction

Different distributions of pockets of retained austenite were randomly distributed within the martensitic aggregate for a volume fraction of 5% (Figure 4.1). It is initially assumed that the austenite grain had a cube Euler orientation of (0°, 0°, 0°). The contours for the normalized (by the initial mobile dislocation density) mobile dislocation densities and the normalized (by the initial immobile dislocation density) immobile dislocation densities corresponding to the most active slip system of the martensite and retained austenite aggregate at a nominal strain of 20% are shown in Figure 4.3. For the most active slip system of martensite \((\bar{1}12)[1\bar{1}1]\), the maximum normalized mobile dislocation density is \(2.0 \times 10^7\), and the maximum normalized immobile dislocation density is \(1.8 \times 10^5\). The evolution of dislocation densities along selected blocks results in the localization of plastic slip (Figure 4.4a). The dislocation density at the interface between martensite blocks and retained austenite pockets is a maximum, and this is likely due to the interaction of the martensitic slip systems and the retained austenite slip systems. Based on the K-S orientation relationship, the slip systems \{110\}<111> in martensite should be aligned with the slip systems \{111\}<110> in austenite. However, the \{112\}<111> slip systems in martensite are incompatible with the austenite slip systems, which can impede dislocation density transmission between martensite blocks and retained austenite interfaces. For the most active slip system in austenite of \((1\bar{1}1)[011]\), the normalized mobile dislocation density is \(2.0 \times 10^6\), and the normalized immobile dislocation density is \(1.0 \times 10^4\), which are much lower than those in martensite. This can be due to the initial cube orientation of the austenite grain
and the lower number of available f.c.c. slip-systems in comparison with the available b.c.c. slip-systems.

The accumulated plastic slip at a nominal strain of 20% is shown in Figure 4.4a. The maximum accumulated slip is 0.5, and it occurs within the retained austenite pockets. The tensile loading direction is aligned along the [010]γ direction, which can result in a maximum resolved shear stress along the [011]γ directions. The slip-direction [011]γ of the f.c.c. retained austenite is also parallel to the long direction of martensitic laths and blocks, and parallel to the slip direction [111]α based on the K-S OR. The retained austenite grains are at the martensite inter-lath and block boundary, and the long direction should, therefore, be parallel to that of martensite. This would align the austenite slip systems with the maximum resolved shear stress along the long direction of the martensitic blocks and retained austenite grains, which would result in the shear-strain localization of plastic slip. Furthermore, due to the incompatibility of the b.c.c. slip system (112)[111] and the f.c.c. slip system (111)[011], the accumulation of plastic slip occurs at the b.c.c.-f.c.c. interface, which is also exacerbated by the geometrical softening associated with the lattice rotation of both slip-systems (Figure 4.4b).

The interaction density on slip system α, which relates the increase in immobile dislocation density due to junction formation on the slip system relative to the decrease of mobile dislocation density, can be defined as

\[
\rho_{\text{int}}^\alpha = \int \gamma \left( g_{\text{mter}}^\alpha \rho_m^\alpha + \frac{g_{\text{imob}}^\alpha}{b} \sqrt{\rho_{\text{im}}^\alpha - \rho_{\text{mter}}^\alpha} \rho_m^\alpha - \frac{g_{\text{imob}}^\alpha}{b} \sqrt{\rho_{\text{im}}^\alpha} \rho_m^\alpha \right) dt, \quad (4.1)
\]
which can be used to characterize the dominant interaction mechanism on the active slip systems in the crystalline material. Values of $\rho_{\text{intr}}^\alpha < 0$ indicate that the annihilation of dislocation-density junctions is dominant, while values of $\rho_{\text{intr}}^\alpha > 0$ indicate that the formation of dislocation-density junctions is dominant (Shanthraj and Zikry 2012). The normalized (by the initial immobile dislocation density) total interaction dislocation density at a nominal strain of 20% is shown in Figure 4.4c. The maximum normalized total interaction dislocation density is $1.0 \times 10^5$, which occurs in the retained austenite. This indicates that the dominant interaction mechanism in retained austenite is the formation of dislocation junctions, which results in the localization of plastic slip and hardening of retained austenite. The normalized total interaction dislocation density around the periphery of retained austenite pockets in martensite is $-1.0 \times 10^4$, which indicates that the dominant interaction mechanism is the annihilation of dislocation junctions. This can soften martensite, which can render it more susceptible to shear-strain localization.

The normalized (by the static yield stress of martensite) normal stress is shown in Figure 4.4d. The maximum value is 14, which occurs at the interface of martensite and retained austenite. The incompatibility of slip systems in these regions can impede dislocation density transmission, and it would result in these high local stresses. These localized areas of retained austenite with such high stresses may transform to martensite, which can relax these stress accumulations, and inhibit crack nucleation (Jacques 2001). The normal stresses in the retained austenite are much lower, almost by a factor of 5.0, which is an indication of the toughness (as opposed to its strength) of the retained austenite.
4.2.2 Effects of Parent Austenite Orientation

The effects of the initial austenite orientation on the inelastic deformation of the martensite-austenite microstructures have also been investigated. The martensite blocks and retained austenite volume fractions and distributions are the same as before, but the parent austenite Euler angle orientations were varied. Two cases were investigated, one case with a low initial Euler angles of \((2^\circ, 4^\circ, 8^\circ)\), and a second case with a high initial Euler angles of \((15^\circ, 25^\circ, 35^\circ)\).

The contours for the normalized mobile dislocation densities and the normalized immobile dislocation densities corresponding to the most active slip system of martensite and retained austenite, for the Euler angles of \((2^\circ, 4^\circ, 8^\circ)\) at a nominal strain of 20\%, are shown in Figure 4.5. The most active slip systems for the martensite blocks and retained austenite pockets are the same as those for the Euler angles \((0^\circ, 0^\circ, 0^\circ)\). For the most active slip system in martensite of \((\bar{1}12)[1\bar{1}1]\), the maximum normalized mobile dislocation density is \(2.8 \times 10^7\), which is higher than the cube orientation case by approximately 40\%. The maximum normalized immobile dislocation density, for the low angle case, is \(2.4 \times 10^5\), which is 33\% higher than the cube case. These larger immobile and mobile dislocation densities are obviously due to the higher incompatibilities of the slip-systems between the retained austenite and the martensite blocks.

The accumulated plastic slip, lattice rotation, and normalized total interaction dislocation density, for the low Euler angle case at a nominal strain of 20\%, are shown in Figure 4.6a-c. The maximum plastic slip is 0.55, and the maximum normalized total interaction dislocation density is \(1.1 \times 10^5\), which is 10\% higher than the cube orientation.
case. The maximum lattice rotation is 30°, which is higher than the cube orientation case by approximately 20%. These maximum values occur in the retained austenite regions adjacent to the interface of martensite and retained austenite (Figure 4.6a-c). The higher positive values of the total interaction dislocation density indicate that more dislocation density junctions can form, which results in the hardening of the retained austenite. The maximum normalized normal stress is 20 (Figure 4.6d), and these high stresses are due to the slip system incompatibility between the retained austenite and martensite.

The contours for the normalized mobile dislocation densities and the normalized immobile dislocation densities corresponding to the most active slip system of martensite and retained austenite, for the high Euler angle case at a nominal strain of 20%, are shown in Figure 4.7. The most active slip system in martensite is (2\(\bar{1}\)1)[11\(\bar{1}\)], and the most active slip system in the retained austenite pockets is (1 \(\bar{1}\)1)[\(\bar{T}\)01], which are not the same as the cube orientation case and the low Euler angle case.

Some of \{110\}<111> slip systems in martensite, which are compatible with f.c.c. austenite slip systems, are highly active, as indicated by the high immobile and mobile dislocation densities. This compatibility can result in plastic accumulation as shown in Figure 4.8a. The accumulated plastic slip, lattice rotation, normalized total interaction dislocation density, and normalized normal stress, for this high Euler angle case at a nominal strain of 20%, are shown in Figure 4.8. The accumulated plastic slip is uniformly distributed in martensite, and the maximum value is 0.5. The maximum lattice rotation is 35°, and it occurs in the retained austenite pockets (Figure 4.8b). The normalized total interaction dislocation densities have an average value of 5.0 \(\times\) 10\(^4\) in the retained austenite pockets, and -1.0 \(\times\) 10\(^4\)
in the martensite blocks (Figure 4.8c). This indicates that fewer dislocation-density junctions form in retained austenite, and more dislocation-density junctions are annihilated in martensite, which can result in shear strain localization and soften the material. The maximum normalized normal stress is 12, and it occurs in the martensitic blocks. The stresses are significantly lower than that of the cube orientation by approximately 14%, and 40% lower than the low Euler angle case. These changes in behavior are due to the compatibility of the slip systems and the domination of annihilation processes due to dislocation-density interactions at the interface of martensite blocks and retained austenite pockets.

4.2.3 Dynamic Behavior

In this section, we investigate the dynamic behavior of martensitic steel with retained austenite. The martensite blocks and retained austenite volume fractions and distributions are as before, and the parent austenite with a low Euler angle orientation of (2°, 4°, 8°) was used. A displacement load at a steep slope, such that a nominal strain rate of 5000s\(^{-1}\) results along the tensile axis (Figure 4.1). The nominal strain-rate was obtained by scaling the nominal strain over an appropriate time-scale. The nominal stress-strain curves are shown in Figure 4.9. The oscillations at high strain rate occur due to stress wave reflection along the free and fixed boundary.

The accumulated plastic slip, lattice rotation, normalized temperature (normalized by the martensite melting temperature of 1700K) and the normalized normal stresses, at a nominal strain of 10%, are shown in Figure 4.10. The maximum plastic slip is 0.4, and it occurs within the retained austenite pockets. The large values of plastic slip are as a result of
geometrical softening and thermal softening. The geometrical softening occurs due to large lattice rotations (Figure 4.10b). The maximum value of lattice rotation is 25°. In addition to the geometrical softening, adiabatic heating results in a thermal accumulation (Figure 4.10c). It is assumed in our approach that the thermal accumulation is due to adiabatic heating, and the rate of change of temperature is obtained from the balance of energy (Eq. 2.12). The highest value of normalized temperature is 0.32, and it occurs at the interface of martensite blocks and retained austenite pockets. This increase in temperature further indicates that due to adiabatic heating, the material can soften. These two softening mechanisms would lead to shear strain localization, but it is a material competition with the dynamic strain hardening, which results in large normalized normal stresses of approximately 13 (Figure 4.10d).

4.3 Conclusions

Newly developed dislocation-density based evolution equations are coupled to a multiple-slip crystal plasticity formulation, and a framework is established that relates immobile and mobile dislocation-density evolution to austenitic and martensitic crystallographic orientations and behavior. Specialized FE methodologies were then used to investigate the effects of retained austenite, parent austenite grain orientations, and quasi-static and dynamic loading rates on deformation and failure in martensitic steel.

For the cube orientation case, the dominant slip system in martensitic blocks is \(\{\overline{1}12\}\langle1\overline{1}1\rangle\), which is incompatible with the retained austenite (f.c.c.) slip systems. The interfaces between martensite blocks and retained austenite pockets can impede dislocation density transmission, and result in local strengthening at the interface. The dominant
interaction mechanism was predicted to be the formation of dislocation junctions in austenite pockets, and the annihilation of dislocation junctions around the periphery of retained austenite in the martensitic blocks. This would result in the hardening of the austenitic pockets and the softening of martensitic blocks, which can render the martensitic blocks more susceptible to shear-strain localization. Furthermore, the high local stresses at the interface of martensite and retained austenite may induce a martensitic transformation, which can relax stress accumulations and inhibit crack nucleation.

In comparison with the cube orientation case, the low Euler orientation of the parent austenite grain does not change the dominant slip system, but exacerbates the incompatibility of slip system. This resulted in an increase of dislocation densities, plastic slips, and lattice rotations, and the formation of more dislocation junctions in retained austenite. The high Euler orientation of the parent austenite grain changes the dominant slip system in comparison with the cube orientation case and the low Euler angle case. Some of \{110\}<111> slip systems, which are compatible with f.c.c. austenite slip systems, were activated. This results in the annihilation of more dislocation junctions in martensite, and subsequently softens the material.

The effects of dynamic load have been investigated for a strain rate of 5000 s\(^{-1}\). The coupled effects of the geometrical and thermal softening accelerate shear strain localization. As the strain-rate is increased, the material strain hardens, and this is a competing effect with the thermal and geometrical softening mechanisms.
## 4.4 Tables and Figures

Table 4.1: Material Properties

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<tr>
<th>Properties</th>
<th>Retained austenite</th>
<th>Martensite</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young’s modulus, $E$</td>
<td>100 GPa</td>
<td>228 GPa</td>
</tr>
<tr>
<td>Static yield stress, $\tau_y$</td>
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<td>517 MPa</td>
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<tr>
<td>Poisson’s ratio, $\nu$</td>
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<td>Reference strain rate, $\dot{\gamma}_{ref}$</td>
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<td>Critical strain rate, $\dot{\gamma}_{critical}$</td>
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<td>$10^4$ s$^{-1}$</td>
</tr>
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<td>Burger vector, $b$</td>
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</tr>
<tr>
<td>Saturation dislocation density, $\rho_s$</td>
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<td>$1.0 \times 10^{16}$ m$^{-2}$</td>
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<td>Fraction of plastic energy to heat, $\chi$</td>
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<td>Geometric parameter, $f_0$</td>
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Figure 4.1 Microstructural model and retained austenite pocket, block/packet arrangement
Figure 4.2 Nominal stress-strain curve for experimental and numerical model
Figure 4.3 Mobile and immobile dislocation densities at a nominal strain of 20% for, (a) and 
(b) most active slip system in martensite ($\overline{1}12$)[$1\overline{1}$], (c) and (d) most active slip system in 
retained austenite ($1\overline{1}$)[011].
Figure 4.4 Behavior at a nominal strain of 20%, (a) shear slip, (b) lattice rotation, (c) normalized total interaction dislocation density, (d) normalized normal stress.
Figure 4.5 Mobile and immobile dislocation densities at a nominal strain of 20% for the low Euler angle case of (2°, 4°, 8°) for, (a) and (b) most active slip system in martensite (\(\overline{1}12\)[1 1 1]), (c) and (d) most active slip system in retained austenite (1\(\overline{1}1\)[0 1 1]).
Figure 4.6 Behavior at a nominal strain of 20% for the low Euler angle case of $(2^\circ, 4^\circ, 8^\circ)$, (a) shear slip, (b) lattice rotation, (c) normalized total interaction dislocation density, (d) normalized normal stress.
Figure 4.7 Mobile and immobile dislocation densities at a nominal strain of 20% for the high Euler angle case of (15°, 25°, 35°) for, (a) and (b) most active slip system in martensite (2 Ġ1)[111], (c) and (d) most active slip system in retained austenite (1 Ġ1)[Γ01].
Figure 4.8 Behavior at a nominal strain of 20\% for the high Euler angle case of \((15^\circ, 25^\circ, 35^\circ)\), (a) shear slip, (b) lattice rotation, (c) normalized total interaction dislocation density, (d) normalized normal stress.
Figure 4.9 Nominal stress-strain curves for different parent austenite orientations
Figure 4.10 Behavior at a nominal strain of 10% for the low Euler angle case of \((2^\circ, 4^\circ, 8^\circ)\) at a strain rate of \(5000 \text{ s}^{-1}\), (a) shear slip, (b) lattice rotation, (c) normalized temperature, (d) normalized normal stress.
CHAPTER 5: Microstructural Crack Nucleation and Propagation in High Strength Martensitic Steels

In this chapter, a dislocation-density based multiple-slip crystalline plasticity formulation, a dislocation-density grain boundary (GB) interaction scheme, and an overlapping fracture method were used to investigate crack nucleation and propagation in martensitic steel with retained austenite for both quasi-static and dynamic loading conditions. A failure criterion based on the normal component of traction on the microstructural cleavage planes is developed (Chapter 3.1). The formulation accounts for variant morphologies, orientation relationships, and retained austenite that are uniquely inherent to lath martensitic microstructures. The interrelated effects of dislocation-density evolution ahead of crack front and the variant distribution of martensitic blocks on crack nucleation and propagation are investigated.

5.1 The Model

The multiple-slip dislocation-density-based crystal plasticity formulation is coupled to the specialized FE method to investigate microstructural fracture of martensitic steel with distributions of retained austenite. The martensitic orientation and microstructure are represented as outlined in Chapter 2.6. In this study, 40 martensitic blocks are distributed randomly within 14 packets from one parent austenite grain. The variant arrangements, representing the orientation relationships between the parent austenite grain and martensitic blocks, are based on experimental EBSD observations (Morito et al., 2003; Kitahara et al., 2006). Two different variant distributions are used, as shown in Figure 5.1. It is assumed that
the retained austenite has a volume fraction of 5% (Thomas, 1978), and that the pockets of retained austenite are randomly distributed inside the martensite blocks, or between the blocks and the packets (Figure 5.1). It is also assumed that the retained austenite pockets has the same grain orientation as the parent austenite grain. The material properties (Table 5.1) that are used are representative of low-carbon martensitic steel and austenitic stainless steel (Byun et al., 2004).

The parent austenite grain is oriented based on the loading plane of \((0 0 1)_\gamma\) and a loading direction of \([0 1 0]_\gamma\). The effects of orientations of parent austenite grain on dislocation-density interaction at the interface of martensite (b.c.c.) and retained austenite pockets (f.c.c.), have been investigated in our previous paper (Wu et al., 2013). Here the high Euler angles \((15^\circ, 25^\circ, 35^\circ)\), representing the orientations of parent austenite grain, are used. The Kurdjumov-Sachs (K-S) OR is adopted as the martensite OR, and \(\{111\}_\gamma\) is assumed as the habit plane. A convergent plane strain FE mesh of 4893 elements was used with a specimen size of \(3.2 \text{ mm} \times 6.4 \text{ mm}\) with tensile loading conditions with a constrained bottom surface (Figure 5.1).

5.2 Results and Discussion

5.2.1 Dislocation-Density Evolution Ahead of Crack Front

Dislocation evolution ahead of crack front, and the effects of retained austenite on dislocation evolution and crack propagation have been investigated. The variant distribution, as shown in Figure 5.1a, and a pre-existing crack with the normalized initial crack length of \(a/w\) of 0.1 (Figure 5.2a) were used, where \(a\) is the crack length and \(w\) is the specimen width.
Based on Eqs. 2.14 and 2.15, the effects of dislocation-density corresponding to different slip systems can be delineated. $\dot{\rho}^{(e)}_{\text{generation}}$ is the mobile dislocation density generation rate, $\dot{\rho}^{(e)}_{\text{annihilation}}$ is the immobile dislocation density annihilated rate, $\dot{\rho}^{(e)}_{\text{interaction}}$ and $\dot{\rho}^{(e)}_{\text{interaction+}}$ are interaction rates related to the formation and destruction of junctions (Shanthraj and Zikry, 2011). The total dislocation-density generation ($\rho_{\text{generation}}$), interaction ($\rho_{\text{interaction}}$), and annihilation ($\rho_{\text{annihilation}}$) terms can be obtained, through integration of these rate terms and summation over all slip systems. Based on this, we can determine how the mobile and immobile terms evolve due to dislocation-density generation, interaction, and annihilation.

The normalized (by the initial immobile dislocation density of martensite) dislocation density generation at a nominal strain of 2% is shown in Figure 5.2a. Dislocations generate ahead of the crack front due to the activation of slip-systems. The maximum normalized dislocation-density generation is $3.5 \times 10^4$, and it occurs in retained austenite pockets, which indicates that plastic deformation first occurs in retained austenite pockets, due to its lower yield stress. With the increase of loading, crack begins to propagate as a sharp crack (Figure 5.2b). The normalized dislocation-density generation ahead of the main crack front, at a nominal strain of 6.2%, is approximately $7.0 \times 10^4$. When the crack propagates near a retained austenite pocket, the inherent ductility of the retained austenite pockets results in dislocation-density generation, which blunts the crack (Figure 5.2c). At a nominal strain of 12%, the maximum normalized dislocation-density generation ahead of the main crack front is $5.0 \times 10^5$, which is approximately 7 times of that for the sharp crack at 6.2% nominal strain, and occurs in a retained austenite pocket (Figure 5.2d).
This accumulation of dislocation-density generation leads to large shear slip accumulations with maximum values of 0.5 (Figure 5.3a). These plastic zones blunt the crack, which is consistent with experimental observations (see, for example, Higashida et al., 2000). Furthermore, the high normal stresses adjacent to the retained austenite pockets, ahead of crack front (Figure 5.3b), with maximum normalized (by the static yield stress of martensite) values of 10, can induce martensitic transformation (Bilmes et al., 2001). The associated volumetric expansion of this transformation can close the crack, relieve stresses at the crack front, and absorb strain energy that can drive crack propagation. Therefore, the retained austenite pockets can significantly improve the fracture toughness of materials.

5.2.2 Quasi-Static Crack Nucleation

In this section, the effects of dislocation-GB interaction on crack nucleation, of variant distribution of martensitic blocks on crack growth have been investigated. Two cases were investigated, Case I with a variant distribution shown in Figure 5.1a, and Case II with a variant distribution shown in Figure 5.1b. These two cases were chose to see if changes in variant arrangement would inhibit crack growth and failure.

The normalized immobile dislocation densities, and GBTF corresponding to the active slip system in martensite \( \{1\overline{2}1\}[111] \), for Case I at a nominal strain of 2.6%, are shown in Figure 5.4a-b. The normalized immobile dislocation density at the block boundary, denoted by the red circle in Figure 5.4a, is approximately \( 5.0 \times 10^3 \). The low GBTF at that block boundary (Figure 5.4b) represents the high incompatibility of slip systems, which can impede dislocation-density transmission and result in high local stresses, as shown in Figure
5.4c. The normalized normal stress at the block boundary, denoted by the red circle, is approximately 5.0. The maximum normalized (by the static yield stress of martensite) cleavage stresses on the three cleavage planes {100} are shown in Figure 5.4d. The distributions of cleavage stresses for Case I are much continuous due to the arrangement of variants from the same Bain variant group. This results in low misorientations of cleavages planes between martensitic blocks, and increases the coherence length on cleavage planes (Guo et al., 2004), which would result in crack propagation and a lower fracture toughness.

The favorable orientation of cleavage planes, represented by the large normalized cleavage stress with a maximum value of 4.5, denoted by the red circle in Figure 5.4d, results in a crack nucleating at the block boundary at a nominal strain of 6.2% (Figure 5.5a). After crack nucleation, the crack cuts through retained austenite pockets and propagates to the left free boundary (Figure 5.5b-c), which leads to a large sharp drop in the nominal stress-strain curve (Figure 5.8). The right crack front is impeded by the high strength martensitic block near the right free boundary, which is indicated by a high normalized normal stress of 16. Eventually, due to the rotation of the cleavages planes, the crack propagates to the right free boundary at a nominal strain of 12% (Figure 5.5d).

The normalized immobile dislocation densities, and GBTF corresponding to the active slip system in martensite ($\bar{2}11$)[111], for Case II at a nominal strain of 2.8%, are shown in Figure 5.6a-b. For regions with high dislocation density and low GBTF, dislocation-densities pile up at the block boundary, which results in high normal stresses (Figure 5.6c). The normalized normal stress at the block boundary, denoted by the red circle in the figure, is approximately 5.5. Combined with the favorable orientation of the cleavage
planes, which is indicated by a high normalized cleavage stress of 4.0 on the cleavage planes of \{100\} (Figure 5.6d), a crack first nucleates at the martensitic block boundary at a nominal strain of 5.8% (Figure 5.7a). In comparison with the distribution of cleavage stresses in Case I, the distribution of cleavage stresses in Case II is not continuous, due to the arrangement of variants from different Bain variant groups. This can create the large misorientations of cleavage planes between martensitic blocks, refine the coherence length along cleavage planes that governs fracture, and improve fracture toughness by deflecting cleavage crack (Wang et al., 2008).

After crack nucleation, the crack propagates to the left free boundary (Figure 5.7b). Due to the large misorientations of cleavage planes \{100\} between adjacent martensitic blocks, the first crack is blunted, which is indicated by a high normalized normal stress of 12. Meanwhile a second crack nucleates, which can relax stresses (Figure 5.7b). This second crack propagates along the right direction, cuts through a retained austenite pocket, and reaches the right free boundary (Figure 5.7c-d), which is indicated by a sharp drop in nominal stress-strain curve (Figure 5.8). Meanwhile, the left crack front for the second crack is blunted due to the large misorientations of the cleavage planes. This results in large plastic deformations, high normalized normal stress ahead of crack front at a value of 11 (Figure 5.7d), and material hardening (Figure 5.8).

The crack nucleation sites, the nominal strain for crack nucleation, and crack propagation path are significantly different for Cases I and II. For Case I, only one crack nucleates, and it propagates rapidly and smoothly along a planar front due to the low misorientations of cleavage planes between martensitic blocks, which would decrease
fracture resistance. For Case II, two cracks nucleate, and both of them are blunted due to the large misorientations of cleavages planes, which would improve overall fracture toughness. Therefore, crack nucleation and inhibition of failure can be controlled through controlling variant distributions.

5.2.3 Dynamic Behavior

In this section, the dynamic crack nucleation and propagation of martensitic steel with retained austenite have been investigated. The variant distribution for Case II (Figure 5.1b) was used and a nominal strain-rate of 5,000s$^{-1}$ was applied along the tensile axis.

The normalized normal stress at a nominal strain of 0.6% is shown in Figure 5.9a. The maximum normalized normal stress is approximately 4.0, and occurs at the interface of a martensitic block and a retained austenite pocket. Stress wave effects can be seen at the bottom of the model, which results in large stress oscillations due to wave reflection at the free and fixed boundaries (Figure 5.11). A crack nucleates at the martensitic block boundary at a nominal strain of 4.4% (Figure 5.9b). In comparison with the quasi-static crack nucleation case, the dynamic crack nucleates at the same site, but at a lower nominal strain (Figure 5.11). The left crack front then propagates to the left free boundary, while the right crack front is blunted. Simultaneously, another two cracks nucleate, one in the middle of the model, and the other at the bottom (Figure 5.9c). The middle crack is blunted, while the bottom crack propagates to the right free boundary due to the low misorientations of cleavage planes (Figure 5.9d), which leads to the unloading of the stresses (Figure 5.11).

The nucleation of cracks at lower nominal strains in comparison with the quasi-static case, is a result of the material competition mechanisms between strain rate hardening and
thermal softening associated with dynamic loading conditions. The accumulated plastic slip and normalized temperature (normalized by the martensite melting temperature of 1700K), at a nominal strain of 10%, are shown in Figure 5.10. The maximum plastic slip is approximately 0.55, and occurs ahead of crack front. The thermal accumulation is assumed to be mainly due to adiabatic heating, and the rate of change of temperature is obtained from the balance of energy (Eq. 2.12). The highest value of normalized temperature is 0.6, and it occurs ahead of the crack front. This softening behavior eventually surmounts the dynamic strain rate hardening, and results in the propagation of the cracks.

5.3 Conclusions

Newly developed dislocation-density based evolution equations are coupled to a multiple-slip crystal plasticity formulation, and a framework is established that relates immobile and mobile dislocation-density evolution to austenitic (f.c.c.) and martensitic (b.c.c.) crystallographic orientations and behavior. A microstructurally-based failure criteria and overlapping element method are used to investigate dislocation-density evolution ahead of crack front, the effects of dislocation-GB interaction and variant distributions on crack nucleation and propagation, and the effects of dynamic loading rates on microstructural fracture.

Low transmission GBs or block boundaries can lead to dislocation-density pile-ups, which result in high local stresses. These high stresses combined with favorable orientations of cleavage planes would result in crack nucleation. Variant distributions affect the misorientations between cleavages planes and martensitic and austenitic slip planes. These orientations affect how stresses are resolved on cleavage planes, and subsequent crack
nucleation, propagation, and rupture. Dislocation-density generation ahead of crack front can induce plastic deformations, and blunt crack propagation. In comparison with quasi-static fracture nucleation and growth, dynamic cracks nucleate at lower nominal strain, and this is because the thermal softening surmounts the dynamic strain rate hardening. These quasi-static and dynamic predictions indicate that fracture toughness can be improved, and crack nucleation can be inhibited by controlling the distribution of variant orientations and retained austenite pockets.
### 5.4 Tables and Figures

Table 5.1: Material Properties

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<th>Martensite</th>
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<td>$3.0 \times 10^{-10}$m</td>
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<td>$5\tau_y$</td>
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Figure 5.1 Microstructural model and distribution of variants in martensitic blocks, (a) variant distribution for Case I, (b) variant distribution for Case II.
Figure 5.2 Dislocation generation at, (a) 2% nominal strain, (b) 6.2% nominal strain, (c) 8% nominal strain, (d) 12% nominal strain.
Figure 5.3 Behavior at 12% nominal strain, (a) shear slip, (b) normal stress
Figure 5.4 Behavior for Case I at 2.6% nominal strain, (a) immobile dislocation density for the active slip system in martensite \((1\bar{2}1)[111]\), (b) GB transmission factor for slip system \((1\bar{2}1)[111]\), (c) normal stress, (d) maximum stress on cleavage planes \(\{100\}\).
Figure 5.5 Normal stress for Case I at, (a) 6.2% nominal strain, (b) 7.2% nominal strain, (c) 9% nominal strain, (d) 12% nominal strain showing crack nucleation and propagation.
Figure 5.6 Behavior for Case II at 2.8% nominal strain, (a) immobile dislocation density for the active slip system in martensite (\(\overline{2}11\))[111], (b) GB transmission factor for slip system (\(\overline{2}11\))[111], (c) normal stress, (d) maximum stress on cleavage planes \{100\}. 
Figure 5.7 Normal stress for Case II at, (a) 5.8% nominal strain, (b) 9.6% nominal strain, (c) 11.2% nominal strain, (d) 14% nominal strain showing crack nucleation and propagation.
Figure 5.8 Stress-strain curves for the two cases.
Figure 5.9 Normal stress for variant distribution Case II at a strain rate of 5000/s at, (a) 0.6% nominal strain, (b) 4.4% nominal strain, (c) 10% nominal strain, (d) 12.6% nominal strain showing crack nucleation and propagation.
Figure 5.10 Behavior for variant distribution Case II at a strain rate of 5000/s at 10% nominal strain, (a) shear slip, (b) normalized temperature.
Figure 5.11 Stress-strain curves for dynamic and quasi-static case.
In this chapter, a dislocation-density-based multiple-slip crystalline plasticity formulation, and an overlapping fracture method were used to investigate the effects of $M_23C_6$ carbide precipitates and block/packet size on microstructural dynamic fracture in martensitic steels. A failure criterion based on the normal component of traction on the microstructural cleavage planes is developed (Chapter 3.1). The formulation accounts for variant morphologies, orientation relationships that are uniquely inherent to lath martensitic microstructures and carbide precipitates. The interrelated effects of dislocation-density evolution and thermal evolution due to the coupled thermo-mechanical effects of adiabatic heating and heat conduction on crack nucleation and propagation were investigated.

6.1 The Model

The multiple-slip dislocation-density-based crystal plasticity formulation was coupled to the nonlinear FE method to investigate the effects of $M_23C_6$ carbide precipitates on microstructural dynamic crack nucleation and growth in martensitic steels. To represent the microstructure of martensite, we used a combination of blocks and packets, which is based on the approach developed by Hatem and Zikry (2010). Blocks are collections of laths with low misorientation, and packets are collections of blocks that have the same habit plane (Morito et al., 2003; Morito et al., 2006). To investigate the effects of martensitic block/packet size on microstructural dynamic fracture, two models were used, one with 18 blocks with 6 packets, and the other with 40 blocks with 14 packets (Figure 6.2). The variant
arrangements, representing the ORs between the parent austenite grain and martensitic blocks, were based on experimental EBSD observations (Morito et al., 2003; Kitahara et al., 2006). It was assumed that the $M_{23}C_6$ carbide precipitates had a volume fraction of 2%, and that they were mainly distributed along block/packet boundaries (Abe, 2008; Taneike et al., 2004; Kipelova et al., 2013). It was also assumed that the $M_{23}C_6$ carbide precipitates had a cube-cube orientation relationship with the parent austenite grain (Shtansky et al., 2000; Song et al., 2010; Padilha and Rios, 2002). The material properties (Table 6.1) that are used are representative of low-carbon martensitic steel and $M_{23}C_6$ carbide precipitates (Jiang, 2008). It was assumed here that the M element is chromium.

The parent austenite grain was oriented based on the loading plane of $(0 0 1)_{\gamma}$ and a loading direction of $[0 1 0]_{\gamma}$. It was assumed that the parent austenite grain had high Euler angles of $(15^\circ, 25^\circ, 35^\circ)$. The Kurdjumov-Sachs (K-S) OR was adopted as the martensite OR, and $\{111\}_{\gamma}$ was assumed as the habit plane. A convergent plane strain FE mesh of 4582 elements was used with a specimen size of $3.2 \, \text{mm} \times 6.4 \, \text{mm}$, and a displacement load was applied on top surface at a nominal strain rate of $5000 \, \text{s}^{-1}$ with a constrained bottom surface (Figure 6.2).

### 6.2 Results and Discussion

#### 6.2.1 Microstructural Dynamic Fracture

The effects of $M_{23}C_6$ carbide precipitates on dislocation-density evolution, plastic deformation and dynamic fracture, have been investigated in this section. To elucidate the local microstructural mechanisms, the normalized (by the initial immobile dislocation density of martensite) immobile dislocation density and GBTF for the most active slip system in
martensite (211)[111], at a nominal strain of 1.8%, are shown in Figure 6.3a-b. The maximum immobile dislocation density was 2200, and it occurred at the interface of martensite and carbide precipitate (Figure 6.3a). The high incompatibility of slip system, represented by the low GBTF at the interface of carbide precipitates and martensite, and martensitic blocks boundaries (Figure 6.3b), can impede dislocation density transmission and result in high local stresses (Figure 6.3c). The maximum normalized (by the static yield stress of martensite) normal stress was 5, which occurred in carbide precipitates due to their higher strength, and martensitic block boundaries due to the incompatibilities of slip systems. The maximum shear slip occurred in martensite with a maximum value of 0.05 (Figure 6.3d). In comparison with the normal stress and shear slip in martensite, carbide precipitates had higher normal stress and lower plastic deformation, which increased the strength of materials.

The high normal stresses around the peripheries of the carbide precipitates resulted in large stresses on the cleavage planes of {100} (Figure 6.4a). The maximum normalized cleavage stress was 4.5, and it occurred around the carbide precipitate, as indicated by the red circle in Figure 6.4a. This high cleavage stress resulted in a crack nucleating at the interface of carbide precipitate and martensite at a nominal strain of 2.6% (Figure 6.4b). After crack nucleation, the crack propagated, which led to the unloading of the nominal stress strain curve (Figure 6.10). When the crack intersected the block/packet boundaries, it was blunted due to the deflection caused by the misorientations of cleavage planes (Wang et al., 2008; C. Wang et al., 2007; Guo et al., 2004), as indicated by the large normal stress of 7 (Figure 6.4c). With increases in loading, the right crack front then propagated to the free boundary, and the left crack front was blunted by the high strength martensite (Figure 6.4d).
When the crack was blunted at the block/packet boundaries, the local high stresses ahead of crack front activated martensitic slip systems. The normalized immobile dislocation density, for the active slip system \( (\overline{1}10)[11\overline{1}] \) at a nominal strain of 3.8%, is shown in Figure 6.5a. The maximum normalized immobile dislocation density was \( 2.2 \times 10^4 \), which occurred ahead of crack front. This high dislocation density resulted in large shear slips with a value of 0.16, as denoted by the red circle in Figure 6.5b, and this large plastic deformation can blunt crack and inhibit crack growth (Figure 6.9).

As the shear slip results (Figure 6.5b) indicate, there were large changes over small length scales, which is an indication that gradients of plastic strain can lead to the formation of geometrically necessary dislocations (GNDs) loops, which can relax strain gradients (Rezvanian et al., 2007; Kubin and Mortensen, 2003). For large deformation of crystalline materials, the formula for calculating GND densities (Elkhodary and Zikry, 2011) can be obtained as

\[
\rho_{\text{screw}}^{(\alpha)} = -\frac{1}{b^{(\alpha)}} l^{(\alpha)} \cdot \nabla \gamma^{(\alpha)},
\]

\[
\rho_{\text{edge}}^{(\alpha)} = -\frac{1}{b^{(\alpha)}} s^{(\alpha)} \cdot \nabla \gamma^{(\alpha)},
\]

where \( \rho_{\text{screw}}^{(\alpha)} \) are GND screw dislocation densities and \( \rho_{\text{edge}}^{(\alpha)} \) are GND edge dislocation densities for slip system \( \alpha \), \( l^{(\alpha)} \) is the dislocation line vector, \( s^{(\alpha)} \) is the slip direction, and \( \gamma^{(\alpha)} \) is the shear strain.

The normalized (by the initial immobile dislocation density of martensite) GND screw dislocation densities for the most active slip system \( (12\overline{1})[\overline{1}11] \), are shown in Figure
6.5c-d. The arrangement of GND screw dislocation densities is in the form of loops, and the dislocation density lines and loops are equivalent to the experimentally observed dislocation lines and loops (Elkhodary and Zikry, 2011). Figure 6.5c shows that several dislocation density loops were nucleated from the crack front at a nominal strain of 3.2%. The maximum value of GND screw dislocation densities was 35, and it occurred ahead of crack front, and where the direction of crack path had been deflected (Figure 6.5c). With the increase of loading, the loops expand, and new dislocation density loops were generated from the crack front (Figure 6.5d). Furthermore, the maximum value of GND screw dislocation densities increased from 35 at a nominal strain of 3.2% (Figure 6.5c) to 70 at a nominal strain of 3.8% (Figure 6.5d). The generation of dislocation loops can relieve tensile stresses, blunt cracks, and improve fracture toughness (Higashida et al., 2000; Higashida et al., 2008), which can inhibit crack growth (Figure 6.9). In comparison with statistically stored dislocation (SSDs) densities (Figure 6.5a), GND screw dislocation densities evolved as loops, while SSD dislocation densities were accumulated ahead of the crack front. GND screw dislocation densities were also three orders of magnitude less than SSD dislocation densities, but as the predictions indicate they were high enough to blunt the crack front.

Large dislocation generation from the crack front resulted in large plastic work, as shown in Figure 6.6a. The maximum plastic work was \(2.6 \times 10^9\) J, and it occurred ahead of the blunted crack front. The maximum normalized (by the martensite melting temperature of 1700K) adiabatic temperature was 0.6 (Figure 6.6b), and this high adiabatic temperature ahead of crack front resulted in large temperature gradients, and this had an effect on heat conduction. The normalized temperature change due to heat conduction is shown in Figure
6.6c. The maximum normalized temperature change was 0.06, and the positive value means heat was diffusing out of the region. Temperature changes were insignificant in other regions, due to the small time scale of $1.0 \times 10^{-5}$ s of this dynamic loading case. The total temperature due to adiabatic heat and conduction is shown in Figure 6.6d, with a maximum value of 0.55, which occurred ahead of the crack front.

6.2.2 Size Effects: Dynamic Fracture with Refined Blocks

In this section, a model with 40 martensitic blocks, which had a smaller block size, was used to investigate the effects of refinement of block size on crack path and velocity, and fracture toughness under dynamic loading conditions with a strain rate of 5000/s applied on the top surface (Figure 6.2b). The normalized immobile dislocation density and GBTF, for the active slip system $(0\bar{1}1)[111]$ at a nominal strain of 2.4%, are shown in Figure 6.7a-b. The maximum immobile dislocation density was 2800, and it occurred at the interface of martensite and carbide precipitate, as indicated by the arrow in Figure 6.7a. The dislocation-density was also impeded by the high strength carbide precipitate, as represented by the low GBTF at the interface (Figure 6.7b), and this resulted in high local normal stresses around the carbide precipitate with a maximum value of 5.5 (Figure 6.7c). Similar to the case with 18 blocks, the carbide precipitates had higher normal stresses and lower plastic deformation (Figure 6.7d) due to their higher strength.

The high local stresses caused by the high strength carbide precipitate, led to a crack nucleating at the interface of carbide precipitates and martensite at a nominal strain of 7.6% (Figure 6.8a). After crack nucleation, this crack then propagated. The maximum normal
stress was 10, which occurred ahead of crack front (Figure 6.8b). Then the right crack front was blunted at the block/packet boundary due to the misorientations of \{100\} cleavage planes, as indicated by the large shear slip, which attained a maximum of 0.5 (Figure 6.8c). This large plastic deformation resulted in large plastic work, which subsequently led to high temperatures with a maximum normalized value of 0.44 (Figure 6.8d).

In comparison with the case with 18 blocks, the crack path is deflected due to the higher frequency of block/packet boundaries. This is consistent with experimental observations (Wang et al., 2008). The frequent crack deflection at block/packet boundaries can absorb more energy and inhibit crack growth. The crack length curve (Figure 6.9) also indicates that the crack propagated at a much lower rate in comparison with the 18 block case, which increased fracture toughness significantly (Figure 6.10).

**6.3 Conclusions**

A dislocation-density-based crystal plasticity formulation and an overlap dynamic fracture approach were used to investigate thermo-mechanical dynamic fracture in martensitic steels. A microstructurally-based failure criterion was used to investigate the combined effects of M_{23}C_{6} carbide precipitates, block/packet sizes, adiabatic heat and thermal conduction on microstructural fracture nucleation and propagation.

M_{23}C_{6} carbide precipitates resulted in higher local normal stresses and lower plastic deformation, which increased the overall strength. The high strength carbide precipitates impeded dislocation-density transmission, and this resulted in high local stresses around the carbide precipitates, which led to large crack opening mode stresses on cleavage planes of \{100\}, and resulted in crack nucleation at the interface of martensite and carbide precipitates.
When cracks intersected block/packet boundaries, the cracks were blunted due to the misorientations of cleavage planes at the block boundaries. The high local stresses ahead of crack front activated slip systems, which generated dislocation-densities, and resulted in large plastic deformation. This also blunted crack propagation. These large plastic accumulations ahead of crack front resulted in large plastic work, which led to high temperatures. Heat conduction had minor effects on temperature distribution due to the small time scale in dynamic case. Block/packet refinement increased the frequency of crack deflection at block/packet boundaries, which inhibited crack growth, and significantly increased fracture toughness.
### 6.4 Tables and Figures

Table 6.1: Material Properties

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Figure 6.1 A schematic diagram of the carbide precipitates, $M_{23}C_6$, in martensitic steels
Figure 6.2 Microstructural model and distribution of variants in martensitic blocks, (a) case I with 18 blocks, (b) case II with 40 blocks
Figure 6.3 Behavior at a nominal strain of 1.8%, (a) immobile dislocation density for slip system (\(\overline{2}11\))[111], (b) GB transmission factor for slip system (\(\overline{2}11\))[111], (c) normal stress, (d) shear slip
Figure 6.4 (a) maximum stress on cleavage planes {100} at a nominal strain of 1.8%, normal stress at a nominal strain of, (b) 2.6%, (c) 3.8%, (d) 6.6% showing crack nucleation and growth
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CHAPTER 7: Hydrogen Embrittlement in High Strength Martensitic Steels

In this chapter, a stress assisted hydrogen diffusion model, a dislocation-density-based multiple-slip crystalline plasticity formulation, and an overlapping fracture method were used to investigate hydrogen diffusion and embrittlement in lath martensitic steels with distributions of $\text{M}_2\text{C}_6$ carbide precipitates. A microstructural failure criterion based on cleavage planes (Chapter 3.1), and a failure criterion based on hydrogen assisted fracture planes (Chapter 3.2), were used to investigate the competition mechanism between cleavage fracture and hydrogen diffusion assisted fracture along different crystallographic planes. The formulation accounts for variant morphologies, and orientation relationships that are uniquely inherent to lath martensitic microstructures. The interrelated effects of martensitic block and packet boundaries and carbide precipitates on hydrogen diffusion, hydrogen assisted crack nucleation and growth, were investigated. Stresses along the three cleavage planes and the six hydrogen embrittlement fracture planes were monitored, such crack nucleation and growth occurred along energetically favorable planes.

7.1 The Model

The multiple-slip dislocation-density-based crystal plasticity and the fracture formulations were coupled within the nonlinear FEM framework to investigate hydrogen assisted crack nucleation and growth in martensitic steels with distributions of $\text{M}_2\text{C}_6$ carbide precipitates. We used a combination of blocks and packets to represent the martensite’s microstructure. This approach is based on the approach developed by Hatem and Zikry.
Blocks are collections of laths with low misorientation, and packets are collections of blocks that have the same habit plane (Morito et al., 2003; Morito et al., 2006). In this study, 40 martensitic blocks were distributed randomly within 14 packets from one parent austenite grain. The variant arrangements, representing the orientation relationships between the parent austenite grain and martensitic blocks, were based on experimental EBSD observations (Morito et al., 2003; Kitahara et al., 2006). It was also assumed that the $\text{M}_{23}\text{C}_6$ carbide precipitates had a volume fraction of 2%, and that they were mainly distributed along block/packet boundaries (Abe, 2008; Taneike et al., 2004; Kipelova et al., 2013). The $\text{M}_{23}\text{C}_6$ carbide precipitates, are f.c.c. and assumed to have a cube-cube orientation relationship with the parent austenite grain (Shtansky et al., 2000; Song et al., 2010; Padilha and Rios, 2002), which means they are fully coherent and coincident with the austenite orientations. The material properties (Table 7.1) that are used are representative of low-carbon martensitic steel and carbide precipitates $\text{M}_{23}\text{C}_6$ (Jiang, 2008; Olden, Thaulow and Johnsen, 2008).

The parent austenite grain was oriented based on a loading plane of $(0\ 0\ 1)_\gamma$ and a loading direction of $[0\ 1\ 0]_\gamma$. The parent austenite grain was assumed as having a cube Euler orientation of $(0^\circ, 0^\circ, 0^\circ)$. The Kurdjumov-Sachs (KS) OR was adopted as the martensite OR, and $\{111\}_\gamma$ was assumed as the habit plane. An initial hydrogen concentration of 1 ppm was chosen, and a constant hydrogen concentration of 10 ppm was applied on the left surface of the model. A convergent plane strain FE mesh of 4931 elements was used with a specimen size of 3.2 mm × 6.4 mm, and a displacement load was applied on top surface at a nominal strain rate of $1.0 \times 10^{-5}$ s$^{-1}$ (Figure 7.1).
7.2 Results and Discussion

7.2.1 Hydrogen Diffusion

In this section, we will discuss how hydrogen diffusion is affected by microstructural effects, such as carbide precipitates and martensitic block boundaries. The hydrogen concentration at a nominal strain of 2%, corresponding to a time of 2000s, is shown in Figure 7.2a. Hydrogen diffused and accumulated around the precipitates, as indicated by the hydrogen concentration of 9 ppm, which is slightly less than the specified boundary condition of 10 ppm. With increases in time and loading, hydrogen continued to diffuse and accumulate at the precipitates. The maximum hydrogen concentration at a nominal strain of 6% was approximately 18 ppm, and it occurred around the carbide precipitate, which is denoted by the red circle (Figure 7.2b). The high concentration of hydrogen around the precipitate is related to pressure (cf. Eq. 2.36). This can be seen in Figure 7.2c, where the normalized (by the static yield stress of martensite) tensile pressure around the precipitate was 4.5, and this pressure accumulation resulted in large pressure gradients. The normalized norm ($L^2$ norm) of the pressure gradient around the precipitates was approximately $2.4 \times 10^4$ (Figure 7.2d), and this large pressure gradient can generate a stress driven flux of hydrogen toward the precipitate (Miresmaeili et al., 2010), which can result in hydrogen accumulation.

The large pressure gradient can be due to microstructural defects, such as dislocation-densities (see, for example, Shanthraj and Zikry, 2012). The normalized (by the initial immobile dislocation density of martensite) immobile dislocation density and GBTF, corresponding to the active slip system in martensite (1 $\bar{1}$ 2)[$\bar{1}$ 11] at a nominal strain of 6%, are shown in Figure 7.3a-b. The maximum normalized immobile dislocation density was 2.0
× 10^4, which occurred around the peripheries of the carbide precipitates. Slip system incompatibilities, as represented by the low GBTF at the interface of precipitate and martensite, and martensitic blocks boundaries (Figure 7.3b), impeded dislocation density transmission and resulted in high local stresses (Figure 7.3c). The maximum normalized (by the static yield stress of martensite) normal stress was 8, and occurred around the precipitates. These high local stresses around the precipitates further activated slip systems, and promoted martensitic inelastic deformation as indicated by the accumulation of shear slip, which attained a maximum of 0.14 (Figure 7.3d).

7.2.2 Hydrogen Diffusion Assisted Fracture

In this section, hydrogen diffusion assisted fracture has been investigated, and compared with the case without hydrogen embrittlement. As discussed in Chapter 7.2.1, carbide precipitate can impede dislocation density transmission and result in high local stresses around the precipitate. These high local stresses can not only lead to hydrogen accumulation, which decreases critical fracture stress, but also resolve large stress components perpendicular to the favorable fracture planes, which act as a driving mechanism for crack nucleation and growth along the favorable planes. It was assumed that cleavage fracture can occur along the three {100} planes, and that hydrogen diffusion assisted fracture can occur along the six {110} planes (Shibata et al., 2012). Therefore, the stresses on all these nine planes were monitored to determine whether cleavage assisted fracture or diffusion assisted fracture would occur. The maximum normalized cleavage stress on the three cleavage planes {100} at a nominal strain of 1% is shown in Figure 7.4a. The maximum normalized cleavage stress of 3.2 occurred within the carbide precipitates, while
the cleavage stress in martensite had a lower value of 2.2. The maximum normalized fracture stress, on the six hydrogen embrittlement fracture planes \{110\} at a nominal strain of 1\% is shown in Figure 7.4b. The maximum normalized value was approximately 3.4, and it occurred at the interface of martensite and the carbide precipitates. The embrittlement due to the accumulation of hydrogen around the carbide precipitates and the large stresses on the \{110\} fracture planes resulted in a crack nucleating at a nominal strain of 1.8\% (Figure 7.4c). Crack nucleation, at such a low nominal strain, is an indication of embrittlement. After crack nucleation, the crack propagated with a small crack opening displacement (Figure 7.4d). The maximum normal stress at a nominal strain of 2.2\% was 4.5, and it occurred ahead of crack front.

The high local normal stress resulted in large pressure and pressure gradients ahead of the crack front. The maximum normalized tensile pressure was 2 (Figure 7.5a), and the maximum normalized norm of pressure gradient was \(1.4 \times 10^4\) (Figure 7.5b). These high pressure gradients ahead of crack front would generate a stress driven flux of hydrogen toward the crack front, which resulted in the accumulation of hydrogen ahead of crack front at a concentration of 11 ppm (Figure 7.5c). The high concentration of hydrogen embrittled martensitic blocks, and it would result in a large reduction of the critical fracture stress on hydrogen embrittlement fracture planes \{110\} as indicated by the value of 0.28 ahead of the crack front (Figure 7.5d). In combination with high crack opening-mode stresses, this accelerated crack growth.

The nominal stress-strain curves for the hydrogen embrittlement case and for the case without embrittlement are shown in Figure 7.6. In comparison with the case without
embrittlement, the crack nucleated at a much lower nominal strain and propagated at a faster rate. The differences in crack nucleation and propagation between the hydrogen embrittlement case and the case without embrittlement are related to how hydrogen diffuses at the interfaces of the martensitic blocks and the carbide precipitates, which results in embrittlement.

The normalized total dislocation density generations for the hydrogen embrittlement case and for the case without embrittlement are shown in Figure 7.7a-b. The maximum total dislocation density generation for the hydrogen embrittlement case, at a nominal strain of 2.8%, was \(8.0 \times 10^4\) (Figure 7.7a), and it occurred ahead of crack front. The maximum total dislocation density generation for the case without embrittlement, at a nominal strain of 10%, was \(4.5 \times 10^5\) (Figure 7.7b), which was approximately 5.5 times of that for the hydrogen embrittlement case. This indicates that accumulation of hydrogen ahead of the crack front suppressed dislocation density generation, which is consistent with the predictions from molecular dynamics simulations (Song and Curtin, 2013). This high dislocation density generation resulted in large plastic deformation. The maximum shear slip for the hydrogen embrittlement case was 0.22 (Figure 7.7c), while the maximum shear slip for the case without embrittlement was 0.55 (Figure 7.7d), which was 2.5 times of that for the hydrogen embrittlement case. Furthermore, the fracture paths for these two cases were different, since lath martensite fractured on \{110\} planes for the hydrogen embrittlement cases (Shibata et al., 2012; Nagao et al., 2012; Kim and Morris, 1983), and on \{100\} cleavage planes without hydrogen embrittlement (Guo et al., 2004; Morris, 2011).
As the shear slip results (Figure 7.7c-d) indicated, there are large changes over such small length scales, which is an indication that gradients of plastic strain can lead to the formation of geometrically necessary dislocations (GNDs), which can relax strain gradients (Rezvanian et al., 2007; Kubin and Mortensen, 2003). For crystalline materials, the formula for calculating GND densities (Rezvanian et al., 2007; Elkhodary and Zikry, 2011) can be obtained as Eq. 6.1.

The normalized (by the initial immobile dislocation density of martensite) GND screw dislocation densities for the most active slip system \((\mathbf{T10}[1\mathbf{1}\mathbf{T}]\) for the hydrogen embrittlement case, for the local region denoted by the red circle in Figure 7.7c, are shown in Figure 7.8a-b. The GND screw dislocation densities evolve as loops, and the GND dislocation density lines and loops are equivalent to the actual dislocation lines and loops (Elkhodary and Zikry, 2011; Rezvanian et al., 2007). Figure 7.8a shows one dislocation density loop with a maximum value of 35 nucleated from a carbide precipitate at a nominal strain of 1.7\%, and then several small dislocation density loops with the same values were generated by the propagating crack (Figure 7.8b). The normalized GND screw dislocation densities for the most active slip system \((\mathbf{110}[1\mathbf{T}1]\), for the case without embrittlement at a nominal strain of 6\%, for the local region denoted by the red circle in Figure 7.7d, are shown in Figure 7.8c. Dislocation density loops nucleated from the crack front. As the nominal strain increases, the loops expanded, and new dislocation density loops were emitted from crack front (Figure 7.8d). Furthermore, the maximum normalized value of GND screw dislocation densities increased from 35 at 6\% nominal strain (Figure 7.8c) to 180 at 8.4\% nominal strain (Figure 7.8d). The emission of dislocation loops ahead of crack front can relax
tensile stresses, blunt the cracks, and improve fracture toughness (Higashida et al., 2000; Higashida et al., 2008), which retarded crack growth (Figure 7.9). The hydrogen embrittlement case had fewer dislocation density loops and lower dislocation density values, which further indicates that the diffusion of hydrogen suppressed the emission of dislocation loops and embrittled martensite, and resulted in cracks propagation at low nominal strains (Figure 7.9). In comparison with the behavior of statistically stored dislocations (SSDs) densities (Figure 7.7a-b), GND screw dislocation densities evolved as loops, while SSD dislocation densities evolved as accumulations. The GND screw dislocation densities were 3 orders of magnitude less than SSD dislocation densities.

7.2.3 Hydrogen Embrittlement with A Pre-existing Crack

In this section, the effects of a model with a pre-existing crack on hydrogen embrittlement have been investigated, and a pre-existing crack with the normalized initial crack length of $a/w$ of 0.1 was used, where $a$ is the crack length and $w$ is the specimen width. The pressure and norm of pressure gradient at a nominal strain of 0.3% are shown in Figure 7.10a-b. The stress accumulation caused by the pre-existing crack resulted in large tensile pressures ahead of the crack front with a maximum normalized value of 1.6 (Figure 7.10a), which subsequently led to large pressure gradients. The maximum norm of pressure gradient was approximately 8000, and it occurred ahead of crack front (Figure 7.10b), which would generate a stress assisted hydrogen flux toward the crack front, and it resulted in the accumulation of hydrogen with maximum concentrations of 9 ppm (Figure 7.10c). This high concentration of hydrogen embrittled the martensitic blocks, as indicated by the large
reduction of the critical fracture stress at a value of 0.26 (Figure 7.10d), which resulted in crack propagation and growth at low nominal strains (Figure 7.12).

The normal stress at a nominal strain of 2% for the hydrogen embrittlement case is shown in Figure 7.11a. At such a low nominal strain, the crack had already cut through the model with a small crack opening displacement. Figure 7.11b shows the normal stress at the same nominal strain for the case without hydrogen embrittlement. The crack had propagated a short distance, cut through one carbide precipitate, then was blunted by the high strength martensitic block, as indicated by the large normalized normal stress of 5.5 ahead of the crack front (Figure 7.11b) and the crack extension curve (Figure 7.12). Crack paths for these two cases were significantly different due to the different fracture planes of cleavage and hydrogen embrittlement.

As noted earlier, hydrogen embrittlement is related to dislocation-density evolution and plastic deformation. The normalized immobile dislocation densities for the most active slip system $\{112\}[1\bar{1}1]$, at a nominal strain of 2% for the hydrogen embrittlement case, are shown in Figure 7.13a. The maximum dislocation density was approximately 5000, and it occurred when the crack changed orientation due to the misorientation of martensitic blocks. The maximum normalized immobile dislocation density for the most active slip system $\{11\bar{2}\}[111]$, at a nominal strain of 4% for the case without embrittlement, was $6.0 \times 10^4$ (Figure 7.13b), which occurred ahead of crack front, and was 12 times of that for the hydrogen embrittlement case. The maximum shear slip for the hydrogen embrittlement case was 0.05 (Figure 7.13c), while for the case without embrittlement it was 0.4 (Figure 7.13d), which was 8 times of that for the hydrogen embrittlement case. These results further
substantiate that hydrogen can suppress dislocation activity, embrittle martensite, and result in crack propagation at low nominal strains due to lower plastic deformation and dislocation-density evolution and accumulation. In comparison with the hydrogen embrittlement case, without a pre-existing crack (Figure 7.4), this case resulted in higher local tensile pressures and hydrogen accumulations (Figure 7.10), which accelerated embrittlement and crack growth (Figure 7.12), and resulted in failure at a lower strain (Figure 7.11a).

7.3 Conclusions

A stress-assisted hydrogen diffusion model has been coupled to a dislocation-density-based, multi-slip crystal plasticity formulation to investigate the effects of microstructure on hydrogen diffusion and embrittlement in martensitic steels with and without pre-existing cracks. A microstructurally-based failure criterion and overlapping element method were then used to investigate hydrogen-assisted crack nucleation and propagation in martensitic steels with distributions of $M_{23}C_6$ carbide precipitates.

The predictions indicate that low transmission martensitic block boundaries and carbide precipitates impeded dislocation density transmission, resulted in large tensile pressure and pressure gradients, and led to the accumulation of hydrogen, which locally embrittled martensitic steels. Large opening-mode stresses resulted in crack nucleation at low nominal strains along $\{110\}$ planes. Stresses on all the three cleavage planes and the six hydrogen embrittlement planes were monitored for critical values, such that crack nucleation and growth would occur along the most preferential planes. The high tensile stresses ahead of the crack fronts resulted in large pressures and pressure gradients, which led to hydrogen accumulation, a significant reduction of the critical fracture stress, and an acceleration of
crack propagation. Dislocation-densities, due to geometrically necessary screw dislocation loops ahead of the crack fronts relaxed tensile stresses, blunted cracks, and retarded crack propagation. In the absence of hydrogen diffusion and embrittlement, cracks nucleated and propagated along the \{100\} planes and had significantly different orientations and paths in comparison with the hydrogen embrittlement case. The pre-existing crack in hydrogen embrittlement case resulted in higher local tensile pressures and hydrogen accumulations, which accelerated embrittlement and crack growth, and resulted in failure at a lower strain in comparison with the hydrogen embrittlement case without a pre-existing crack.
### 7.4 Tables and Figures

Table 7.1: Material Properties

<table>
<thead>
<tr>
<th>Properties</th>
<th>Carbide Precipitates, $\text{M}_{23}\text{C}_6$</th>
<th>Martensite</th>
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<tr>
<td>Young’s modulus, $E$</td>
<td>357 GPa</td>
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<td>Static yield stress, $\tau_y$</td>
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<td>Poisson’s ratio, $\nu$</td>
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<td>Rate sensitivity parameters, $m$</td>
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<td>Reference strain rate, $\dot{\gamma}_{\text{ref}}$</td>
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</tr>
<tr>
<td>Critical strain rate, $\dot{\gamma}_{\text{critical}}$</td>
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<td></td>
</tr>
<tr>
<td>Burger vector, $b$</td>
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<td>$3.0 \times 10^{-10}$ m</td>
</tr>
<tr>
<td>Initial immobile dislocation density $\rho_{\text{ini}}^0$</td>
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<td>$1.0 \times 10^{10}$ m$^{-2}$</td>
</tr>
<tr>
<td>Initial mobile dislocation density $\rho_{\text{m}}^0$</td>
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<td>$1.0 \times 10^7$ m$^{-2}$</td>
</tr>
<tr>
<td>Saturation dislocation density, $\rho_s$</td>
<td>$1.0 \times 10^{14}$ m$^{-2}$</td>
<td>$1.0 \times 10^{16}$ m$^{-2}$</td>
</tr>
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<td>Fracture stress on ${100}$ planes, $\sigma_{\text{frac}}$</td>
<td>$2\tau_{y,\text{precipitate}}$</td>
<td>$5\tau_{y,\text{martensite}}$</td>
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<tr>
<td>Initial fracture stress on ${110}$ planes, $\sigma_{c:0}$</td>
<td>$2\tau_{y,\text{precipitate}}$</td>
<td>$4\tau_{y,\text{martensite}}$</td>
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<tr>
<td>Hydrogen diffusion coefficient, $D$</td>
<td>$2.0 \times 10^{-16}$ m$^2$/s</td>
<td>$8.2 \times 10^{-10}$ m$^2$/s</td>
</tr>
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</table>
Figure 7.1 Microstructural model and carbide precipitates $\text{M}_{23}\text{C}_6$, block/packet arrangement.
Figure 7.2 Hydrogen diffusion behavior, (a) hydrogen concentration at 2% nominal strain, (b) hydrogen concentration at 6% nominal strain, (c) pressure, (d) norm of pressure gradient.
Figure 7.3 Behavior at 6% nominal strain, (a) immobile dislocation density for the active slip system (1 T2)[T11], (b) GB transmission factor for slip system (1 T2)[T11], (c) normal stress, (d) shear slip.
Figure 7.4 Diffusion assisted hydrogen cracking behavior, (a) maximum stress on \{100\} planes at 1\% nominal strain, (b) maximum stress on \{110\} planes at 1\% nominal strain, (c) normal stress at 1.8\% nominal strain, (d) normal stress at 2.2\% nominal strain.
Figure 7.5 Hydrogen embrittlement behavior at 2.2% nominal strain, (a) pressure, (b) norm of pressure gradient, (c) hydrogen concentration, (d) reduction of critical fracture stress on \{110\} planes.
Figure 7.6 Stress-strain curves for the hydrogen embrittlement case, and the case without embrittlement.
Figure 7.7 Comparison between the hydrogen embrittlement case and the case without embrittlement, total dislocation density generation, (a) for the hydrogen embrittlement case at 2.8% nominal strain, (b) for the case without embrittlement at 10% nominal strain; shear slip, (c) for the hydrogen embrittlement case at 2.8% nominal strain, (d) for the case without embrittlement at 10% nominal strain.
Figure 7.8 Comparison of GND dislocation density loop between the hydrogen embrittlement case and the case without embrittlement, GND screw dislocation density of slip system $(\overline{1}0)[1\overline{1}1]$ for the hydrogen embrittlement case, (a) at 1.7% nominal strain, (b) at 2.8% nominal strain; GND screw dislocation density of slip system $(110)[1\overline{1}1]$ for the case without embrittlement, (c) at 6% nominal strain, (d) at 8.4% nominal strain.
Figure 7.9 Comparison of crack length for the hydrogen embrittlement case and the case without embrittlement.
Figure 7.10 Hydrogen embrittlement behavior for the case with a pre-crack at 0.3% nominal strain, (a) pressure, (b) norm of pressure gradient, (c) hydrogen concentration, (d) reduction of critical fracture stress on \{110\} planes.
Figure 7.11 Comparison of normal stress at 2% nominal strain with a pre-crack for, (a) the hydrogen embrittlement case and (b) the case without embrittlement.
Figure 7.12 Comparison of crack length for the hydrogen embrittlement case and the case without embrittlement, with a pre-crack.
Figure 7.13 Comparison between the hydrogen embrittlement case and the case without embrittlement, (a) the immobile dislocation density for the active slip system \((\bar{1}12)[\bar{1}1]\), for the hydrogen embrittlement case at 2% nominal strain, (b) the immobile dislocation density for the active slip system \((11\bar{2})[111]\), for the case without embrittlement at 4% nominal strain, (c) shear slip, for the hydrogen embrittlement case at 2% nominal strain, (d) shear slip, for the case without embrittlement at 4% nominal strain.


CHAPTER 8: Transgranular and Intergranular Fracture in Bicrystal Martensitic Steels

In this chapter, a dislocation-density based multiple-slip crystalline plasticity formulation, a dislocation-density grain boundary (GB) interaction scheme for dislocation-density transmission and impedance at GB, and an overlapping fracture method were used to investigate the effects of misorientations on transgranular (TG) and intergranular (IG) fracture in bicrystal martensitic steels with $\Sigma 3$ and $\Sigma 11$ boundaries. Failure criteria based on the normal component of traction on microstructural cleavage planes of $\{100\}$ for TG fracture (Chapter 3.1), and GB planes for IG fracture (Chapter 3.3) were used to analyze the competition mechanism between TG and IG fracture. The formulation accounted for variant morphologies, and orientation relationships that are uniquely inherent to lath martensitic steels.

8.1 The Model

The multiple-slip dislocation-density-based crystal plasticity formulation was coupled to the specialized FE method to investigate the effects of misorientations, represented by coincident site lattice (CSL) GB (Figure 8.1), on TG and IG fracture in bicrystal martensitic steels. To model the microstructure of martensite, we used a combination of blocks and packets, which is based on the approach developed by Hatem and Zikry (2010). Blocks are collections of laths with low misorientation, and packets are collections of blocks that have the same habit plane (Morito et al., 2003; Morito et al., 2006). Two bicrystal models were used, one with $\Sigma 3$ boundary based on the misorientations of martensitic variant 1 and 2, and the other with $\Sigma 11$ boundary based on martensitic variant 1 and 6 (Kitahara et al., 2006), as
shown in Figure 8.2. The variant arrangements, representing the orientation relationships between the parent austenite grain and martensitic blocks, were based on experimental EBSD observations (Morito et al., 2003; Kitahara et al., 2006). The material properties (Table 8.1) that are used are representative of low-carbon martensitic steel.

The parent austenite grain was oriented based on the loading plane of (0 0 1)$_\gamma$ and a loading direction of [0 1 0]$_\gamma$. It was assumed that the parent austenite grain had high Euler angles of (20°, 30°, 40°). The Kurdjumov-Sachs (K-S) OR was adopted as the martensite OR, and {111}$_\gamma$ was assumed as the habit plane. A convergent plane strain FE mesh of 5000 elements was used with a specimen size of 0.5 mm × 1.0 mm, and a displacement load was applied for a quasi-static nominal strain rate on top surface with symmetric boundary condition (Figure 8.2). A pre-existing crack with the normalized initial crack length of a/w of 0.1 was used, where $a$ is the initial crack length, and $w$ is the specimen width.

8.2 Results and Discussion

8.2.1 Microstructural Fracture in Bicrystals with $\Sigma 3$ Boundary

The crack opening mode stresses on microstructural cleavage planes of {100} and GB planes were monitored and compared with the critical fracture stresses for failure to investigate the competition mechanism between TG and IG fracture. To elucidate the microstructural mechanisms at block boundaries, the normalized (by the initial immobile dislocation density of martensite) immobile dislocation density and GBTF for the most active slip system in martensite (110)[1 1 1], at a nominal strain of 1%, are shown in Figure 8.3a-b. The maximum dislocation density was 2400, and it occurred ahead of crack front. The low
misorientation \( \Sigma 3 \) boundary resulted in dislocation-density transmission across block boundary, which is represented the high GB transmission factor with a maximum value of 0.9. This would result in low stresses at block boundary and inhibit IG fracture, and then TG fracture would be the dominant failure mechanism (Figure 8.3c), which is consistent with experimental observations (Su et al., 2002; Suzuki et al., 2011). The TG crack was blunted by the high strength martensite, which is indicated by a large normalized (by the static yield stress of martensite) normal stress of 6, as shown in Figure 8.3c. With increases in loading, strain energy accumulated and finally built up, which drove crack propagation (Figure 8.3d) and led to a sharp drop in nominal stress-strain curve (Figure 8.7).

The stress accumulation ahead of blunted crack would activate slip systems and result in large dislocation density generation. The normalized total dislocation density generation at a nominal strain of 6.6% is shown in Figure 8.4a. The maximum total dislocation density generation was approximately \( 6.0 \times 10^4 \), and it occurred where crack changed directions and was blunted. Large dislocation density generation resulted in large plastic deformation with a maximum value of 0.16 (Figure 8.4b), which blunted crack, inhibited crack growth, and improved fracture toughness significantly (Figure 8.7). Besides large plastic deformation, lattice rotations also had a large value of 18° (Figure 8.4c), and it occurred where crack changed propagation directions and was blunted. This large lattice rotation would rotate the cleavages planes to a favorable orientation for crack growth, and combined with the stress accumulations, crack finally propagated (Figure 8.3d).
8.2.2 Microstructural Fracture in Bicrystals with $\Sigma11$ Boundary

In this section, crack propagation in bicrystal with $\Sigma11$ boundary was investigated and compared with the case with $\Sigma3$ boundary. The normalized immobile dislocation density and GBTF for the most active slip system in martensite (110)[1 $\bar{1}$1], at a nominal strain of 0.8%, are shown in Figure 8.5a-b. The immobile dislocation density ahead of crack front was approximately 400, as shown in Figure 8.5a. The high misorientation $\Sigma11$ boundary would impede dislocation-density transmission, which is represented by a low GB transmission factor of 0.5 (Figure 8.5b). This led to high normal stresses at block boundary, and resulted in IG fracture (Figure 8.5c). The stress accumulation ahead of crack front with a maximum value of 5 (Figure 8.5c) and the straight crack path along block boundary accelerated crack growth (Figure 8.5d), and decreased fracture toughness significantly (Figure 8.7).

The normalized total dislocation density generation at a nominal strain of 1.8% is shown in Figure 8.6a. The total dislocation density generation at the fracture surface regions was approximately 600, which was only 1 percent of that in $\Sigma3$ boundary. Lower dislocation density generation led to lower plastic deformation, and the shear slip at the fracture surface regions was 0.02, which was one eighth of that in $\Sigma3$ boundary. This low plastic deformation would further accelerate crack growth and decrease fracture toughness (Figure 8.7). The maximum lattice rotation was 1.5° (Figure 8.6c), which was one twelfth of that in $\Sigma3$ boundary, and this low lattice rotation was caused by the straight crack path along block boundary for IG fracture.
8.3 Conclusions

A dislocation-density GB interaction scheme was coupled to a dislocation-density based multi-slip crystal plasticity formulation to investigate the effects of misorientations on dislocation-density transmission and impedance, and TG and IG fracture in bicrystal martensitic steels. Failure criteria based on the stresses on cleavage planes and GB planes were used to characterize the competition mechanism between TG and IG fracture.

For Σ3 block boundary, dislocation-density transmission was dominant, which is represented by a large GB transmission factor. This high dislocation-density transmission resulted in low stresses at block boundary, inhibited IG fracture, and led to TG fracture. The TG crack had large dislocation density generation and plastic deformation, which blunted crack, inhibited crack propagation, and increase fracture toughness significantly. For Σ11 block boundary, dislocation-density impedance was dominant, which is represented by a low GB transmission factor, resulted in high stresses at block boundary, and led to IG fracture. In comparison with the TG crack, the IG crack propagated along the straight block boundary, and had much lower dislocation-density generation and plastic deformation, which accelerated crack growth and decreased fracture toughness significantly.
### 8.4 Tables and Figures

Table 8.1: Material Properties

<table>
<thead>
<tr>
<th>Properties</th>
<th>Martensite</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young’s modulus, $E$</td>
<td>228 GPa</td>
</tr>
<tr>
<td>Static yield stress, $\tau_y$</td>
<td>517 MPa</td>
</tr>
<tr>
<td>Poisson’s ratio, $\nu$</td>
<td>0.3</td>
</tr>
<tr>
<td>Rate sensitivity parameters, $m$</td>
<td>0.01</td>
</tr>
<tr>
<td>Reference strain rate, $\dot{\gamma}_{ref}$</td>
<td>0.001 s$^{-1}$</td>
</tr>
<tr>
<td>Critical strain rate, $\dot{\gamma}_{critical}$</td>
<td>$10^4$ s$^{-1}$</td>
</tr>
<tr>
<td>Burger vector, $b$</td>
<td>$3.0 \times 10^{-10}$ m</td>
</tr>
<tr>
<td>Initial immobile dislocation density $\rho_{im}^0$</td>
<td>$1.0 \times 10^{10}$ m$^{-2}$</td>
</tr>
<tr>
<td>Initial mobile dislocation density $\rho_m^0$</td>
<td>$1.0 \times 10^7$ m$^{-2}$</td>
</tr>
<tr>
<td>Saturation dislocation density, $\rho_s$</td>
<td>$1.0 \times 10^{16}$ m$^{-2}$</td>
</tr>
<tr>
<td>Fracture stress, $\sigma_{frac}$</td>
<td>$5\tau_{y,\text{martensite}}$</td>
</tr>
<tr>
<td>Fracture stress on GB planes, $\sigma_{gb}$</td>
<td>$5.5\tau_{y,\text{martensite}}$</td>
</tr>
</tbody>
</table>
Figure 8.1 CSL grain boundary
Figure 8.2 Microstructural bicrystal model and distribution of variants in martensitic blocks, (a) case I with $\Sigma 3$ boundary, (b) case II with $\Sigma 11$ boundary.
Figure 8.3 (a) immobile dislocation density and (b) GB transmission factor for slip system \((\bar{1}10)[11\bar{1}]\) at a nominal strain of 1%, normal stress at, (c) 6% nominal strain, (d) 6.6% nominal strain showing crack growth.
Figure 8.4 Behavior at a nominal strain of 6.6%, (a) total dislocation-density generation, (b) shear slip, (c) lattice rotation.
Figure 8.5 (a) immobile dislocation density and (b) GB transmission factor for slip system (110)[1 1 1] at a nominal strain of 0.8%, normal stress at, (c) 1.2% nominal strain, (d) 1.8% nominal strain showing crack growth.
Figure 8.6 Behavior at a nominal strain of 1.8%, (a) total dislocation-density generation, (b) shear slip, (c) lattice rotation.
Figure 8.7 Stress-strain curves for case I with \(\Sigma 3\) boundary and case II with \(\Sigma 11\) boundary
CHAPTER 9: Recommendations for Future Research

1. **Intergranular (IG) fracture in polycrystalline microstructures**: IG failure criterion has been developed and applied to bicrystal martensitic steels, presented in Chapter 8. It is necessary to study IG fracture in polycrystalline steels alloys. To investigate IG fracture in polycrystalline microstructures, IG crack propagation in triple-junctions needs to be addressed in detail.

2. **Competition between IG and Transgranular (TG) fracture in polycrystalline microstructures**: The effects of misorientations on IG and TG fracture in bicrystal martensitic steels have been discussed in Chapter 8. Due to the different misorientations in polycrystalline microstructures, the transition from IG to TG fracture, or vice versa, can occur. Sukumar et al. (2003) have investigated transition from IG to TG brittle fracture in polycrystalline microstructures using extended finite element method, but that investigation did not account for the underlying microstructural mechanisms, such as dislocation-GB interactions, and their effects on TG and IG fracture.

3. **IG stress corrosion cracking (IGSCC) in crystalline steel alloys**: Stainless steels obtain corrosion resistance through chromium, since chromium can incorporate a protective film (Bruemmer and Was, 1994; Duarte et al., 2013). For stainless steels at high temperature, chromium diffusion and precipitation at GB result in chromium depletion, which leads to oxidation at GB in corrosive environment. GBs become brittle and fracture (King et al., 2008). An oxygen diffusion model can be
incorporated into the current crystal plasticity framework to investigate microstructural effects on IGSCC.

4. **Microstructural fracture analysis for duplex, TRIP and ferritic steels**: The current framework is general, and can be applied to investigate large plastic deformation, dynamic fracture and hydrogen embrittlement in other steel alloys.

5. **3-D microstructure representation and simulation**: The slip system and fracture planes are in 3-D configuration. Currently the model is 2 dimensional, and the fracture planes are projected onto 2-D plane. It is important to extend the current 2-D model to 3-D to obtain the influence from the out of plane direction.
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