Dynamic fracture predictions of microstructural mechanisms and characteristics in martensitic steels

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Abstract

A dislocation-density-based multiple-slip crystalline plasticity formulation, and an overlapping fracture method were used to investigate the effects of carbide precipitates, $M_{23}C_6$, and martensitic block size on dynamic fracture in martensitic steels. The interrelated effects of dislocation-density evolution, orientation relations (ORs), adiabatic heating, and heat conduction on fracture behavior were investigated. Precipitates interfaces are shown to be the sites of crack nucleation due to dislocation-density impedance. Dislocation-densities are also shown to relieve tensile stresses and blunt crack propagation. These predictions indicate that the size refinement of martensitic blocks increases crack deflection at block/packet boundaries, which can significantly improve fracture toughness.

Keywords: Carbide precipitates $M_{23}C_6$, Lath martensite, Dislocation-density, Crack nucleation

1. Introduction

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 due to martensitic steel's unique lath microstructure, and this microstructure can be characterized in terms of lath, block and packet substructures, and its ORs with parent austenite grain [1,2]. The strength and toughness of lath martensitic steel are strongly related to block and packet size [3,4]. Refinement of the block and packet size can improve the strength and toughness, as the block and packet boundaries act as obstacles to dislocation transmission and crack propagation [5,6]. Experimental investigations have indicated that block and packet refinement can be effective in improving fracture resistance [7,8].

The strength of steels can be increased through introduction of precipitates [9–11], since these fine precipitates can impede dislocation movement. This strength improvement is related to the size, volume fraction, distribution, and crystal structure of precipitates [12–14]. In addition to improving the strength, these hard precipitates can reduce the ductility and fracture toughness of steels [15,16]. Experimental observations have, however, indicated that the hard precipitates can act as the sites of crack nucleation [17–19].

In martensitic steels, various precipitates including $M_{23}C_6$, M_6C , M_7C_3 , MX and M_2X are frequently observed, where M denotes a metallic element, and X denotes carbon or nitrogen atoms [3,20,21]. A primary precipitate is the carbide precipitate $M_{23}C_6$, where M is mainly chromium, Cr , and it can be replaced with Fe , Mo , Ni [22,23]. The carbide precipitates $M_{23}C_6$ mainly occur at martensitic block and packet boundaries, and at parent austenite grain boundaries [24,25]. The carbide precipitates $M_{23}C_6$ have face centered cubic (f.c.c.) crystal structure, and have cube-to-cube ORs with parent austenite grains [26,27]. Since they tend to coarsen easily due to solubility of iron and chromium, the

carbide precipitates $M_{23}C_6$ have a relatively large size of 0.1 – 0.3 μm with a volume fraction of approximately 2% [28].

These experimental investigations, furthermore, indicate that the interrelated microstructural effects of martensitic block/packet size and carbide precipitates $M_{23}C_6$ have a significant influence on the strength, ductility, and fracture toughness. The objective of the present work, therefore, is to develop an integrated framework that can incorporate microstructural features of lath martensite and carbide precipitates $M_{23}C_6$, to investigate the effects of carbide precipitates and block/packet size on microstructural dynamic fracture. In the proposed approach, we account for variant morphologies and ORs that are uniquely inherent to lath martensitic microstructures and carbide precipitates $M_{23}C_6$. A dislocation-density grain boundary (GB) interaction scheme that accounts for dislocation transmission and impedance across martensitic block and packet boundaries has been developed, and it is incorporated within the dislocation-density based crystalline plasticity formulation [29–31]. A fracture method based on the overlapping element method of Wu and Zikry [32] and Hansbo A. and Hansbo P. [33] has been used to generate failure surfaces, on experimentally observed cleavage planes, as a function of microstructural characteristics, dislocation-density evolution, and martensitic block orientations. This formulation is then used to investigate microstructural dynamic fracture in lath martensitic steels with distributions of carbide precipitates $M_{23}C_6$.

This paper is organized as follows: the dislocation-density based crystalline plasticity formulation, the derivation of the dislocation-density GB interaction, the thermo-mechanical coupling model, and a brief introduction of carbide precipitates $M_{23}C_6$ are presented in Section 2, the microstructurally-based failure criterion, and the

numerical implementation of overlapping element method for fracture are outlined in Section 3, the results are presented and discussed in Section 4, and a summary of the results and conclusions are given in Section 5.

2. Constitutive Formulation

In this section, only a brief outline of the multiple-slip crystal plasticity rate-dependent constitutive formulation and the evolution equations for the mobile and immobile dislocation-densities, which are coupled to the constitutive formulation, are presented. A detailed presentation is given by Shanthraj and Zikry [30].

2.1. Multiple-slip dislocation-density based crystal plasticity formulation

The dislocation-density based crystal plasticity constitutive framework used in this study is based on a formulation developed by Zikry [29], Shanthraj and Zikry [34], and Wu et al. [35], and a brief outline will be presented here. It is assumed that the velocity gradient is decomposed into a symmetric deformation rate tensor D_{ij} and an anti-symmetric spin tensor W_{ij} [36]. The tensors D_{ij} and W_{ij} are then additively decomposed into elastic and inelastic components as

$$D_{ij} = D_{ij}^* + D_{ij}^p, \quad W_{ij} = W_{ij}^* + W_{ij}^p, \quad (1)$$

The superscript $*$ denotes the elastic part, and the superscript p denotes the plastic part.

W_{ij}^* includes the rigid body spin. The inelastic parts are defined in terms of the crystallographic slip-rates as

$$D_{ij}^p = \sum_{\alpha} P_{ij}^{(\alpha)} \dot{\gamma}^{(\alpha)}, \quad \text{and} \quad W_{ij}^p = \sum_{\alpha} \omega_{ij}^{(\alpha)} \dot{\gamma}^{(\alpha)}, \quad (2)$$

where α is summed over all slip-systems, and $P_{ij}^{(\alpha)}$ and $\omega_{ij}^{(\alpha)}$ are the symmetric and anti-symmetric parts of the Schmid tensor in the current configuration respectively.

A power law relation can characterize the rate-dependent constitutive description on each slip system as

$$\dot{\gamma}^{(\alpha)} = \dot{\gamma}_{ref}^{(\alpha)} \left[\frac{\tau^{(\alpha)}}{\tau_{ref}^{(\alpha)}} \right] \left[\frac{|\tau^{(\alpha)}|}{\tau_{ref}^{(\alpha)}} \right]^{\frac{1}{m}-1}, \quad (3)$$

where $\dot{\gamma}_{ref}^{(\alpha)}$ is the reference shear strain-rate which corresponds to a reference shear stress $\tau_{ref}^{(\alpha)}$, and m is the rate sensitivity parameter. $\tau^{(\alpha)}$ is the resolved shear stress on slip system α . The reference stress used is a modification of widely used classical forms [37] that relate reference stress to immobile dislocation-density ρ_{im} as

$$\tau_{ref}^{(\alpha)} = \left(\tau_y^{(\alpha)} + G \sum_{\beta=1}^{nss} b^{(\beta)} \sqrt{a_{\alpha\beta} \rho_{im}^{(\beta)}} \right) \left(\frac{T}{T_0} \right)^{-\xi}, \quad (4)$$

where $\tau_y^{(\alpha)}$ is the static yield stress on slip system α , G is the shear modulus, nss is the number of slip systems, $b^{(\beta)}$ is the magnitude of the Burgers vector, and $a_{\alpha\beta}$ are Taylor coefficients which are related to the strength of interactions between slip-systems [38–40]. T is the temperature, T_0 is the reference temperature, and ξ is the thermal softening exponent, which is chosen as 0.3.

2.2. Mobile and immobile dislocation density evolution equations

Following the approach of Zikry and Kao [41], it is assumed that, for a given deformed state of the material, the total dislocation-density, $\rho^{(\alpha)}$, can be additively decomposed into a mobile $\rho_m^{(\alpha)}$ and an immobile dislocation-density, $\rho_{im}^{(\alpha)}$. Furthermore, the mobile and immobile dislocation-density rates can be coupled through the formation and destruction of junctions as the stored immobile dislocations act as obstacles for evolving mobile dislocations. This is the basis for taking the evolution of mobile and immobile dislocation densities as

$$\frac{d\rho_m^\alpha}{dt} = |\dot{\gamma}^\alpha| \left(\frac{g_{sour}^\alpha}{b^2} \left(\frac{\rho_{im}^\alpha}{\rho_m^\alpha} \right) - g_{minter}^\alpha \rho_m^\alpha - \frac{g_{immob-}^\alpha}{b} \sqrt{\rho_{im}^\alpha} \right), \quad (5)$$

$$\frac{d\rho_{im}^\alpha}{dt} = |\dot{\gamma}^\alpha| \left(g_{minter+}^\alpha \rho_m^\alpha + \frac{g_{immob+}^\alpha}{b} \sqrt{\rho_{im}^\alpha} - g_{recov}^\alpha \rho_{im}^\alpha \right), \quad (6)$$

where g_{sour} is a coefficient pertaining to an increase in the mobile dislocation-density due to dislocation sources, g_{minter} are coefficients related to the trapping of mobile dislocations due to forest intersections, cross-slip around obstacles, or dislocation interactions, g_{recov} is a coefficient related to the rearrangement and annihilation of immobile dislocations, and g_{immob} are coefficients related to the immobilization of mobile dislocations.

2.3. Determination of dislocation density evolution coefficients

To couple the evolution equations for mobile and immobile dislocation densities to the crystal plasticity formulation, the non-dimensional coefficients in Eqs. (5, 6) were determined as functions of the crystallography and deformation mode of the material, by

considering the generation, interaction and recovery of dislocation densities as discussed in Shanthraj and Zikry [30]. These expressions are summarized in Table 1,

Table 1. g coefficients in equation (5-6)

g Coefficients	Expression
g_{sour}^{α}	$b^{\alpha} \varphi \sum_{\beta} \sqrt{\rho_{im}^{\beta}}$
g_{mter-}^{α}	$l_c f_0 \sum_{\beta} \sqrt{a_{\alpha\beta}} \left[\frac{\rho_m^{\beta}}{\rho_m^{\alpha} b^{\alpha}} + \frac{\dot{\gamma}^{\beta}}{\dot{\gamma}^{\alpha} b^{\beta}} \right]$
g_{immob-}^{α}	$\frac{l_c f_0}{\sqrt{\rho_{im}^{\alpha}}} \sum_{\beta} \sqrt{a_{\alpha\beta}} \rho_{im}^{\beta}$
g_{mter+}^{α}	$\frac{l_c f_0}{\dot{\gamma}^{\alpha} \rho_m^{\alpha}} \sum_{\beta, \gamma} n_{\alpha}^{\beta\gamma} \sqrt{a_{\beta\gamma}} \left[\frac{\rho_m^{\gamma} \dot{\gamma}^{\beta}}{b^{\beta}} + \frac{\rho_m^{\beta} \dot{\gamma}^{\gamma}}{b^{\gamma}} \right]$
g_{immob+}^{α}	$\frac{l_c f_0}{\dot{\gamma}^{\alpha} \sqrt{\rho_{im}^{\alpha}}} \sum_{\beta} n_{\alpha}^{\beta\gamma} \sqrt{a_{\beta\gamma}} \rho_{im}^{\gamma} \dot{\gamma}^{\beta}$
g_{recov}^{α}	$\frac{l_c f_0}{\dot{\gamma}^{\alpha}} \left(\sum_{\beta} \sqrt{a_{\alpha\beta}} \frac{\dot{\gamma}^{\beta}}{b^{\beta}} \right) e^{\left(\frac{-H_0 (1 - \sqrt{\frac{\rho_{im}^{\alpha}}{\rho_s^{\alpha}}})}{kT} \right)}$

where f_0 , and φ are geometric parameters. H_0 is the reference activation enthalpy, ρ_s is the saturation density and the average junction length, l_c , can be approximated as

$$l_c = \frac{1}{\sum_{\beta} \sqrt{\rho_{im}^{(\beta)}}}, \quad (7)$$

An interaction tensor, $n_{\alpha}^{\beta\gamma}$, is introduced and defined as having a value of 1 if dislocations on slip-systems β and γ interact to form an energetically favorable junction on slip system α , and a value of 0 if there are no interactions. This interaction tensor is

used to map the dislocation-density interactions with the corresponding slip system, and the energy criterion based on Frank's rule is used to determine the formation of junctions. Junction formation is different for b.c.c. (martensite) and f.c.c. (carbide precipitates $M_{23}C_6$) structures, and details are given in Shanthraj and Zikry [34].

2.4. 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 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 [42–45]. The energy required to produce the residual dislocation at the boundary is considered as the energy barrier for thermally activated dislocation transmission [46,47]. The constitutive relation Eq. (3) has been modified at the boundary through the introduction of a GB transmission factor (GBTF) based on the energy barrier as

$$\dot{\gamma}^{(\alpha)} = \dot{\gamma}_{ref}^{(\alpha)} \left[\frac{\tau^{(\alpha)}}{\tau_{ref}^{(\alpha)}} \right] \left[\frac{\tau^{(\alpha)}}{\tau_{ref}^{(\alpha)}} \right]^{\frac{1}{m}-1} GBTF^{(\alpha)}, \quad (8)$$

where $GBTF^{(\alpha)} = e^{\left(\frac{U_{GB}^{(\alpha)}}{kT} \right)}$. It can range from 0 to 1, where 0 corresponds to full blockage and 1 corresponds to full transmission. $U_{GB}^{(\alpha)}$ is the internal energy for slip system α due to the activation of a Frank-Read source in the presence of a GB, k is the Boltzmann constant, and T is the absolute temperature. Based on a line tension model developed by

Koning et al. (2002), this energy barrier due to GB residual dislocations, for incoming and outgoing slip systems α and β , can be postulated as

$$U_{GB}^{(\alpha\beta)} = \kappa G \Delta b_{eff}^2 \Delta_2, \quad (9)$$

where κ is approximately equal to 0.5, G is the shear modulus, Δb_{eff} 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. Δ_2 is the length of residual dislocation, and it is a function of the resolved shear stress for the outgoing slip system β . Details for calculation of Δb_{eff} and Δ_2 are given in Shanthraj and Zikry [42] and Koning et al. [48]. Dislocation-density transmission is considered on the most energetically favorable outgoing slip system by using the lowest value of the energy, on all active outgoing slip systems, as

$$U_{GB}^{(\alpha)} = \min_{\beta} U_{GB}^{(\alpha\beta)}, \quad (10)$$

2.5. Thermo-mechanical coupling

For dynamic loading condition, the adiabatic heating generation, $q_{mechanical}$, due to plastic work is given as

$$q_{mechanical} = \chi \sigma'_{ij} D_{ij}^p, \quad (11)$$

where χ is the fraction of plastic work transformed to heat energy, and σ'_{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

$$\rho c_p \dot{T} = \lambda \nabla^2 T + q_{mechanical} \quad (12)$$

where ρ is the mass density, c_p is the specific heat capacity, and λ is the thermal conduction coefficient. The discretized finite element heat conduction equation is given as [49]

$$[C][\dot{T}] + [K][T] = [R_T] \quad (13)$$

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.

2.6. Carbide precipitates $M_{23}C_6$

Precipitates in martensitic steels have a significant effect on strength and toughness. A primary precipitate is carbide precipitate $M_{23}C_6$. These carbide precipitates have f.c.c. crystal structure, and mainly locate at martensitic block/packet boundaries, as shown in Fig. 1. These carbide precipitates have cube to cube orientation relationships with parent austenite grain, which can be described as $\{001\}_{\gamma} // \{001\}_{M_{23}C_6}$ and $\langle 100 \rangle_{\gamma} // \langle 100 \rangle_{M_{23}C_6}$. The slip systems for carbide precipitates $M_{23}C_6$ are the same as f.c.c. slip systems.

3. Microstructural failure criterion and numerical implementation of overlapping element method

3.1. Microstructurally-based failure criterion

The inherent fracture mode in martensitic steel is cleavage on $\{100\}_{\alpha'}$ planes [6]. To account for this as 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 Wu and Zikry [32] as

$$n_{cleave} = [T]_3 [T]_2 [T]_1 n_{cleave, \alpha'}, \quad (14)$$

where $[T]_1$, relates an observed OR to a theoretical OR, such as Kurdjumov-Sachs (KS) and Nishiyama-Wassermann (NW) ORs, the second transformation, $[T]_2$, relates the martensite OR to the parent austenite Euler grain orientation, and the third transformation, $[T]_3$, relates the parent austenite Euler grain orientation to the global coordinates.

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 as $\dot{n}_{cleave} = W^* n_{cleave}$. The normal component of the traction acting on each cleavage plane has a direct influence on fracture along that plane [50,51]. 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 a critical fracture stress σ_{frac} to determine failure. The failure criterion is then given by

$$t_{cleave} > \sigma_{frac}, \quad (15)$$

where $t_{cleave} = \max_{\{100\}_{\alpha'} \text{ planes}} \langle n_{cleave}^T [\sigma] n_{cleave} \rangle$.

3.2. Computational implementation of overlapping element method

We follow the approach of Wu and Zikry [32] and Hansbo A. and Hansbo P. [33], and consider one element with a crack defined implicitly by $f(X)=0$. This divides the element domain into two subdomains with areas A_{e1} and A_{e2} . The direction of crack propagation would be along the most favorable cleavage plane [5,7]. 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} , corresponding to one of the two subdomains for the original cracked element, is considered as active. Details for implementation of overlapping element method are given in Wu and Zikry [32].

3.3. Computational techniques for dislocation-density-based 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 [29] and Shanthraj and Zikry [30] 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 dislocation densities. For dynamic deformations, a lumped mass, one point integration, trapezoidal rule, and a stiffness based hourglass control are used.

4. Results and discussion

The multiple-slip dislocation-density-based crystal plasticity formulation was coupled to the nonlinear FE method to investigate the effects of carbide precipitates $M_{23}C_6$ 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 [52]. Blocks are collections of laths with low misorientation, and packets are collections of blocks that have the same habit plane [1,2]. 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 (Fig. 2). The variant arrangements, representing the ORs between the parent austenite grain and martensitic blocks, were based on experimental EBSD observations [1,53]. It was assumed that the carbide precipitate $M_{23}C_6$ had a volume fraction of 2%, and that they were mainly distributed along block/packet boundaries [24,25,28]. It was also assumed that the carbide precipitate $M_{23}C_6$ had a cube-cube orientation relationship with the parent austenite grain [22,26,54]. The material properties (Table 2) that are used are representative of low-carbon martensitic steel and carbide precipitates $M_{23}C_6$ [55]. 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 s^{-1} with a constrained bottom surface (Fig. 2).

Table 2 Material Properties

Properties	Carbide Precipitate M_{23}C_6	Martensite
Young's modulus, E	357 GPa	228 GPa
Static yield stress, τ_y	1.65 GPa	517 MPa
Poisson's ratio, ν	0.3	0.3
Rate sensitivity parameters, m	0.01	0.01
Reference strain rate, $\dot{\epsilon}$	0.001 s^{-1}	0.001 s^{-1}
Critical strain rate, $\dot{\epsilon}$	10^4 s^{-1}	10^4 s^{-1}
Burger vector, b	$3.0 \times 10^{-10} \text{ m}$	$3.0 \times 10^{-10} \text{ m}$
Initial immobile dislocation density ρ_{im}^0	$1.0 \times 10^{10} \text{ m}^{-2}$	$1.0 \times 10^{10} \text{ m}^{-2}$
Initial mobile dislocation density ρ_m^0	$1.0 \times 10^7 \text{ m}^{-2}$	$1.0 \times 10^7 \text{ m}^{-2}$
Saturation dislocation density, ρ_s	$1.0 \times 10^{14} \text{ m}^{-2}$	$1.0 \times 10^{16} \text{ m}^{-2}$
Fracture stress, σ_{frac}	$2\tau_{y_precipitate}$	$5\tau_{y_martensite}$
Thermal conduction coefficient, λ	$19 \text{ Wm}^{-1}\text{K}^{-1}$	$25 \text{ Wm}^{-1}\text{K}^{-1}$

4.1 Microstructural dynamic fracture

The effects of carbide precipitates M_{23}C_6 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 $(\bar{2}11)[111]$, at a nominal strain of 1.8%, are shown in Figs. 3(a-b). The maximum immobile dislocation density was 2200, and it occurred at the interface of martensite and carbide precipitate (Fig. 3(a)). The high incompatibility of slip system,

represented by the low GBTF at the interface of carbide precipitates and martensite, and martensitic blocks boundaries (Fig. 3(b)), can impede dislocation density transmission and result in high local stresses (Fig. 3(c)). 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 (Fig. 3(d)). 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 $\{100\}$ (Fig. 4(a)). The maximum normalized cleavage stress was 4.5, and it occurred around the carbide precipitate, as indicated by the red circle in Fig. 4(a). This high cleavage stress resulted in a crack nucleating at the interface of carbide precipitates and martensite at a nominal strain of 2.6% (Fig. 4(b)). After crack nucleation, the crack propagated, which led to the unloading of the nominal stress strain curve (Fig. 10). When the crack intersected the block/packet boundaries, it was blunted due to the deflection caused by the misorientations of cleavage planes [6–8], as indicated by the large normal stress of 7 (Fig. 4(c)). 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 (Fig. 4(d)).

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 $(\bar{1}10)[11\bar{1}]$ at a nominal strain of 3.8%, is

shown in Fig. 5(a). The maximum normalized immobile dislocation density was 2.2×10^4 , 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 Fig. 5(b), and this large plastic deformation can blunt crack and inhibit crack growth (Fig. 9).

As the shear slip results (Fig. 5(b)) 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 [56,57]. For large deformation of crystalline materials, the formula for calculating GND densities [58] can be obtained as

$$\begin{aligned}\rho_{screw}^{(\alpha)} &= -\frac{1}{b^{(\alpha)}} l^{(\alpha)} \cdot \nabla \gamma^{(\alpha)}, \\ \rho_{edge}^{(\alpha)} &= -\frac{1}{b^{(\alpha)}} s^{(\alpha)} \cdot \nabla \gamma^{(\alpha)},\end{aligned}\tag{16}$$

where $\rho_{screw}^{(\alpha)}$ are GND screw dislocation densities and $\rho_{edge}^{(\alpha)}$ are GND edge dislocation densities for slip system α , $l^{(\alpha)}$ 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 $(12\bar{1})[\bar{1}11]$, are shown in Figs. 5(c-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 [58]. Fig. 5(c) 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 (Fig. 5(c)). With the increase of loading, the loops expand, and new dislocation density loops were generated from the crack front (Fig. 5(d)). Furthermore, the maximum value of GND screw dislocation densities increased from 35 at a nominal strain of 3.2% (Fig. 5(c)) to 70 at a nominal strain of 3.8% (Fig. 5(d)). The generation of dislocation loops can relieve tensile stresses, blunt cracks, and improve fracture toughness [59,60], which can inhibit crack growth (Fig. 9). In comparison with statistically stored dislocation (SSDs) densities (Fig. 5(a)), 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 Fig. 6(a). The maximum plastic work was 2.6×10^9 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 (Fig. 6(b)), 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 Fig. 6(c). 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 1.0×10^{-5} s of this dynamic loading case. The total temperature due to adiabatic heat and conduction is shown in Fig. 6(d), with a maximum value of 0.55, which occurred ahead of the crack front.

4.2 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 (Fig. 2(b)). 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 Figs. 7(a-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 Fig. 7(a). The dislocation-density was also impeded by the high strength carbide precipitates, as represented by the low GBTF at the interface (Fig. 7(b)), and this resulted in high local normal stresses around the carbide precipitates with a maximum value of 5.5 (Fig. 7(c)). Similar to the case with 18 blocks, the carbide precipitates had higher normal stresses and lower plastic deformation (Fig. 7(d)) due to their higher strength.

The high local stresses caused by the high strength carbide precipitates, led to a crack nucleating at the interface of carbide precipitates and martensite at a nominal strain of 7.6% (Fig. 8(a)). After crack nucleation, this crack then propagated. The maximum normal stress was 10, which occurred ahead of crack front (Fig. 8(b)). Then the right crack front was blunted at the block/package boundary due to the misorientations of $\{100\}$ cleavage planes, as indicated by the large shear slip, which attained a maximum of 0.5 (Fig. 8(c)). This large plastic deformation resulted in large plastic work, which subsequently led to high temperatures with a maximum normalized value of 0.44 (Fig. 8(d)).

In comparison with the case with 18 blocks, the crack path is deflected due to the higher frequency of block/package boundaries. This is consistent with experimental

observations [7]. The frequent crack deflection at block/packet boundaries can absorb more energy and inhibit crack growth. The crack length curve (Fig. 9) also indicates that the crack propagated at a much lower rate in comparison with the 18 block case, which increased fracture toughness significantly (Fig. 10).

5. Conclusions

A dislocation-density-based crystal plasticity formulation and an overlapping 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 carbide precipitates $M_{23}C_6$, block/packet sizes, adiabatic heat and thermal conduction on microstructural fracture nucleation and propagation.

Carbide precipitates $M_{23}C_6$ 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.

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List of figures

Fig. 1 A schematic diagram of the carbide precipitates, $M_{23}C_6$, in martensitic steels

Fig. 2 Microstructural model and distribution of variants in martensitic blocks, (a) case I with 18 blocks, (b) case II with 40 blocks

Fig. 3 Behavior at a nominal strain of 1.8%, (a) immobile dislocation density for slip system $(\bar{2}11)[111]$, (b) GB transmission factor for slip system $(\bar{2}11)[111]$, (c) normal stress, (d) shear slip

Fig. 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

Fig. 5 Behavior at a nominal strain of 3.8%, (a) immobile dislocation density for slip system $(\bar{1}10)[11\bar{1}]$, (b) shear slip, GND screw dislocation density for slip system $(12\bar{1})[\bar{1}11]$ at a nominal strain of, (c) 3.2%, (d) 3.8%

Fig. 6 Thermal evolution behavior at a nominal strain of 6.6%, (a) plastic work, (b) adiabatic temperature, (c) temperature change due to heat conduction, (d) total temperature

Fig. 7 Behavior at a nominal strain of 2.4%, (a) immobile dislocation density for slip system $(0\bar{1}1)[111]$, (b) GB transmission factor for slip system $(0\bar{1}1)[111]$, (c) normal stress, (d) shear slip

Fig. 8 Normal stress at a nominal strain of, (a) 7.6%, (b) 9.2% showing crack nucleation and growth, (c) shear slip and (d) total temperature at a nominal strain of 9.4%

Fig. 9 Comparison of crack length curves

Fig. 10 Nominal stress-strain curves at a strain rate of 5000/s

Fig. 1 A schematic diagram of the carbide precipitates, $M_{23}C_6$, in martensitic steels

Fig. 2 Microstructural model and distribution of variants in martensitic blocks, (a) case I with 18 blocks, (b) case II with 40 blocks

Fig. 3 Behavior at a nominal strain of 1.8%, (a) immobile dislocation density for slip system $(\bar{2}11)[111]$, (b) GB transmission factor for slip system $(\bar{2}11)[111]$, (c) normal stress, (d) shear slip

Fig. 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

Fig. 5 Behavior at a nominal strain of 3.8%, (a) immobile dislocation density for slip system $(\bar{1}10)[11\bar{1}]$, (b) shear slip, GND screw dislocation density for slip system $(12\bar{1})[\bar{1}11]$ at a nominal strain of, (c) 3.2%, (d) 3.8%

Fig. 6 Thermal evolution behavior at a nominal strain of 6.6%, (a) plastic work, (b) adiabatic temperature, (c) temperature change due to heat conduction, (d) total temperature

Fig. 7 Behavior at a nominal strain of 2.4%, (a) immobile dislocation density for slip system $(0\bar{1}1)[111]$, (b) GB transmission factor for slip system $(0\bar{1}1)[111]$, (c) normal stress, (d) shear slip

Fig. 8 Normal stress at a nominal strain of, (a) 7.6%, (b) 9.2% showing crack nucleation and growth, (c) shear slip and (d) total temperature at a nominal strain of 9.4%

Fig. 9 Comparison of crack length curves

Fig. 10 Nominal stress-strain curves at a strain rate of 5000/s