Engineering Fracture Mechanics 145 (2015) 54–66

Contents lists available at ScienceDirect

Engineering Fracture Mechanics

journal homepage: www.elsevier.com/locate/engfracmech

# Dynamic fracture predictions of microstructural mechanisms and characteristics in martensitic steels

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ARTICLE INFO

*Article history:*
Received 27 December 2014
Received in revised form 28 May 2015
Accepted 1 June 2015
Available online 8 July 2015

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

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.



## 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

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http://dx.doi.org/10.1016/j.engfracmech.2015.06.002
0013-7944/

[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 and Hansbo [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

$$D_{ij} = D^{*}_{ij} + D^{p}_{ij}, \quad W_{ij} = W^{*}_{ij} + W^{p}_{ij} \tag{1}$$

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

$$D^{p}_{ij} = \sum_{\alpha} P^{(\alpha)}_{ij} \dot{\gamma}^{(\alpha)}, \quad \text{and} \quad W^{p}_{ij} = \sum_{\alpha} \omega^{(\alpha)}_{ij} \dot{\gamma}^{(\alpha)} \tag{2}$$

where $\alpha$ is summed over all slip-systems, and $P^{(\alpha)}_{ij}$ and $\omega^{(\alpha)}_{ij}$ 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

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

where $\dot{\gamma}^{(\alpha)}_{ref}$ is the reference shear strain-rate which corresponds to a reference shear stress $\tau^{(\alpha)}_{ref}$, 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 $\rho_{im}$ as

$$\tau^{(\alpha)}_{ref} = \left( \tau^{(\alpha)}_{y} + G \sum_{\beta=1}^{nss} b^{(\beta)} \sqrt{a_{\alpha\beta} \rho^{(\beta)}_{im}} \right) \left( \frac{T}{T_0} \right)^{-\xi}, \tag{4}$$

where $\tau^{(\alpha)}_{y}$ is the static yield stress on slip system $\alpha$, $G$ 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 $\xi$ is the thermal softening exponent, which is chosen as 0.3.