Micromechanical simulation for texture induced uncertainty in fatigue damage incubation using crystal plasticity model

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Abstract

Crystallographic texture of wrought aluminum alloys has significant influence on the fatigue damage incubation and small-crack growth in the high cycle fatigue (HCF) regime. HCF lives have demonstrated fairly large scatters due to the random textural feature and its stochastic interaction with fatigue damage evolution. The fatigue life of an individual specimen is deterministic, which manifests the specific microstructure in the specimens and its interference with fatigue. In this paper, micromechanical simulations were conducted to quantify the grain orientation and grain boundary mismatch effects to fatigue damage incubation in a wrought 7075-T651 Al alloy. Fatigue damage incubated at fractured intermetallic particles near or at the surface [Xue et al. 2007]. Many intermetallic particles fractured after a few initial loading cycles; however, only one or a few fractured particles induced a crack into the matrix. One of these microcracks eventually grew and became a dominate crack and caused the final failure. The size of the particles, the orientation of the grain in which the particle resides, the particle spatial location to the grain boundary, the mismatch of the grain boundary, and the interaction of all these factors comprise the primary reason for the fatigue damage incubation. But no systematic investigation exists to provide general guideline for fatigue design and structural prognosis applications.

In this research, a crystal plasticity constitutive model is implemented to simulate the microplasticity at the fractured intermetallic particles in single crystal and bicrystals, in which the crystallographic orientation mimics the typical rolling texture. The spatial location of the particle with respect to the grain and grain boundary is designed to represent those observed on the fractographs fatigued in the high cycle fatigue regime. The non-uniform loading distribution due to the heterogeneity of textured alloy is investigated by simulating on a representative unit cell with grain size and orientation taken from the realistic stereomicrograph of the sample. This approach is an initial high-order mechanistic multistage fatigue modeling approach, which can be implemented to estimate the uncertainty of the fatigue life prediction and fatigue life distribution using Monte Carlo simulation. Eventually, the reliability of fatigue life predictions will be accessed and the model evaluated as a mathematically rigorous tool for the structural integrity prognosis of aerospace structures that use wrought aluminum alloys.

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1. Introduction

Wrought aluminum alloys are primary materials in aerospace and automotive structures. Multistage fatigue (MSF) models that incorporate microstructural features and fatigue mechanisms have been developed for a variety of aluminum and magnesium alloys for high strength, lightweight applications since 2000. The initial MSF model was developed for the high cycle fatigue of a cast aluminum A356-T6 alloy [McDowell, et al., 2003], based on micromechanics simulations [Gall, et al., 2000 & 04; Fan, et al., 2001 & 03] and small-scale experiments of small crack growth [Shiozawa, et al., 1997]. The MSF model was further applied to a series of case Al and Mg alloys [Xue, et al., 2007c,d] based on the systematically evaluated microstructure-fatigue damage relations [Horstemeyer, et al., 2002 & 2004; Mayer, et al., 2003 & 05]. The influence of texture, in terms of grain sizes and orientations, was incorporated into the small crack growth modeling in the MSF model for the wrought 7075-T651 Al alloy [Xue, et al., 2007a,b], based on micromechanical simulations and experimental observations [Potirniche & Daniewicz; 2003, Lankford 1983; Lankford, et al., 1983 & 84; Newman 1983; Shijev, 1997 & 99] for application in the structural health prognosis of aging aircrafts. However, the texture effects on the fatigue damage incubation have not been systematically investigated.

The physics of single-crystal plasticity deformation was established since the 1920s [Taylor & Elam, 1923; Schmid 1924; Bishop & Hill, 1951]. Rigorous and rational formulations for complex crystal plasticity laws were developed in late the 60s and 70s [Hill, 1966; Rice, 1971; Asaro & Rice, 1977, to name a few key contributors]. Since then, many studies to simulate deformation in grains and polycrystalline metals were conducted following crystal kinematics described by Asaro (1983a) and the rate-dependent formulation developed by Peirce et al. (1983). The efficiency and accuracy of simulation models depends on discretization of the crystal aggregates. At least 10–30 elements per grain are required to capture the main features of localization at grain boundaries in polycrystals [Teodosiu et al., 1991; Watanabe et al., 1998; Nakamachi et al., 2000; Bhattacharyya et al., 2001].

Observations have illustrated strong heterogeneities of plastic strain at grain junction lines and at grain boundaries. Several computations account for the compatibility at grain boundaries. The local stress equilibrium demonstrated satisfactory simulation results in agreement with observations and highlight stress concentration at grain boundaries (Becker and Panchanadeeswaran, 1995; Zisman and Rybin, 1998; Bate, 1999; Harder, 1999; Schroeter and McDowell, 2003).

In this paper, we will thoroughly acquire the knowledge of grain orientation and 3-d topology and shape and location of inclusions and implement the McGinty-McDowell’s crystal plasticity model with weighted convergence criterion, McGinty 2001[18] such that deformation localization at the grain boundaries and the inclusion particles will be captured in predicting the fatigue damage evolution and the small crack growth.

Nomenclature

\( F, F_o, F_p \) deformation gradient tensor
\( L, L_o, L_p \) velocity gradient tensor
\( \overline{L} \) velocity gradient tensor in the intermediate configuration
\( B_o, \overline{B}, B \) initial, intermediate, current configuration
\( \dot{\gamma} \) shear strain rate
\( \alpha, \beta \) slip system index
\( s, m \) slip direction and slip plane normal - unit vectors
\( \overline{D} \) plastic deformation rate in the intermediate configuration
\( \nu \) Jaumann rate for stress tensor
\( \sigma \) Jaumann rate for stress tensor
2. Crystal Plasticity Constitutive Model

A single crystal region, such as a region in a grain, deforms from an initial configuration \( B_0 \), noted by coordinate space \( (X) \), to the current configuration \( B \), noted as coordinate \( (x) \), with the mapping between configurations defined by \( x = \chi(X) \). The total deformation gradient tensor is defined as \( F = \frac{\partial x_i}{\partial x_j} \). The micro-kinematic hypotheses of the classical theory are implemented to decompose the total deformation into an elastic and plastic part through an intermediate configuration, such that the deformation gradient tensor is decomposed into

\[
F = F^e F^p
\]

(1)

where \( F_p \) represents the disarrangement of atoms due to slip, while \( F_e \) represents stretching and rotation of the atomic lattice, as shown in Fig. 1.

Fig. 1. The decomposition of deformation gradient tension

In an incremental process, the velocity gradient in the current configuration is defined as \( L_{ij} = \frac{\partial v_i}{\partial x_j} \) and written as the sum of the elastic and plastic parts:

\[
L = F F^{-1} = L^e + L^p
\]

(2)

where the individual velocity gradient tensor is defined as

\[
L^e = F^e F^{e^{-1}}, \quad L^p = F^p F^{p^{-1}}, \quad \overline{L} = F^F F^{F^{-1}}
\]

(3)
where the velocity gradient tensor in the intermediate configuration is direct related to the shear along the slip system as

$$ \overline{\mathbf{L}} = \sum_\alpha \gamma^\alpha \left( \mathbf{s}^\alpha \otimes \mathbf{m}^\alpha \right) $$

(4)

Here, \( \gamma^\alpha \) is the slip rate at the \( \alpha \) slip system (\( \alpha = 1, 2, \ldots, n \)), while \( \mathbf{s}^\alpha \) and \( \mathbf{m}^\alpha \) are orthogonal unit vectors that represent the corresponding slip direction and slip-plane normal. The rate of plastic deformation tensor in the intermediate configuration can be written as

$$ \overline{\mathbf{D}}' = \sum_\alpha \gamma^\alpha \left( \mathbf{s}^\alpha \otimes \mathbf{m}^\alpha \right)_{\text{sym}} $$

(5)

The stress–strain response involves the Jaumann rate of the Piola-Kirchoff stress related to the elastic deformation rate by means of the elastic stiffness tensor \( \mathbf{C} \), i.e.,

$$ \dot{\mathbf{v}} = \mathbf{C} : (\mathbf{D} - \mathbf{D}') $$

(6)

For an FCC single crystal, the elastic stiffness matrix represented in the crystal’s local coordinate system requires three elastic constants, namely, \( C_{11}, C_{12}, \) and \( C_{44} \). The resolved shear stress on slip system \( \alpha \) is found directly from the Cauchy stress tensor by

$$ \tau^\alpha = \mathbf{\sigma} : (\mathbf{s}^\alpha \otimes \mathbf{m}^\alpha) $$

(7)

The general plastic flow rule was adopted in various forms for crystal plasticity [Asaro, 1983]. The following rate-dependent flow rule was employed to calculate the plastic slip increments:

$$ \dot{\gamma}^\alpha = \dot{\gamma}_0 \left[ \frac{\tau^\alpha - \chi^\alpha}{g^\alpha} \right] \frac{1}{m} \text{sgn} \left( \tau^\alpha - \chi^\alpha \right) $$

(8)

where 1/m is the strain rate sensitivity and \( g^\alpha \) and \( X^\alpha \) represent the isotropic and kinematic hardening for the slip system \( \alpha \), respectively, defined below as functions of the accumulated plastic strains on each slip system,

$$ \dot{\mathbf{g}}^\alpha = H \sum_\beta q^{\alpha\beta} \left| \dot{\gamma}^\beta \right| - R g^\alpha \sum_\beta \left| \dot{\gamma}^\beta \right|, \quad \dot{\chi}^\alpha = h\dot{\gamma}^\alpha - r\dot{\chi}^\alpha \left| \dot{\gamma}^\alpha \right| $$

(9)

where \( H, R, h \) and \( r \) are material properties defining static hardening and dynamic recovery behaviors. Self hardening modifier \( q^{\alpha\beta} \) is set as to 1 for \( \alpha = \beta \), and Ladent hardening modifier \( q^{\alpha\beta} = 1.4 \) for \( \alpha \neq \beta \). Crystallographic texture is then further updated to the current configuration:

$$ \mathbf{s} = \mathbf{F} \cdot \mathbf{s}, \quad \mathbf{m}^\alpha = \mathbf{m}_s \cdot \mathbf{F}^{-1} $$

(10)

For details regarding the computational procedure see McGinty [2002].
3. Microstructural Simulation Results and Discussion

The texture of the 7075-T651 is first modeled using an optical image, as shown in Figure 2a, that gives the grain arrangement, together with intermetallic particles in a two-dimensional review. An image recognition program, written using Matlab, was implemented to identify the grain boundary and take off all the intermetallic particles. An in-house grain boundary treatment code, written using Python associated with ABAQUS, was implemented to smooth and regulate the grain boundaries, with the final geometry shown in Figure 2b. In this initial simulation, the grain orientation is randomly assigned to each grain by selecting between crystallographic orientations from typical rolling texture. The geometry was meshed with a fairly fine element, as shown in Figure 2c.

Fig. 2. (a) Microsection of rolled 7075-T651, (b) microstructural ABAQUS model with local orientation, (c) meshed geometry

The geometry is regarded as a representative volume element (RVE), which is embedded into an isotropic elastic media with the elastic properties identical to the 7075-T651 Al alloy, as shown in Figure 3a. Such a simple displacement boundary condition can be applied. The plastic strain contour is shown in Figure 3b. Localized high strain field in some grain becomes obvious. Even some limited localized plastic slip can be identified. Without considering the effects of the intermetallic particles, the localized plastic deformation concentration should be associated with the fatigue initiation location.
4. Summary

A Crystal plasticity model was developed and encoded in the form of a user-defined material subroutine in ABAQUS. The texture representative volume element was developed based on a two-dimensional optical image. An initial micromechanical simulation was conducted, and the localized plastic deformation was obtained. True texture, with grain orientation measured using EBSD, will be used in future simulation endeavors.

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