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A crystal plasticity-based study of the relationship between microstructure and ultra-high-cycle fatigue life in nickel titanium alloys

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ABSTRACT

Nickel Titanium (NiTi) alloys are often used in biomedical devices where failure due to mechanical fatigue is common. For other alloy systems, computational models have proven an effective means of determining the relationship between microstructural features and fatigue life. This work will extend the subset of those models which were based on crystal plasticity to examine the relationship between microstructure and fatigue life in NiTi alloys. It will explore the interaction between a spherical inclusion and the material's free surface along with several NiTi microstructures reconstructed from 3D imaging. This work will determine the distance at which the free surface interacts with an inclusion and the effect of applied strain of surface-inclusion interaction. The effects of inclusion–inclusion interaction, matrix voiding, and matrix strengthening are explored and ranked with regards to their influence on fatigue life.

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1. Introduction

Nickel Titanium (NiTi) alloys are often used in biomedical devices such as stents [1,2] and artificial heart valves [3]. Failure of such devices due to mechanical fatigue has caused negative clinical outcomes [4] and has potential to increase healthcare cost and patient trauma if device replacement is needed. More fatigue resistant NiTi alloys will help to mitigate these issues.

Quantitative understanding of NiTi microstructures' effect on fatigue performance will allow for the design of improved alloys at a more rapid pace than with *trial-and-error* development approaches.

A computational model offers the ability to assess the sensitivity of fatigue life to microstructural parameters in a controlled manner. This work will perform such a study. It will explore the potency of generic microstructures to nucleate fatigue cracks in a NiTi system, and it will address microstructures specific to drawn NiTi tubes which are used in many biomedical applications [1].

Specifically this work will focus on determining a plastic strain-based damage parameter around non-metallic inclusions in a NiTi alloy using computational crystal plasticity (CP). Unlike phenomenological plasticity models that capture observed trends in material behavior based on macroscale experimental data, CP predicts anisotropic plastic deformation based on slip mechanisms in crystal systems.

A number of studies have used CP modeling to explore fatigue nucleation around inclusions. Parametric studies of microstructural parameters were performed by Shenoy et al. [5] using CP. They used a 2D finite element model to study the effects of inclusion aspect ratio, spacing, and distance to free surface on crack incubation life for nickel superalloys. Kumar et al. [6] studied Ni_3-Al precipitates in single crystal nickel superalloys. They used CP to model strain distributions around large arrays of square precipitates and showed the effect of precipitate volume fraction on fatigue driving force. Wang et al. [7] studied fatigue crack incubation for interacting inclusions in separate grains of an aluminum 7075 alloy. Their analysis used CP to study 3D geometries extruded from circular and elliptical inclusion geometries. Alley and Neu [8] used a combined austenite to martensite phase transformation and CP model to study 3D cuboid and cubic inclusions in a 41100 steel, showing the effect of retained austenite on a plastic strain-based damage parameter. Hochhalter et al. [9] used CP to study a number

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of non-local nucleation metrics around ellipsoidal inclusions in 7075-T651 aluminum; they also applied these metrics to cracked Al_7Cu_2Fe particles which were reconstructed from 2D images. Prasannavenkatesan et al. [10] used a 3D CP model to study the effects of hard Al_2O_3, soft La_2O_2S and pores on fatigue life in martensitic gear steels. Salajegheh et al. [11] determined the probability of failure in the nickel superalloy IN100, using a 2D crystal plasticity model of 2 μm inclusions. While all of these works studied fatigue crack nucleation around inclusions using CP, none focused specifically on NiTi.

Other crystal plasticity models, such as those of Wang et al. [12], Manchiraju and Anderson [13], Manchiraju et al. [14], Yu et al. [15–18], and Paranjape and Anderson [19] have focused specifically on NiTi but did not study fatigue or inclusions[1].

Two final studies of note are that of Przybyla et al. [20] and Salajegheh et al. [21]. Przybyla et al. [20] used a 2D model to determine a strain-based damage parameter as a function of surface distance to a hard inclusion in the presence of an oxide layer, which this work will parallel albeit in 3D and without considering surface oxidation. Salajegheh et al. [21] studied the behavior of a strain-based damage parameter with respect to interaction and orientation between inclusions in 2D and orientation between inclusions in 3D; the present work will address similar inclusion interactions based on a NiTi specific microstructure. However, both Przybyla et al. and Salajegheh et al. used an isotopic phenomenological plasticity model rather than CP.

This work will, for the first time, use the microstructure-sensitive fatigue models developed for steels, aluminums, and nickel superalloys combined with CP models of NiTi to address the effects of non-metallic inclusions on NiTi fatigue life.

This work will address the effect of inclusion-surface interactions, inclusion–inclusions interactions, inclusion morphology and an inclusion/matrix interface void on fatigue life. The results of these studies will then be summarized in the contexts of materials design and fatigue resistance improvements for NiTi materials.

2. Fatigue prediction method

Cracks that will ultimately cause fatigue failure can form at a variety of microstructural features such as grain boundaries, surface defects and inclusions [22]. When samples fail at 10^8–10^{10} cycles [23], the failure process is often termed Ultra-High-Cycle Fatigue (UHCF). This scenario is of particular interest for biomedical applications which are frequently in continuous service for up to 20 years[2]. Studies of SUJ2 steel [25–30] have shown that subsurface fatigue nucleation at inclusions becomes the dominant mode of nucleation when samples fail in (or near) the UHCF regime. Also, fatigue crack nucleation at inclusions is a common concern in biomedical materials [31]. For this reason, this work will focus only on inclusions.

The fatigue life of a material can be decomposed into several stages [32]:

$$N = N_{\mathrm{inc}} + N_{\mathrm{MSC}} + N_{\mathrm{PSC}} + N_{\mathrm{LC}}, \tag{1}$$

where N is the total fatigue life, N_{inc} is the number of crack incubation cycles, N_{MSC} is the number of cycles of microstructurally small crack growth, N_{PSC} is the number of cycles of physically small crack growth, and N_{LC} is the number of cycles of long crack growth. Incubation refers to the number of cycles for crack nucleation and growth beyond the influence of the feature or defect where nucleation occurred. Microstructurally small and physically small crack growth are often lumped together into one stage of crack growth beyond microcrack influence but where linear elastic fracture mechanics is invalid [32].

This work will focus on characterizing the potency of NiTi microscale features to incubate fatigue cracks. Based on these results, the fatigue incubation life will be predicted. Lankford and Kusenberger observed that the variation in fatigue life of 4340 steels was dominated by crack initiation; furthermore, McDowell [22] observed that the fatigue life beyond the initial crack site is often an "inconsequential" fraction of fatigue life. Thus, the comparisons of N_{inc} for various microstructures will be considered valid for total fatigue life as well.

This work will link fatigue incubation life to microscale simulation outputs through Goh and McDowell's [33] extension of Fatime and Socie's [34] "Fatigue Indicator Parameter" (*FIP*) given by:

$$\frac{\Delta\gamma^{p}_{\max}}{2}\left(1+\kappa\frac{\sigma_n^{\max}}{\sigma_y}\right) = \tilde{\gamma}_f(2N_{\mathrm{inc}})^{c} = FIP, \tag{2}$$

where $\Delta\gamma^{p}_{\max}$ is the change in maximum cyclic plastic shear strain averaged over a finite volume, and $\sigma_n^{\max}$ is the stress normal to the critical plane of $\gamma^{p}_{\max}$. The parameters c and $\tilde{\gamma}_f$ are Coffin-Manson type calibration parameters and κ is a constant determined to equate *FIP* for uniaxial and torsional loaded specimens [34].

The values of $\Delta\gamma^{p}_{\max}$ and $\sigma_n^{\max}$ are determined from crystal plasticity-based finite element simulations of NiTi microstructures, from which *FIP* is calculated and averaged over a region 10% of the volume of an inclusion in accordance with the procedure in [35]. This volume averaging reduces mesh dependency and introduces a length scale into fatigue life calculations. The "fatigue indicator parameter" gages the potency of microstructural features to incubate fatigue cracks. Calibrating *FIP* values for a given microstructure to fatigue life data using c and $\tilde{\gamma}_f$ establishes a *baseline* microstructure to which other microstructures can be compared. This work will use a microstructure based on 3D imaging as such a *baseline*.

For this study, volume averaging was performed over a cubic region. The edge length of this region has ranged from 1–3 μm in previous simulations of inclusions [5,11,10], but Shenoy et al. suggests that 0.3–1 μm should be a lower bound. This work uses an edge length of 0.23 μm, which is consistent with the procedure in [35], but just below Shenoy et al.'s suggested range. However, the 0.23 μm window amounts to a cubic volume region with faces consisting of 5×5 element. Fig. 9 shows that this is roughly the area of the interface between carbide and void, and thus, is good estimate of the length scale on which damage has been observed.

3. Computational micromechanics

Computational crystal plasticity will act as the constitutive modeling framework for this study. Several versions of computational crystal plasticity exist. Each version differs slightly in its continuum mechanics, hardening laws, calibration methods and algorithmic details. This work will use the CP version of McGinty and McDowell [36,37]. This version employs an *implicit* time integration algorithm for both the material law and finite element method (FEM) kinematic variable updates. The details of this CP version are given in [36] but the basic assumptions of the approach will be discussed below.

The plastic deformation gradient $\boldsymbol{F}$, is multiplicatively decomposed into an elastic $\boldsymbol{F}^{e}$ and plastic $\boldsymbol{F}^{p}$ part as:

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[1] A number of studies (see [18] for a review) model phase transformation in NiTi based on similar concepts to crystal plasticity, these are often called *crystal plasticity* models but do not consider plastic deformation specifically.

[2] The normal resting heart rate for an adult is 60–100 beats per minute [24]. A heart beating at 100 beats per minute for 20 years results in $1,051,898,000$ heart beats ($\approx$ 1 billion). This represents the approximate service life of an artificial heart valve.