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CONTINUUM-ATOMISTIC MODELING FOR CRACK INITIATION AND PROPAGATION IN POLYCRYSTALS

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ABSTRACT

Current research efforts are developing simulation methods at the mesoscopic scale to study fatigue crack initiation and propagation in polycrystals. Geometric models of the microstructure are created using Voronoi tessellations. The grain material is modeled by statistically assigning lattice orientation and elastic or elastic-plastic material properties to each grain in a model. Grain boundaries then naturally arise in the model.

The focus is on the involvement of the grain boundaries in the fracture process and ways of characterizing their resistance to fracture based on atomic scale studies. The goal is to extract grain boundary properties (when possible as a function of their macroscopic parameters) out of atomistic simulations, then summarize and transfer this information across length scales. To model the behavior of the grain boundaries at the mesoscopic scale we consider a coupled, cohesive zone model, where the microscopic information is summarized in the form of traction-displacement relationships.

Finite element analyses are then conducted under monotonic and cyclic loading. Observations are made about where and when cracks initiate, their subsequent trajectory, and the sensitivity of the simulation to the grain and grain boundary constitutive models and their distributions in the polycrystal.

KEYWORDS

Fatigue Crack Initiation, Polycrystal, Multi-scale, simulation, cohesive model

INTRODUCTION

Assuming homogeneity at the macroscopic scale in a metallic component leaves out the details from smaller length-scales that precipitate fatigue crack initiation, a major concern in many applications. For these concerns the details at the polycrystal scale are the features that determine when and where fatigue cracks will initiate and which ones will grow to macro-cracks. As the macroscopic response results from the polycrystal-scale features, properties of polycrystal features such as grain boundaries are in turn dependant on the atomic-scale.

The work presented here investigates statistically modeling the polycrystal geometry and properties in order to study influences on the initiation of fatigue cracks. Outlined in the following section are how the polycrystal geometry is modeled and how the individual grains are constitutively modeled. Then, the coupled, cohesive zone constitutive model used for the grain boundaries is discussed. Finally, an example of a fatigue crack initiation simulation using FRANC2D/L is shown and the results and observations are discussed.

POLYCRYSTAL MODELING

Creating a polycrystal sample begins with defining the geometry of the grains. This is done using a Voronoi tessellation. Polygons are created from a random set of initiation points. Each polygon then represents a grain with an average size held to observed measures from electron back-scattering pattern scans (EBSP). Once the geometry is in place material properties are assigned. Four constitutive relationships for the grain material are currently being evaluated for their impact on the crack initiation process: elastic, isotropic; elastic, orthotropic; elastic-plastic, isotropic (von Mises); elastic-plastic, orthotropic (Hill). For the chosen material model each grain is assigned values of the appropriate parameters sampled from uniform distributions centered on the average macroscopic value. This allows each grain to be a separate realization of the material model.

COUPLED COHESIVE ZONE MODEL

The geometry created by the tessellation determines the locations of the grain boundaries while the material parameters introduce heterogeneity and possible anisotropy. Finally, a cohesive zone model (CZM) is used to describe the strength of the grain boundaries. The CZM is also used as a criterion for initiation of intergranular cracks. The GB's are allowed to decohere after reaching a critical combination of transmitted normal and shear stress, thus gradually initiating a crack. An advantage of using such a model is that initial cracks are not arbitrarily introduced at the beginning of a simulation. Instead cracks naturally occur due to the heterogeneous stress field throughout the sample caused by the geometry and property variations.

CZM's are traction-displacement relationships originally used to describe the damage that occurs in the plastic zone ahead of the crack [1]. In the present case the damage represented by the softening portion of the CZM is used to describe the decohesion of the GB's. The implementation being used in our simulation code, FRANC2D/L [2], is adapted from the coupled, cohesive zone model (CCZM) developed by Tvergaard and Hutchinson [3] where the normal and shear components of the traction and displacement are combined into single measures for each quantity, t and λ, respectively (Figure 1). A key characteristic of the relationship is the area under the curve, G_c, which represents the critical energy release rate.

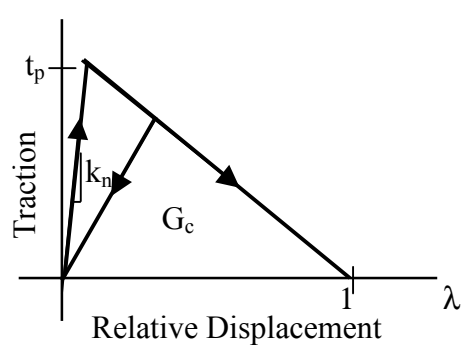


Figure 1: Coupled Cohesive Zone Model

The CCZM begins from a traction potential, Φ, (Eqn. 1) that is a function of the relative normal, δ_n, and tangential, δ_t, displacements between the faces of the GB. λ is a non-dimensional separation measure for the relative opening and sliding normalized to the relative critical displacement values, δ_n^c and δ_t^c, at which the separation is considered a true crack in pure Mode I and pure Mode II (Eqn. 2). When the value of λ reaches 1 this indicates the complete decohesion of the GB and the formation of a true crack. For a given relative displacement between two grains the combined traction, t, transmitted across the GB can be determined from the CCZM. The combined traction can then be decomposed into normal, T_n, and shear, T_t, components by differentiating Φ according to Eqns. 3 and 4, respectively. In the case in which the GB encounters unloading, the CCZM follows the path shown in Figure 1.

$$\Phi(\delta_n \delta_t) = \delta_n^c \int_\lambda t(\lambda')d\lambda' \tag{1}$$

$$\lambda = \left[\left(\frac{\delta_n}{\delta_n^c}\right)^2 + \left(\frac{\delta_t}{\delta_t^c}\right)^2\right]^{1/2} \tag{2}$$

$$T_n = \frac{\partial \Phi}{\partial \delta_n} = \frac{t(\lambda)}{\lambda}\frac{\delta_n}{\delta_n^c} \tag{3}$$

$$T_t = \frac{\partial \Phi}{\partial \delta_t} = \frac{t(\lambda)}{\lambda}\frac{\delta_n^c}{\delta_t^c}\frac{\delta_t}{\delta_t^c} \tag{4}$$

In our simulations the parameters describing the CCZM where determined to either be the same for all GB's in the sample, or to vary from GB to GB. For the orthotropic models, parameters were varied based on the misorientation angle, θ, across the GB shown in Eqn. 7 and Figure 2. For the isotropic grain material models, there is no physical misorientation across GB's. Therefore, the inclination angle, ψ, of the grain boundary with respect to the global X-axis (Figure 3) was chosen as an arbitrary measure with which to introduce variation in G_c. Assuming that G_c varies with the angle θ or ψ changes, the area under the CCZM varied according to Eqn. 5 or Eqn. 6, respectively, in which G_{avg} is the average value of the critical energy release rate and ΔG determines the range of values. The critical normal displacement, δ_n^c, is then held constant at 1μm so that the critical combined traction, t_p, for each GB could be determined.

$$G(\theta) = G_{avg} + \Delta G \cos(4\theta) \tag{5}$$

$$G(\psi) = G_{avg} + \Delta G \cos(4\psi) \tag{6}$$

$$\theta = \beta_1 - \beta_2 \tag{7}$$

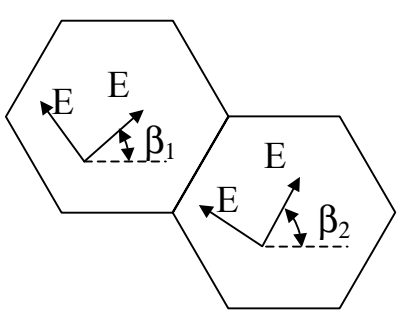


Figure 2: Misorientation angle, θ, calculated according to Eqn. 7 from the material orientation angles, β_i, of neighboring grains.

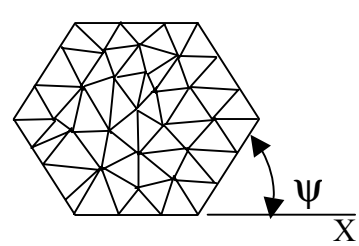


Figure 3: Grain boundary inclination angle measured with respect to the global X-axis.

The form of Eqns. 5 and 6 was chosen based on a Fourier expansion of spherical harmonics. In 3D any periodic function can be written using a Fourier expansion of spherical harmonics of which the present case is a 2D degenerative form. Holding the normal of each grain to be along the (100) direction forces cubic symmetry for a FCC crystal. This results in the cos 4θ(or ψ) form term seen in Eqns. 5 and 6.

In conjunction with this work are efforts to conduct atomistic and quasi-continuum simulations of the fracture of GB's and triple point junctions of grains. These results will be used to guide the determination of parameters of the CCZM as well as give insight into the shape of the CCZM curve and the form of variation as a function of misorientation between grains.

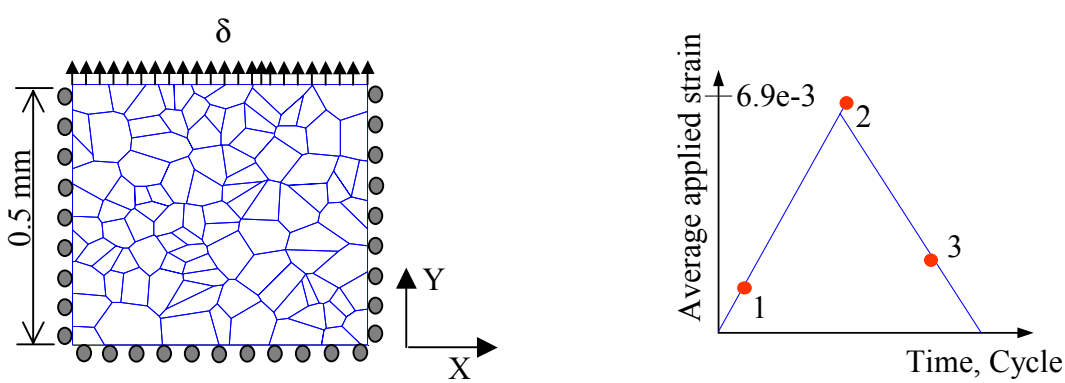
SIMULATION OF FATIGUE CRACK INITIATION

Simulations were run as part of a parametric study to observe the sensitivity of fatigue crack initiation due to the various parameters. Varied parameters included different realizations of grain geometry from the Voronoi tessellations, the four grain material models mentioned previously, different samplings from an orientation distribution function (ODF) for orientations of the orthotropic grains, variation in the range and mean values of the CCZM parameter ΔG, varying load conditions including monotonic and cyclic, and the presence of an initial stress field.

RESULTS

Results discussed here are for the grain geometry, boundary conditions and loading history shown in Figure 4. Individual results will be shown for the points indicated in Figure 4b. The grain material properties for the Hill material model and CCZM parameters are shown in Table 1. The parameters chosen result in the average peak combined strength of the GB's being equal to the average uniaxial yield stress of the grains. This will allow some of the GB's to reach their peak and begin softening, initiating fatigue cracks, before the grains begin to yield and absorb all of the damage to the polycrystal. The current implementation of the Hill yield criterion is limited to perfect plasticity.

As seen in Figure 4, the sample was loaded to 0.69% strain (98% of the macroscopic yield strain) and then unloaded. Figures 5a-c show the deformed mesh of the sample at 0.1%, 0.69%, and 0.2% strain corresponding to the points marked in the loading history (Figure 4b). The circled area in Figure 5b shows the opening of a grain boundary due to decohesion. Figures 5d-f show schematically the approximate corresponding location along the CCZM of the decohering GB's. Since λ has not reached a value of 1 this damaged GB has not yet completely fractured.



(a) (b)

Figure 4: (a) Boundary conditions and loading of polycrystal sample. (b) Loading history.

TABLE 1

GRAIN MATERIAL AND CCZM PARAMETERS

Grain Material		CCZM	
Type	**Elastic-Plastic, Orthotropic (Hill)**	**G_{avg}**	**250 Pa m**
E	**72 GPa**	**ΔG**	**100 Pa m**
σ_{yld1}	**505 MPa**	**Resulting t_{pavg}**	**500 MPa**
σ_{yld2}	**450 MPa**		
σ_{yld12}	**400 MPa**		

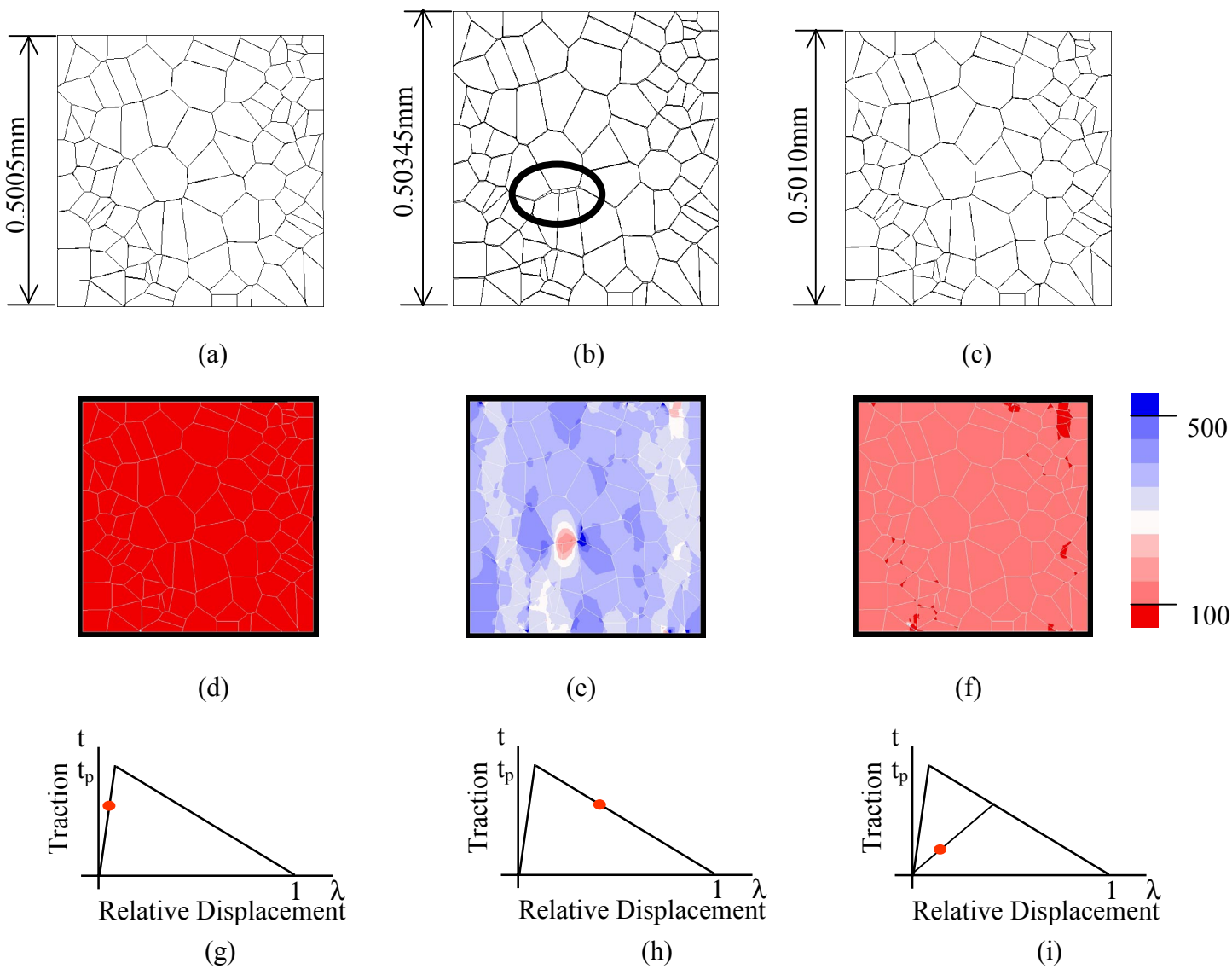


Figure 5: Deformed mesh at 2X magnification for (a) point 1 indicated in Figure 4. (b) point 2 in Figure 4. The circled grain boundaries have begun to decohere. (c) point 3 in Figure 4. (d) σ_{yy} contour plot corresponding to (a). (e) σ_{yy} contour plot corresponding to (b). (f) σ_{yy} contour plot corresponding to (c). (g) Schematic representation of the location on the CCZM of the opening GB at the first load point. (h) Schematic representation of the location on the CCZM of the opening GB at the first load point. (i) Schematic representation of the location on the CCZM of the opening GB at the first load point.

OBSERVATIONS AND CONCLUSIONS

Using a Voronoi tessellation, samples of polycrystalline geometry were created. The grains where statistically assigned material parameters from one of four material models. The GB's where assigned a statistically varying CCZM. Completed polycrystal samples were loaded monotonically and cyclically to observe damage and crack initiation.

In an example shown herein, damage occurs to the sample in the form of GB decohesion before any grains reach yield from macroscopic loading. Local yielding then follows due to stress re-distribution caused by the decohesion process. The use of the CCZM to describe the GB's allows for this type of damage to occur.

Other simulations to be reported include monotonically loaded samples strained to 3% or to failure due to the propagation of a through-crack. In samples using elastic material models damage began once the t_p was reached and progressed to failure as true cracks were created and propagated through the sample. Samples using elastic-plastic material models saw damage in the form of GB decohesion and plastic yielding of the grains. From these simulations the influence of t_p relative to the yield stress of the grains was observed. For the samples using the elastic-plastic, isotropic (von Mises) material model, which allowed for hardening within the grains, a shift from GB damage to grain hardening was observed as t_p was raised to from 0.8 to 1.5 times the average yield stress.

The current ongoing parametric study will yield additional sensitivities to modeling choices and parameter ranges. The collected observation will serve to reduce the parameter space when the current capabilities are transferred to a 3-D framework. Also, the accuracy of parameters for the CCZM, such as t_p or δ^c, needed will be determined though the observed sensitivity. This will guide future atomistic simulations of GB's.

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