

MULTISCALE MODELING OF DAMAGE PROCESSES IN ALUMINUM ALLOYS: GRAIN-SCALE MECHANISMS

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I. Introduction

Traditionally, prognosis of structural behavior has been based on empirical models that homogenize all damage mechanisms occurring within a structural component and recast them in the form of fracture or damage parameters (e.g., G, K, CTOA). The uncertainties that result from the homogenization contribute to the need for high and costly safety factors and material “allowables” and lead to decreased inspection intervals. To facilitate the design of safer, more efficient and reliable structures, a computational modeling framework is needed to represent distinct damage mechanisms, and incorporate knowledge about the stochastic material system and loading. This framework couples damage evolution to structural degradation. Certain components of this framework must be adaptable since, for example, it is vital to continually incorporate the best available physics-based models as knowledge is gained about governing mechanisms. Such a framework can only be developed through the continued expansion of four subjects: physics-based modeling, computational methods, materials science, and test technology.

Inherent to any structural material are distinct physical scales, each characterized by a set of governing mechanisms. Physics-based models that represent these mechanisms need to be continuously improved so that structural simulations are consistently carried out at the highest level of fidelity available. Continued improvements to computational simulation methods that link the various scales are needed so that these physics-based models can be incorporated within a multiscale framework ever more accurately. Test technology and materials science underpins the physics-based modeling.

Useful prognosis of structural behavior is probabilistic due to the inherent variability in materials, loading, manufacturing, environment, etc. In a statistical sense, lower uncertainty in prognoses implies that this inherent variability is understood and incorporated within the analysis. It is the contention of the authors that the incorporation of microstructural detail within the analyses will yield tangible and beneficial improvements to existing prognosis methods. Additionally, the most accurate way to include microstructural variability is to explicitly model a statistically representative geometry of the material. Since it is computationally intractable to represent an entire component with microstructural resolution, multiscale modeling is required.

Traditionally, two main classes of approaches have been developed for multiscale modeling, either continuum or discrete: superposition methods and homogenization methods. Superposition methods decompose the solution space into global and local effects, and then superpose the two results. Solution compatibility must be enforced by prescribing homogeneous boundary conditions for the local solution at the global-local interface. In this procedure, local finite element solutions are superposed with global direct variational solutions, such as the Ritz method, to achieve a more efficient or accurate solution. The homogenization method is a

multiscale expansion method that relies on three assumptions: the continuum structure is formed by a spatial periodicity of the representative volume element (RVE); the solution is locally periodic in the statistical sense, and; macroscopic fields are constant within the RVE. Since the method is based on a spatial periodicity assumption, the calculated material properties are inherently non-local, meaning they are the same everywhere in the global structure. However, the explicit modeling of fatigue cracking, which is considered here, is an inherently localized phenomenon and new multiscale procedures are required as described in Section 2. By including atomistic simulation within a multiscale procedure, the goal is to be able to simulate fatigue crack growth where the only limitation is in our ability to provide the model with physically accurate input.

Specific to aging aircraft, over the past 8 years a multidisciplinary team has been developing a computational framework for the multiscale simulation of damage evolution from incubation at the microscale to component-scale failure by explicitly modeling crack growth at its various stages [2, 3, 11, 12]. Development of the framework was made possible by advances in the statistical modeling of polycrystalline metal microstructures, meshing, multiscale analysis, modeling of constitutive behavior of face-centered cubic (FCC) crystals and interfaces (using cohesive zone models), and test technology for observation, measurement and validation procedures. This team has produced a multiscale framework in which improved physics-based models can be hypothesized, implemented, analyzed and validated. An overview of the existing framework is given in Section 2.

Currently, improvements to existing physics-based models for intra-, inter- and transgranular fracture modes are needed for crack growth simulations in the microstructure. Past research regarding the incorporation of cohesive zone models (CZMs) to simulate these forms of crack growth has focused, to a large extent, on numerical methods for solving the resulting nonlinear systems. This inevitably leads to a choice of CZM parameters that are numerically advantageous rather than being physically meaningful, since the mechanisms that control those parameters are not well-known and have not been quantified. On the other hand, experimental techniques have been established to approximate physically-meaningful parameters for CZMs [8, 15] and usually require an assumed CZM shape and a range of test component configurations. Little focus, however, has been applied to a quantification of how the resulting CZM parameters relate to the process zone mechanisms that are being homogenized, e.g. how does the CZM depend on misorientation angle for transgranular crack growth?

Considering lower length scales, atomistic simulations have shown the capability to predict a CZM based on first principle computation. However, some inherent problems with the use of atomistic simulation to predict a CZM include the high level of idealization of the atomic structure that is required, and the restrictions on length and time scales that can be simulated. The length scales and time scales are typically limited to nanometers and picoseconds, respectively, neither of which are appropriate for real structural components [30]. Therefore, the ability to relate a CZM as predicted by atomistic simulation to a CZM observed through physical experimentation would provide a much needed understanding for modeling of the process zone; basically, such a capability would provide an insight into how molecular dynamics simulation ‘scales.’ Development of this CZM would significantly improve the existing capability to model the early stages of crack growth.

In this paper, a methodology for development of a physically-grounded analysis for modeling the initial stages of crack growth in an aluminum alloy is described. Sections 2 and 3 of the paper are dedicated to the overview and validation of an existing multiscale framework as it pertains to the fatigue of aluminum alloys. Section 4 proposes a method for the aggregation of nanoscale mechanics through the union of experimentation of single- and bi-crystals and structural scale finite element simulation for the improvement of CZMs. Discussed also in Section 4 are the expected advances to be made through the incorporation of nanoscale mechanics into microscale simulation, as well as the limitations to be overcome.

II. Background – A Multiscale, Computational Framework

An existing multiscale modeling framework, the Damage and Durability SIMulator (DDSIM), is the foundation for this effort. DDSIM contains three levels, each of which has a unique level of fidelity and computational demand [11, 12]. For simplicity, let's assume that a finite element analysis has been completed for an entire aircraft structure and that the design engineer is specifically interested in a single structural component, say a wing panel containing large stress concentrations near the bolt-holes. To initiate a multiscale analysis of the wing panel, the engineer provides DDSIM level 1 with the completed finite element analysis (mesh description and nodal stress values) of the model of the critical component, in this case the wing panel. Next, DDSIM level 1 uses a unique method to locate the critical points in the structural component by determining which of the points, if they were to be sites of crack initiation, would result in the shortest fatigue crack propagation life for the component. A low-fidelity, conservative, estimate of fatigue crack propagation life is produced as a result of this initial screening of the structural component. After completion of DDSIM level 1, the engineer can either use this initial estimate of fatigue life, or continue on to DDSIM level 2 which will provide a higher-fidelity estimate of fatigue crack propagation life.

Cracks that are microstructurally large – large with respect to the microstructural features – can be simulated using classical fracture mechanics, such as that used in DDSIM level 2, to provide a reasonable prediction of crack growth trajectory and residual strength [5, 6, 7, 23]. DDSIM level 2 employs FRANC3D (Fracture Analysis Code 3D) for explicit simulation of crack growth within the wing panel using the finite element method and continuum fracture mechanics parameters. At this point, the engineer introduces a crack into the wing panel using FRANC3D, the size of which should be chosen to be larger than characteristic microstructural features of the wing panel material. Finite element analysis is then iteratively used at each crack growth step until component failure is reached.

However, it is commonly observed in fatigue experiments that a given structural component can spend upwards of 90% of its fatigue life reaching that microstructurally large size [26]; read by the inquisitive scientist: “~90% of the knowledge is yet to be gained.” Consequently, the engineer can once again opt to continue the multiscale analysis to yet a higher level of resolution. At the micro-scale, DDSIM level 3 explicitly incorporates microstructural models into the multiscale analysis of the wing panel, where the component- and micro-scale are combined computationally, Figure 1 [11, 12]. DDSIM level 3 is discussed in-depth in the remainder of this section.

At DDSIM level 3, a computational, multiscale modeling technique is used to combine component-scale models and microscale models to represent stress and displacement fields local

to cracks. This approach is designed to couple the component-scale and microscale models so they behave coherently as shown in schematic form in Figure 1. The steps in the approach are: mesh and analyze the component model, determine appropriate boundary conditions for the microstructural model by extracting solution fields from the component model, mesh and analyze the microstructural model using the determined boundary conditions and update the stiffness of the component model to locally represent damage in the microstructure. This approach is repeated until the boundary conditions placed on the microstructure model converge on consecutive iterations.

There are two goals for the multiscale approach: determine physically correct boundary conditions for the microstructural model, and determine an accurate representation of updated stiffness for the component model resulting from damage in the microstructural model. Once the component model's stiffness is updated after the first iteration of Figure 1, the local stress and displacement fields in the component model will redistribute, causing a change in the boundary conditions placed on the microstructural model. Using this method, the region subjected to microstructural modeling in the component model will have the same deformation characteristics as the microstructural model itself. Therefore, this method provides boundary conditions for the microstructural model that accurately represent those physically experienced by the microstructure [2, 3].

To explicitly simulate crack growth at a microstructurally small size, geometric details and material models relevant to that scale need to be considered. Statistically representing grain geometry of aluminum alloy (AA) microstructures is at the forefront of multiscale crack growth simulation, mainly because of its importance to aging aircraft [9,27]. Statistically accurate microstructures are produced by creating voxellated grain structures with the correct distribution of grain sizes and using a multiple-material, marching cubes algorithm to obtain the correct grain morphology via surface smoothing [18, 25, 31]. Once a statistically accurate microstructure has been developed, the finite element method is employed, which necessitates the discretization of the microstructural model. Lagrangian, tetrahedral meshes of the model are created by a fully automated routine [27, 4]. The resulting meshes explicitly represent grain boundaries and are sufficiently refined near small geometrical features to capture local stress gradients.

With the capability to statistically represent, mesh and analyze a microstructure and subsequently couple it with a component-scale model, governing mechanisms at the microstructure must be understood and implemented into the framework to complete the loop of Figure 1. Because of its ubiquitous use in legacy aircraft AA 7075-T651 is considered as a focus problem in much of the development of DDSIM. Three distinct stages of microstructurally small fatigue crack (MSFC) growth have been observed for an AA 7075-T651 microstructure: incubation, nucleation and microstructurally small propagation. For this alloy, the cracking of iron-bearing particles serves as the incubation process. Observations of the microstructure have revealed that only a small percentage of these particles crack and those that crack do so during the first high load cycle. Given this observation, it is attractive to include only the subset of particles that are likely to incubate a crack in a microstructural model, since this will reduce computation time and model complexity while still including the crucial model characteristics. Only the incubation stage of MSFC is discussed in the remainder of this paper.

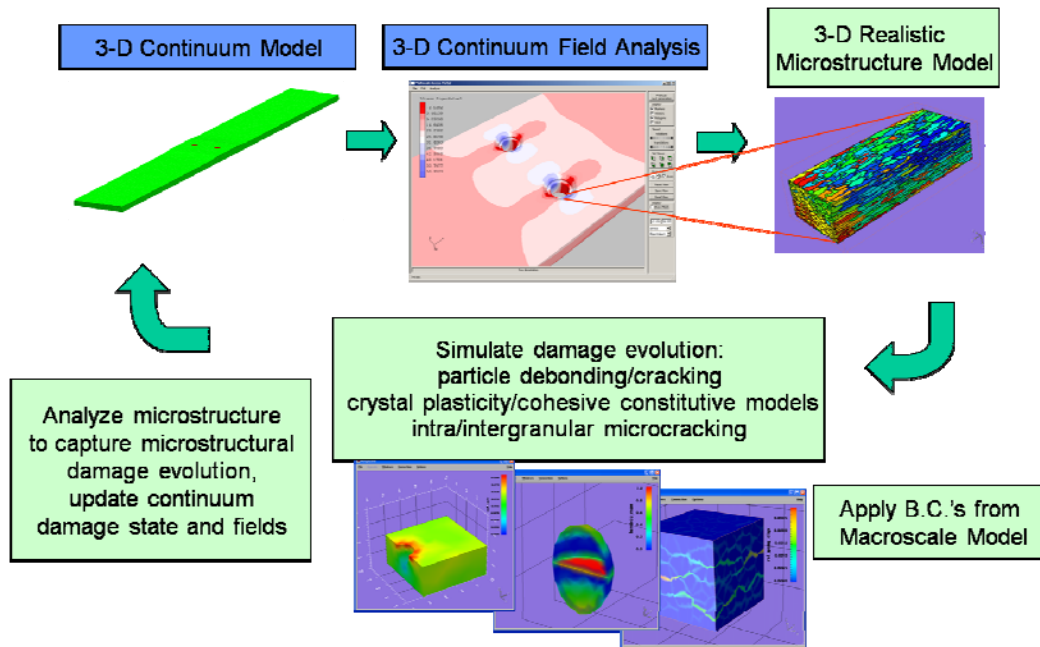


Figure 1: Data flow for the current multiscale framework, DDSIM level 3.

A stress-based criterion is used to determine which of the particles are likely to crack. To determine the stress experienced by an arbitrary particle under load, Bozek *et al.* completed 2592 3D, elasto-crystal plastic finite element analyses to develop a response surface for tensile stress at the particle centroid (point A in Figure 2) as a function of the strain level of the grain in the rolling direction, grain orientation and particle aspect ratio. The baseline model used for generation of the response surface is shown as Figure 2 [3] with respect to the rolling direction (RD), normal direction (ND) and transverse direction (TD).

The boundary conditions applied to the baseline model are intended to emulate strain fields in a grain located within an experimental specimen. Since the baseline model represents a grain embedded within a larger structure and the TD-ND plane at the front of Figure 2 is a free surface, the TD and ND components of strain in the baseline model are non-zero. Specifically, the out-of-plane boundary conditions on surfaces with normals in the TD or ND are between the two extremes of traction-free and constrained in the direction of the face normal. Thus, two sets of boundary conditions that represent these extremes envelope the actual conditions and were considered in the response surface generation. Displacement boundary conditions were applied to the surfaces of the baseline model such that the strain in the RD was 1%.

Three key assumptions/parameterizations inherent to the response surface are:

- (i) Maximum particle tensile stress occurs:
 - a. During the first load cycle (as supported by experimental observation);
 - b. At Point A in the particle, Figure 2 [20];
- (ii) The particle and matrix are perfectly bonded;
- (iii) Particle tensile stress is accurately obtained when:
 - a. Idealizing the particle as semi-ellipsoidal, and;
 - b. Only the influence of the surrounding grain is considered.

For use in the stress-based criterion, a technique for determining particle strength from fracture toughness, particle size and intrinsic flaw size was developed based on linear elastic fracture mechanics. For the calculation of particle tensile strength, the following assumptions were made:

- (i) Particle tensile strength is a function of particle size, due to the presence of inherent particle flaws;
- (ii) An inherent surface flaw exists that lies perpendicular to the loading direction;
- (iii) The inherent flaw size, a_f , is much smaller than the particle size, a_p ;
- (iv) A material constant, C , can be defined as the ratio of inherent flaw size to particle size (a_f / a_p).

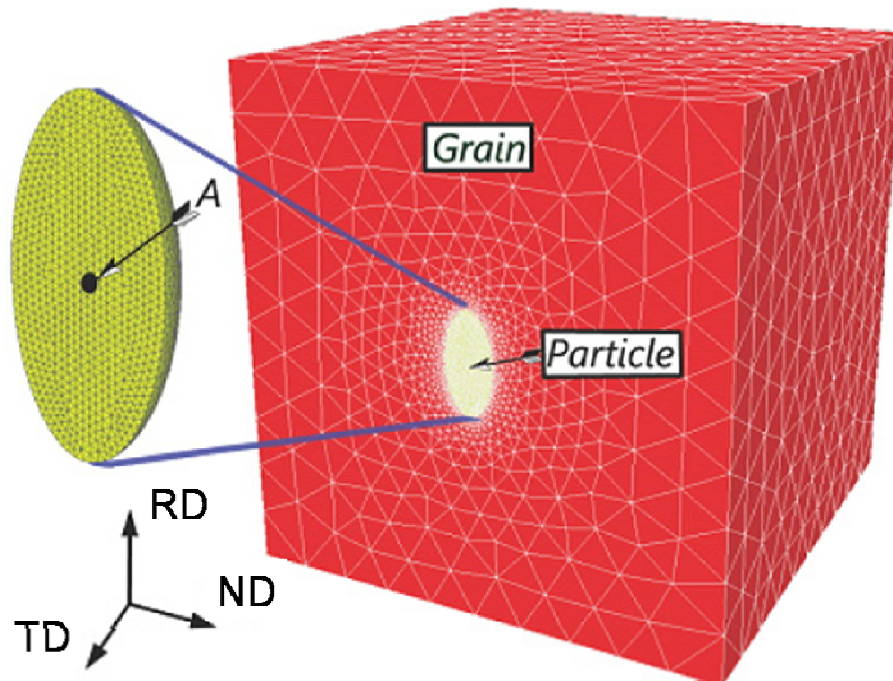


Figure 2: Typical surface mesh on an example baseline structural model used for response surface generation.

Assumption (i) has been commonly used in previous works [9,22]. The flaw is assumed to be oriented perpendicular to the maximum tensile stress, assumption (ii), because this is the orientation that yields the highest Mode I stress intensity factor. In observations of particles for this study, no inherent flaws were visible, which means that either the particles are initially flaw free or that the inherent flaws are too small to see at 20,000X magnification. It is unlikely that the particles are initially flaw free; therefore, assumption (iii) is made. Furthermore, since these flaws are undetectable at the microstructural scale, their actual shape and size is unknown. Thus, for simplicity, the crack shape is assumed to be semi-circular and a_f is assumed to be proportional to a_p , assumption (vi). Therefore a_f and a_p are radii of the inherent flaw and particle, respectively.

Finally, linear elastic fracture mechanics (LEFM) is assumed to be valid since the particles are brittle, with a measured very low average toughness, $0.14 \text{ MPa}\sqrt{\text{m}}$ with a standard deviation of $0.07 \text{ MPa}\sqrt{\text{m}}$ [25]. Fracture toughness values for twelve, iron-bearing, second-phase particles were estimated from a Vickers hardness test with a nano-indenter. With assumption (iii), the initial flaw configuration can be approximated as a semi-circular surface crack in an infinite plate with a critical Mode I stress intensity factor solution given by [21],

$$K_{IC} = 0.73 \sigma_{cr} \sqrt{\pi a_f}, \quad (1)$$

where σ_{cr} is the particle tensile strength.

Solving (1) for σ_{cr} and substituting $C = a_f/a_p$ yields the equation for particle strength used herein,

$$\sigma_{cr} = \frac{K_{IC}}{\sqrt{\pi a_f}} = \frac{K_{IC}}{0.73 \sqrt{\pi C a_p}}. \quad (2)$$

The particle tensile strength can therefore be calculated given the particle toughness, K_{IC} , the material parameter, C , and the particle radius, a_p . The material parameter, C , was calibrated in a previous study [3] and is used here.

The subset of particles to be included in the microstructural model is then determined by querying the response surface for an arbitrary particle configuration and comparing with the calculated strength. Therefore, a physically meaningful distribution of particle configurations is generated based on a sampling of the experimentally observed distribution of grain orientations, particle aspect ratios and sizes. To validate this overall approach to predicting particle cracking within an AA 7075-T651 microstructure, 2 methods are used:

- (i) Statistical Validation - Using a statistical realization of a distribution of particle configurations, based on experimental observation, validation can be made by comparing the predicted percentage of crack particles, as produced by querying the response surface, to that of an actual experiment, where the percentage of cracked particles is directly observed and;
- (ii) Case Study Validation - Obtaining the particle stress field from a finite element model, generated from a directly replicated AA 7075-T651 microstructure, and comparing to the response surface predicted stress. Subsequently, comparing the calculated strength to the computed stress for the replicated model for the prediction of particle cracking of the specific case.

Good agreement for the Statistical Validation, approach (i), between the predicted frequency of particle cracking and two experiments where particle cracking frequency was directly observed was found by Bozek *et al.* [3]. A model for a Case Study Validation, approach (ii), of DDSIM level 3 is discussed in the next section.

III. Framework Validation - Microstructural Modeling

This section addresses validation of the methodology for the prediction of particle cracking frequency as it is a crucial aspect of the above multiscale framework. Specifically, simplifications made pertaining to the exclusion of some geometric detail in the baseline model for response surface generation are tested in this section: compare the level of geometric detail included in the baseline model, Figure 2, to that of an actual AA 7075-T651 microstructure, Figure 3. This is done by directly replicating, discretizing, and analyzing the geometry of an observed AA 7075-T651 microstructure. First, a model that replicates the microstructure is developed and analyzed. Second, validation of the response surface methodology is made by comparing the computed value of particle tensile stress within the replication model at the particle's free surface centroid, analogous to point A in Figure 2, to the value predicted by its parameterization in the response surface.

The value of C calibrated by Bozek *et al.* is used here for calculation of particle strength. By using this value of C and the value of stress predicted by the response surface, a stress-based criterion is used to predict particle cracking. Correctly predicting particle cracking serves as validation of the methodology for the prediction of particle cracking frequency. Of course, validation of such a methodology requires that this procedure be repeated for a number of replication models. This study is currently underway and results will be published in a future paper.

Model Generation and Analysis

The description of a specific microstructural morphology is obtained by orientation imaging microscopy (OIM). The region (grain or particle) boundaries in the resulting image are traced to create a computational replication of the microstructural geometry, Figure 3. This 2-dimensional geometry is then extruded to create a 3-dimensional model. Experimental observations of grain aspect ratio are used to determine the distance for extrusion of the grains, i.e. 2 characteristic dimensions of the grains are known from OIM and the 3rd is computed from an observed average grain aspect ratio. For particle regions, a characteristic radius is computed by fitting a circle to the particle boundary and the radius is used as the extrusion distance. If the particle extrusion depth is less than that of the grain, then there is a void created behind each particle in the model. In this case, the grain that has the greatest area of contact with the particle is used to 'fill in' this resulting void.

The orientation of each grain in the observed microstructure is also determined by OIM. After generation of the 3D geometry, a mesh is generated where elements are assigned material orientations corresponding to experimental observations. In this study, the particle is modeled as a linear elastic, isotropic solid and the grains are modeled as rate-dependent, face-centered cubic (FCC) crystal plastic solids of varying orientation. Particle regions were modeled using the experimentally determined values of Young's modulus and Poisson's ratio of 166.4 GPa and 0.30, respectively. The overall formulation of the grain material model follows the work of Matous and Maniatty [19]. The parameters used for the FCC model were also found from experiment. A detailed discussion of those parameters can be found in [3]. For this model, ABAQUS[®] was used for both the generation and the discretization of the configuration.

An in-house FE analysis code, Finite Element All Wheel Drive (FEAWD), was used to perform the analyses. FEAWD is a parallel driver, which coordinates the partitioning,

formulation, assembly and solution of the resulting nonlinear finite element equations. It is based on standard packages including MPI [28], ParMetis[17], PETSc [1], and the Cornell Fracture Group's FemLib library [8], which contains an implementation of the crystal plasticity model. Ten-noded hybrid tetrahedral elements were used in all models.

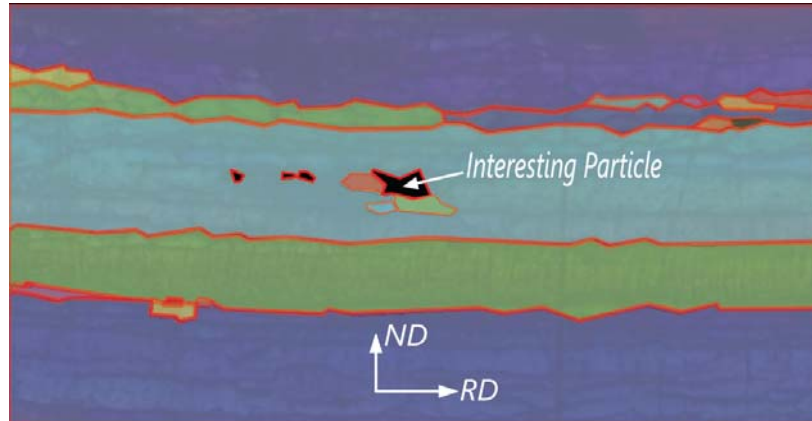


Figure 3: OIM of a rolled aluminum alloy microstructure with traced boundaries shown as thick lines between regions.

Systematic simplifications of the replicated geometry were made to determine the sensitivity of the computed stress in a particle to the surrounding grain geometry. Starting with a detailed replication model, “All Grains,” simplifications were made with varying hypotheses in mind. Those hypotheses pertain to the geometric details that are potentially important to the computation of tensile stress within the particle. The four derivatives of the “All Grains” model considered here are shown in Figure 4, where the name of each derivative corresponds to a hypothesis of the level of geometric detail that is crucial, e.g., “No Small Grains” suggests that only grains above a specific volume are of importance.

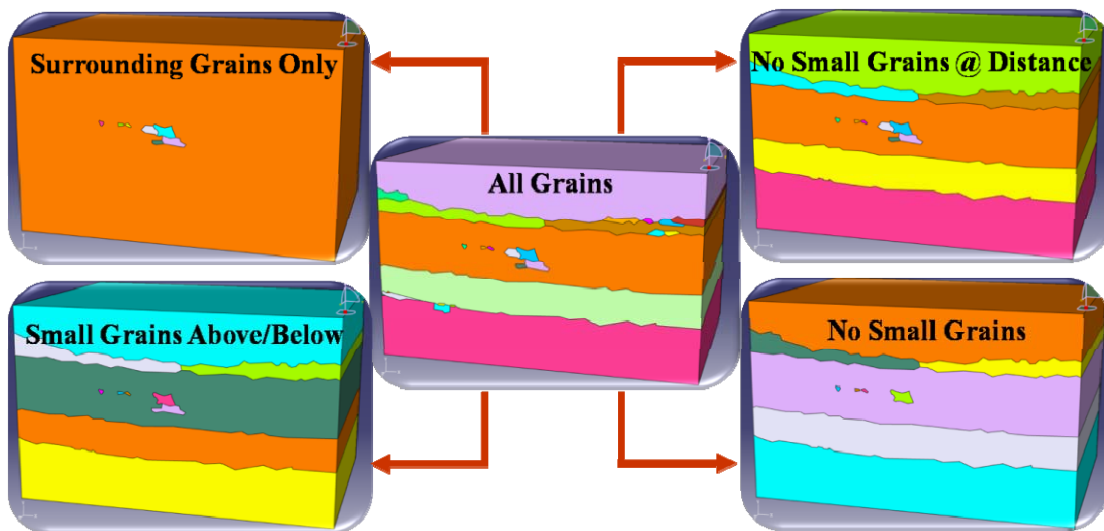


Figure 4: Four possible derivatives of the detailed, replicated microstructure “All Grains”.

In each derivative above, if a grain is considered to be negligible either because of its size or distance from the particle of interest, it is merged with a neighboring grain. Of all of the grains in the neighborhood of the negligible grain, the neighboring grain to be merged is that grain which has the least misorientation relative to the negligible grain.

Boundary conditions on each of the replication models were such that the face shown in Figure 4 was free to move. The remaining 5 faces of the models were fixed in the normal direction to the face. These boundary conditions were enforced to model the constraint that the replication model feels from the surrounding material. Relieving these constraints and enforcing a uniaxial tension state in the RD within the validation model produces another bound of the model stress fields. This study is currently underway and will be published in a future paper. A more accurate representation of the boundary conditions for the microstructural model can be obtained by using the multiscale technique overviewed in Section 2.

Discussion of Results

Analysis of the replication model was carried out using each of the geometric configurations shown in Figure 4. For each configuration, a mesh refinement study was carried out and the convergence of stress, σ_{RD} along Path-A in Figure 5, was used as the criterion. Path-A was chosen for testing convergence since the particle was observed to crack along Path-A during loading and since Path-A contains the particle's free surface centroid, which is the point where a comparison between the baseline model and replication model will be made.

The coarsest mesh used for the "All Grains" case is shown in Figure 5 and contained 200,000 quadratic tetrahedral elements and approximately 2 million degrees of freedom (DOF). In general, considering the various levels of mesh refinement and geometric configurations, the meshed models were between 1 million and 20 million DOF. To run problems of this size, a 340 processor distributed memory cluster was used. Analysis time of the models ranged from 4 hours to 4 days and was strongly dependent on mesh quality, but somewhat counter-intuitively was not as dependent on mesh size or geometric configuration. In practice, the analysis of a coarsely meshed model can take longer than that of a more refined model since integration at the material level requires much smaller load steps for relatively large elements in regions of high stress gradient. The computed RD component of tensile stress for the converged mesh refinement, within the particle of interest, in the "All Grains" model is shown at the upper right of Figure 5. The value of stress at the midpoint of Path-A is used to compare the results of the validation model to the response surface predicted value, since this point is analogous to Point A in Figure 2. To query the response surface, a parameterization of the particle in the validation model is made. This is done by finding the best-fit ellipse to the actual particle geometry. The value of particle tensile stress predicted by the response surface is then obtained using the ellipsoidal parameterization for the actual particle, the surrounding grain orientation and particle strain level. For the parameterized particle, the queried value of σ_{RD} is found to be 886 MPa, which is within 10% of the stress computed within the validation model, 820 MPa, at the midpoint of Path-A.

The dependence of particle tensile stress on geometric simplifications in the replication models is shown in Figure 6. The two most extreme geometric configurations, "All Grains" and "Surrounding Grains Only" (SGO), define the envelope of particle tensile stress along Path-A, Figure 5. Particle tensile stress along Path-A for the other geometric configurations was

bounded by this envelope. This finding supports the assumption made for the generation of the response surface that only the surrounding grain needs to be modeled to obtain an accurate prediction of particle tensile stress.

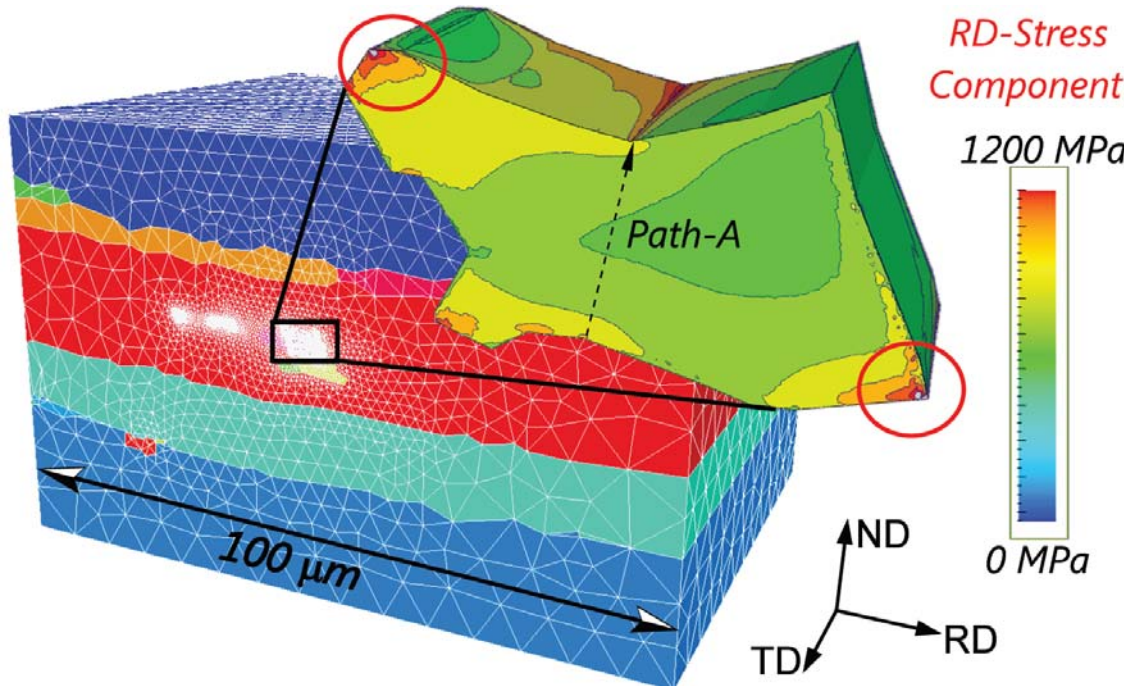


Figure 5: Finite element model (left) and computed tensile stress in the particle (detail) for the replication model.

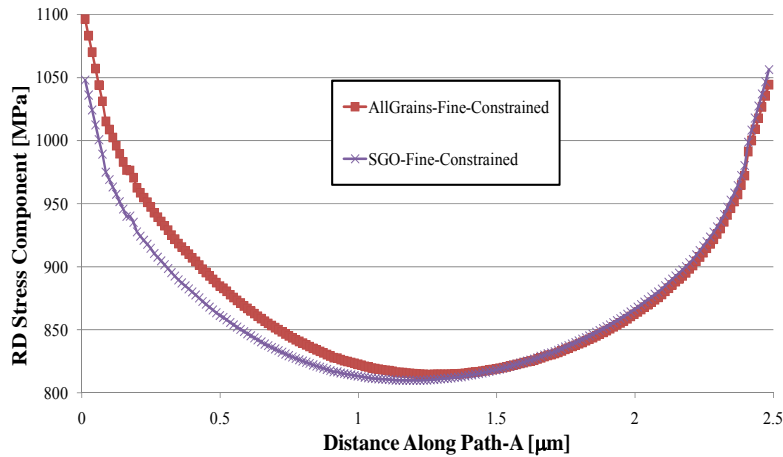


Figure 6: Maximum principal stress along Path-A within the particle of interest.

The particle strength was computed to be between 1200-1320 MPa using the range of values for C reported by Bozek *et al.* [3]. With the strength of the particle much greater than the stress predicted by the response surface, this particle will not crack. However, this particle did crack under load. The range of C values reported by Bozek *et al.* is based on one calibration study and more calibration studies must be done for this material parameter. Also, this investigation implies that particle cracking occurs due to high stresses near the boundary of the particle and not the bulk particle stress retrieved from Point A. Investigations where the gradient of the stress field within the particle is considered will be carried out in a future study.

Also apparent within the particle are the stress concentrations: encircled at the upper left and lower right corners of the particle in Figure 5. These stress concentrations are the effect of: modeling the particle-grain interface as a perfect bond; representing the microstructural geometry by a set of lines that cause sharp angles, extrusion in the TD also causes sharp angles; and modeling the particle as linear elastic. It is likely that the bond between the particle and grain would be severed in regions of high stress near the sharp corners of the particle. CZMs have been used to model separation along similar boundaries in regions of high stress gradients; however, the behavior of this particle-grain interface has not been quantified. This lack of understanding of the constitutive behavior of the interface serves as a motivation to develop CZMs based on small-scale experimentation and physics-based modeling (e.g., atomistic simulation) as will be discussed in Section 4. In addition to improving the fidelity of the replication models, physically-based CZMs will also increase the fidelity of the baseline model for response surface generation.

IV. Approach for Incorporating Physics-Based Modeling and Small-Scale Experiments

As discussed in Section 3, debonding of the second phase particles is believed to have a pronounced influence on their cracking during the incubation phase of damage growth in the AA 7075-T651. Additionally, once a particle cracks in the incubation phase, it sometimes initiates a crack within the aluminum grains that propagates during the nucleation phase of damage growth. Currently, the accuracy of models that are developed to describe these two events is entirely dependent on the fidelity of *assumed* CZM relationships. Ideally, the CZM relationships should be determined using physics-based modeling, small-scale experiment or a combination of both.

Physics-based modeling of fracture ultimately begins at nanometer length scales in which atomistic simulation is used to predict the formation, propagation, and interaction of fundamental damage mechanisms. These mechanisms include dislocation formation and interaction, interstitial void formation, and atomic diffusion. However, modeling atomistic processes quickly becomes computationally intractable as the system size increases. With current computer technology, the computational demands of modeling suitable domain sizes needed to capture nanoscale damage processes (e.g., billions of atoms for classical mechanics-based methods) quickly reaches an upper bound for practical analyses. Thus, multiscale modeling is often employed at the nanoscale to incorporate the required higher physical resolution while maintaining computational efficiency.

Nanoscale simulation enables an understanding of fundamental damage processes that is otherwise unavailable. The information that can be gained at this scale is immediately useful for providing a qualitative foundation for multiscale modeling, and with some additional

assumptions on scaling, can provide a quantitative basis for development of higher-level constitutive relationships [30]. Disadvantages to simulation at the nanoscale include the ability to only model idealized crystal structures composed of materials for which interatomic potentials have been developed and, because of existing computational resources, consideration of only very short time scales ($\sim 10^{-12}$ seconds) and very small domains ($<$ microns). With ever-increasing computer power, it is evident that the long-term ability to use atomistic simulation to improve the fidelity of crack growth simulations will not be limited by computational resources, but by our lack of knowledge in creating atomistic models and providing valid input.

Referring to the left half of Figure 7, NASA Langley Research Center (LaRC) and Brown University are currently developing concurrent multiscale simulation codes that are capable of modeling dislocation and grain boundary deformation modes at the nanoscale [24, 29, 30, 32, 34]. Curtin has developed CADD, a tool that integrates molecular dynamics simulation with dislocation dynamics to seamlessly pass dislocations from an atomistic domain to a continuum domain [24]. NASA LaRC has developed the Embedded Statistical Coupling Method, which also embeds a molecular dynamics region within a finite element domain, but unlike CADD, uses statistical averages to couple the two computational schemes. Each of the components shown at the far left of Figure 7 provide a means to simulating fracture mechanisms based on first-principle computation and, when combined, are capable of predicting CZMs for intra- and inter-granular damage growth.

Referring to the right half of Figure 7, as discussed in Section 3, the ability to develop and analyze multiscale models of actual or statistically representative microstructures within an aircraft structural component currently exists. At the microscale, material models (i.e. crystal plasticity) are represented as a continuum and so mechanisms that govern fatigue crack are only captured in a homogenized sense. However, the tools for crack simulation at these scales are in place and can easily adapt to include improved physics-based models. Effectively, this means that if the ability to represent local damage mechanisms were to be developed then the existing DDSIM framework can still be used.

A computational modeling method to link the simulation capabilities represented by the left and right halves of Figure 7 has been conceptualized for highly idealized configurations for this incorporation of local damage mechanisms [14]. As discussed in [14], the method to connect the microscale and nanoscale models and still maintain computational tractability is to aggregate the damage processes occurring at the nanoscale into a cohesive zone model for microscale fracture simulation. So, although the nanoscale is not explicitly represented in microscale models, the mechanisms occurring at the nanoscale are implicitly represented through the cohesive zone models. However, a similar but much more complicated connection between the statistically generated or experimentally replicated detailed microstructural models discussed in Section 3 and atomistic simulation is yet to be developed. Such a connection would provide the existing DDSIM multiscale framework with another, much needed, level of increased fidelity.

The existing molecular dynamics-based CZMs contain many idealizations (e.g., absence of defects) and cannot be deemed as being quantitative; however, they do improve our understanding of the underlying mechanisms of damage at very small length scales. A means of reconciling this atomistically-derived damage process characterization with experimentally-determined values is needed and is being developed.

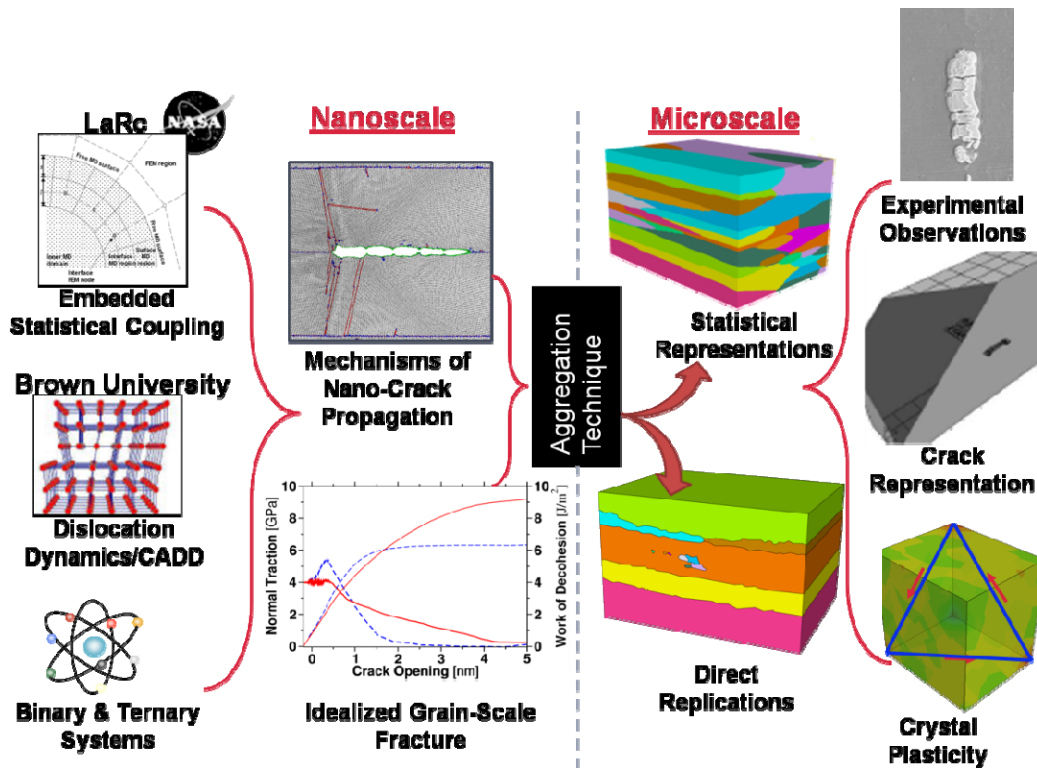


Figure 7: Framework for the integration of existing microstructural modeling tools with existing atomistic simulation tools.

An experimental setup at the NASA Langley Research Center (LaRC) is in place that will provide high-resolution displacement data of single- or bi-crystals under load. The process illustrated in Figure 8 employs atomistic simulation to provide the optimization loop with a prediction of a CZM. This predicted CZM is then used in the simulated experiment as an initial guess within the optimization procedure. The optimization procedure converges to a CZM that produces the best replication of experimental observation. A surface displacement field will be measured using the experimental setup at LaRC and used as the reference solution, \mathbf{u}^{exp} . The surface displacement field is captured using digital image correlation. The loop continues until the simulated displacement field, \mathbf{u}^{sim} , is within a defined tolerance of the experimental field, \mathbf{u}^{exp} .

First, the aggregation process will be employed using an uncracked, single-crystal specimen to compute continuum material model parameters used in an already developed crystal plasticity model [19]. With the crystal plasticity material properties, remotely applied boundary conditions, and displacement field known, calculation of the local traction vs. separation relation at the crack front is facilitated by a finite element model with included cohesive zone elements. The CZM is iterated upon and optimized until a suitable comparison with experimental observation is obtained. The process effectively aggregates the mechanics at the nanoscale into a CZM. Since the resulting CZM is found by comparison with experimentation, a comparison can be made between the predicted CZM parameters given by atomistic simulation and the converged CZM parameters. This comparison will give much needed insight into how atomistic

simulations scale in time. It can be expected from past research that the governing mechanisms near a crack front will be dependent on the orientation of the surrounding microstructure [29, 32]. For this reason, cohesive zone parameters that are dependent on the surrounding orientation will be obtained by repeating the aggregation technique for various crystal orientations. Also, loss of fidelity due to the homogenization of nanoscale mechanics will be a major point of comparison that will serve as a measure of success of the aggregation process.

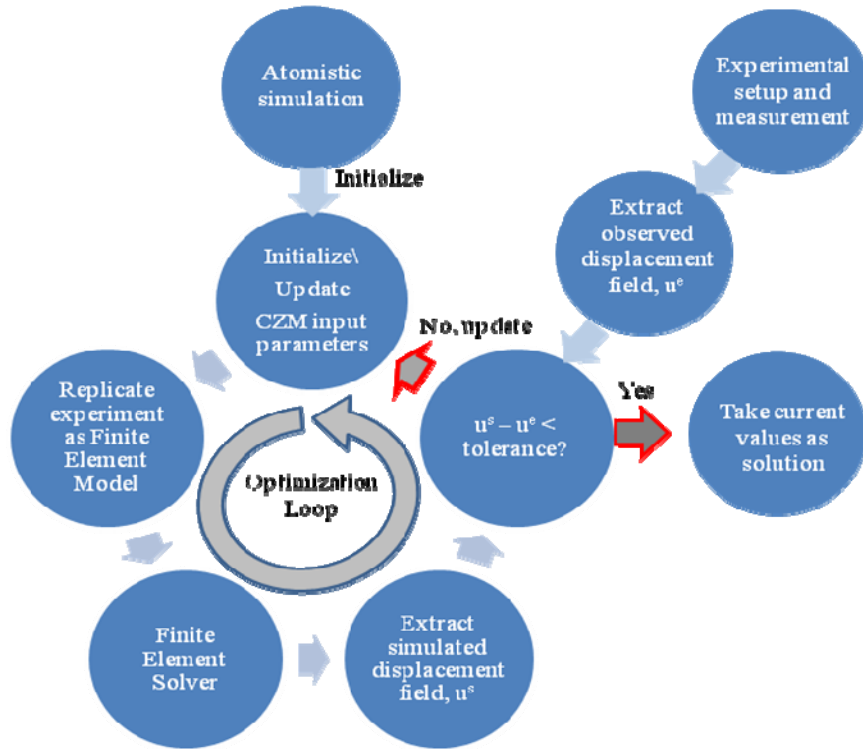


Figure 8: Method for extracting CZM parameters using experimentation and simulation

V. Conclusion

This paper has two goals related to the development of a physically-grounded methodology for modeling the initial stages of fatigue crack growth in an aluminum alloy. The aluminum alloy, AA 7075-T651, is susceptible to fatigue cracking that nucleates from cracked second phase iron-bearing particles. Thus, the first goal of the paper is to validate an existing framework for the prediction of the conditions under which the particles crack. The observed statistics of particle cracking (defined as incubation for this alloy) must be accurately predicted to simulate the stochastic nature of microstructurally small fatigue crack (MSFC) formation. Also, only by simulating incubation of damage in a statistically accurate manner can subsequent stages of crack growth be accurately predicted. To maintain fidelity and computational efficiency, a filtering procedure was developed to eliminate particles that were unlikely to crack. The particle filter considers the distributions of particle sizes and shapes, grain texture, and the configuration of the surrounding grains. This filter helps substantially reduce the number of particles that need to be included in the microstructural models and forms the basis of the future work on the subsequent stages of MSFC, crack nucleation and microstructurally small crack propagation.

A physics-based approach to simulating fracture should ultimately begin at nanometer length scale, in which atomistic simulation is used to predict the fundamental damage mechanisms of MSFC. These mechanisms include dislocation formation and interaction, interstitial void formation, and atomic diffusion. However, atomistic simulations quickly become computationally intractable as the system size increases, especially when directly linking to the already large microstructural models.

Therefore, the second goal of this paper is to propose a method that will incorporate atomistic simulation and small-scale experimental characterization into the existing multiscale framework. At the microscale, the nanoscale mechanics are represented within cohesive zones where appropriate, i.e. where the mechanics observed at the nanoscale can be represented as occurring on a plane such as at grain boundaries or slip planes at a crack front. Important advancements that are yet to be made include:

- an increased fidelity in cohesive zone modeling;
- a means to understand how atomistic simulation scales with time;
- a new experimental methodology for generating empirical models for CZMs and emerging materials; and
- a validation of simulations of the damage processes at the nano-micro scale.

With ever-increasing computer power, the long-term ability to employ atomistic simulation for the prognosis of structural components will not be limited by computation power, but by our lack of knowledge in incorporating atomistic models into simulations of MSFC into a multiscale framework.

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