A Method for Combining Experimentation and Molecular Dynamics Simulation to Improve Cohesive Zone Models for Metallic Microstructures

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Abstract: Fracture processes within a material begin at the nanometer length scale at which the formation, propagation, and interaction of fundamental damage mechanisms occur. Physics-based modeling of these atomic processes quickly becomes computationally intractable as the system size increases. Thus, a multiscale modeling method, based on the aggregation of fundamental damage processes occurring at the nanoscale within a cohesive zone model, is under development and will enable computationally feasible and physically meaningful microscale fracture simulation in polycrystalline metals. This method employs atomistic simulation to provide an optimization loop with an initial prediction of a cohesive zone model (CZM). This initial CZM is then applied at the crack front region within a finite element model. The optimization procedure iterates upon the CZM until the finite element model acceptably reproduces the near-crack-front displacement fields obtained from experimental observation. With this approach, a comparison can be made between the original CZM predicted by atomistic simulation and the converged CZM that is based on experimental observation. Comparison of the two CZMs gives insight into how atomistic simulation 'scales.'

1 Introduction

State-of-practice methods for predicting material fracture are based on empirical models that homogenize damaging mechanisms and recast them in the form of a single fracture or damage parameter, *e.g.*, Crack Tip Opening Angle (CTOA). In general, a damage parameter is asserted to be the driving force for crack propagation, and subsequently, mechanical testing is performed to provide the corresponding critical value for a given material and testing condition. State-of-practice methods for modeling fracture have greatly improved the ability to predict structural failure; however, these methods are inductive and only a small subset of all possible configurations (both material and geometric) can be tested. This results in high uncertainty and safety factors, and necessitates decreased inspection intervals and inefficient design. The state-of-practice methods are fundamentally limited in that a phenomenological governing driving force, such

as CTOA, is initially asserted, and testing is carried out to find the corresponding value of critical material resistance, *i.e.* critical CTOA ($CTOA_c$), that was initially asserted to be the mechanism of consequence. Breaking out of this circular-reasoning loop and developing a more deductive approach enabled by modeling fundamental mechanisms will reduce uncertainty and result in more efficient and reliable structures.

Useful prognosis of structural behavior is probabilistic due to the inherent variability in materials, loading, manufacturing, and environment at all physical scales. 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 a statistical prognosis capability requires quantitative simulation of microstrutural crack growth utilizing physics-based models of intra-, inter-, and transgranular fracture modes for polycrystalline metals. However, it is computationally intractable and arguably unnecessary to represent an entire component with atomistic resolution, especially statistically. Therefore, an approach that leads to mechanistically-based continuum fracture parameters developed via multiscale modeling and various forms of homogenization is desired.

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. Section 2 of this paper discusses a method for improvement of CZMs that is based on the aggregation of experimentally-derived and computationally-simulated response of single- and bi-crystals. In Section 3, a comparison between state-of-practice methods and the methodology presented in Section 2 is given. Section 3 serves as an exercise to illustrate the expected advances to be made through the incorporation of nanoscale mechanics (discontinuum) into microscale simulation (continuum).

2 Molecular dynamics, experimentation, and inverse modeling

The purpose of molecular dynamics (MD) simulation in this study is to reveal and analyze nanoscale processes occurring near a crack front so that they can be incorporated into crack growth simulation through CZMs. As shown in past work, MD simulation can be used to determine a CZM in a statistical sense [8,11,12]. From MD simulation, one can determine the influence that various plastic processes have on crack growth, such as vacancy and void formation, and dislocation nucleation. Crack growth simulation via a finite element model (FEM) can then be improved by incorporating a CZM that takes into account these distinct processes near the crack front. Currently, however, MD simulation is applied to idealized crystal structures composed of materials for which interatomic potentials have been developed and, as such, the analyses tend to be of only qualitative use. Also, current compute power limits the simulations to

very short time scales (fractions of a microsecond) and small spatial domains (fractions of a micron) [10].

Fig. 1 illustrates the extraction of a MD-based CZM representing decohesion along an idealized Σ99 grain boundary in an aluminum bi-crystal [11]. While these MD-predicted CZMs are qualitatively similar to experimentally derived CZMs, they are not quantitatively similar. This is a result of the idealized nature of MD simulation. From Fig. 1, it is seen that MD simulation predicts a CZM with an ultimate tensile traction, σ_c, of nearly 6 GPa and a complete separation distance, λ_c, of approximately 2.4 nm [11] for pure aluminum, whereas in practice, values of around 500 MPa and 20 μm are expected for σ_c and λ_c, respectively, for aluminum alloys [2,4]. The ability to relate a CZM as predicted by MD simulation to a CZM observed through physical experimentation is needed to develop a validated model of the process zone of a crack; such a capability would provide insight into how molecular dynamics simulation 'scales.'

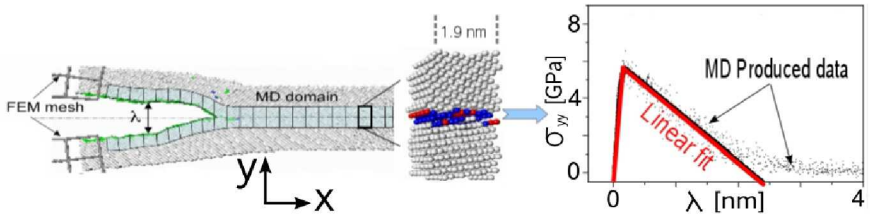

Fig. 1: CZM extraction from MD simulation [11]

To best match the MD simulation spatially, small-scale experiments and highly resolved measurement techniques must be employed. Fig. 2 is an illustration of such an experiment where a fatigue-cracked, single-crystal of 6019 aluminum alloy is being loaded uniaxially in the *y*-direction, and strains in the y-direction are measured using high-resolution (approximately 10 nm displacement resolution) digital image correlation (DIC). In the experimental approach advocated here, single-crystals of pure aluminum, rather than an aluminum alloy, are fabricated and fatigue-cracks are initiated. Upon loading, displacements are measured using DIC in the area surrounding the point at which the crack front intersect the specimen surface. This near-crack displacement field enables observation of the localization of strain at the crack front. MD modeling techniques can then be employed to determine the role that each mechanism plays in the process zone and subsequently its contribution to the CZM.

While MD simulation is capable of providing qualitatively accurate CZMs that account for the contribution of distinct mechanisms, and experimentation can provide high-resolution displacement fields, there is no reconciliation of the

information gained. This reconciliation is the key step to developing a validated model for the process zone. Unfortunately, it is currently computationally intractable to extend the temporal and spatial domains of MD simulation beyond the environs discussed previously, and experimentation certainly cannot measure the movement of each atom, especially on a picosecond scale. Therefore, the methodology developed here aggregates the information gained through MD simulation for application at scales, both temporal and spatial, which lend themselves to experimental validation.

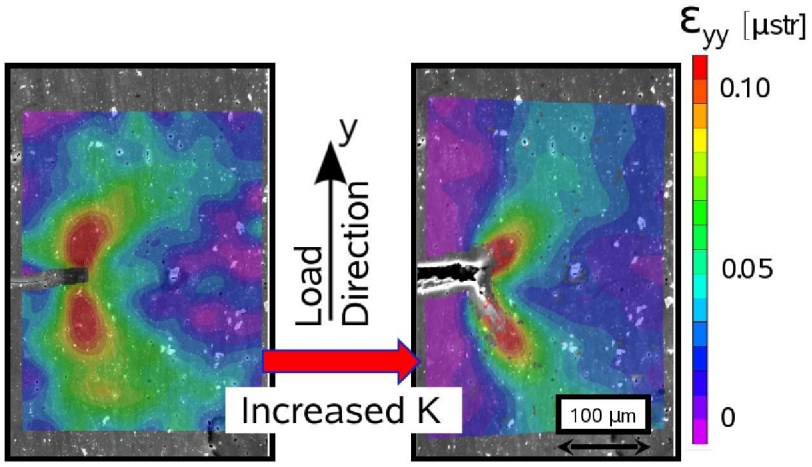

Fig. 2: Digital image correlation produced contours of *y*-direction strain

At this point, an inverse problem has manifested itself; the displacement field has been measured, but one does not know which material model produces that displacement field. Past research regarding the inverse calculation of CZMs to simulate these forms of crack growth has focused, to a large extent, on numerical methods for solving the resulting nonlinear systems [3]. This inevitably has led to a choice of CZM parameters that is numerically advantageous rather than being physically meaningful, since the mechanisms that control those parameters are not well-known and have not been quantified. Concrete and ceramics have been the focus of much past research on calculating CZM parameters using inverse methods. Previously developed methods for these materials are macroscopic in nature, in that the CZM functional form is fixed (usually piecewise linear) and its parameters are calculated using far-field displacement measurements [1,2,4,6,7,9]. Using these macroscopic approaches for inverse calculation of CZMs reproduces well the far-field displacement and total energy dissipation of a system. However, the major goal of the present work is to determine the impact that distinct processes, such as those observed by Horton [5] and others, have on the CZM.

A technique for the inverse calculation of a CZM, Fig. 3, is now formulated using the experimentally measured displacement field near the crack process zone and

an initial guess for the CZM, based on the MD simulation. These initially predicted CZMs are placed within a finite element model that attempts to replicate the configuration, continuum material response, boundary conditions, and loading seen in the experiment. A field of near-crack, surface displacements is measured using the experimental setup and used as the reference solution, $\mathbf{u}_e$. The loop, denoted by the circle in Fig. 3, continues until the corresponding finite element displacement field, $\mathbf{u}_s$, is within a defined tolerance of the experimental field, $\mathbf{u}_e$. The inverse problem-solving technique converges to a CZM that produces the best replication of experimental observation.

The optimization technique employed here for development of the CZM is based on a genetic algorithm. The genetic algorithm technique is employed because of its inherent capability to search for global minima and its ease of parallelization. Initially, a set of CZMs is generated that is closely related to the MD-predicted CZM. An additional set is also generated that varies the CZM parameters by an order of magnitude, which enables a global search of optimal CZM parameters. For each CZM in the population, a finite element model is run; using a computer cluster, each FEM is sent to a different processor so that runtime is greatly reduced. Once the comparison is made between each CZM in the population and the experimentally observed field, if convergence has not been achieved, the genetic algorithm is called to update the population of CZM parameters. It is understood that the outcome of this process is not unique and that the converged solution can, for ill-posed problems, simply be a function of the initial guess. Therefore, subsequent studies will be carried out that investigate the convexity of the search space and the sensitivity to initial predictions of the CZM.

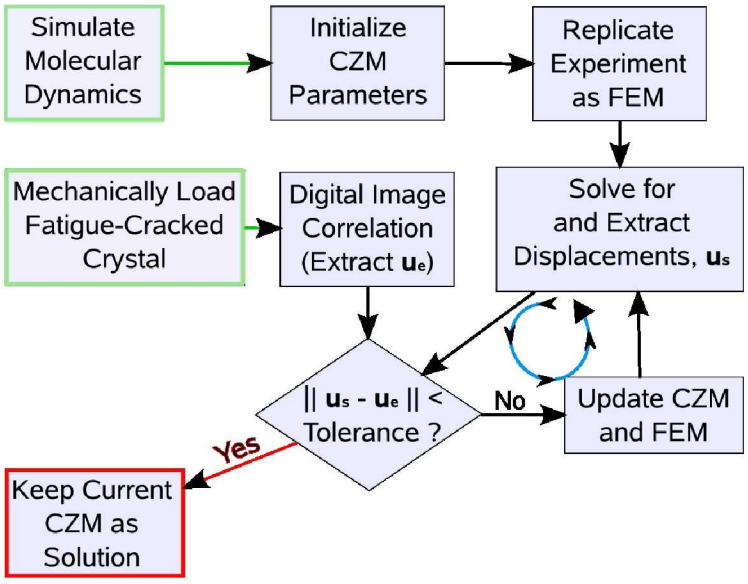

Fig. 3: Inverse approach to finding CZM parameters

3 An illustrative example

In this section, a comparison between state-of-practice methods and the methodology under development is provided. A bicrystal model undergoing intergranular crack growth is used as the basis for comparison, Fig. 4, and was chosen to illustrate the advantage of using a MD-informed CZM during crack growth simulation. Upon loading uniaxially in the y-direction, the two crack tips will begin developing process zones. Let the orientations of Crystal #1 and #2 be such that the interface is symmetric, as in [11,12]. The goal of this comparison is to illustrate the conceptual differences amongst modeling approaches for crack growth simulation rather than to detail quantitative comparison or validation.

In the analogous FEM simulation, the two crystals are assumed to be elasto-plastic with power-law hardening, *i.e.* a Ramberg-Osgood relation, so that stress and strain are given by the Hutchinson, Rice, and Rosengren (HRR) fields, Eqs. 1.

$$\sigma_{ij} = \sigma_o \left(\frac{E}{\alpha \sigma_o^2 I_n} \frac{J}{r} \right)^{\left(\frac{1}{n+1}\right)} \bar{\sigma}_{ij}(\theta, n)$$

$$\varepsilon_{ij} = \alpha \frac{\sigma_o}{E} \left(\frac{E}{\alpha \sigma_o^2 I_n} \frac{J}{r} \right)^{\left(\frac{n}{n+1}\right)} \bar{\varepsilon}_{ij}(\theta, n) \qquad \text{Eqs. 1}$$

In Eqs. 1:
σ_{ij} = stress tensor
ε_{ij} = strain tensor
α, I_n = dimensionless constants
σ_n = yield stress
n = strain hardening exponent
θ = angle about crack tip, Fig. 4
$\bar{\sigma}_{ij}(\theta, n), \bar{\varepsilon}_{ij}(\theta, n)$ = dimensionless functions of θ and n

The state-of-practice methods are well-represented by three different approaches to this problem:

Damage mechanics – where a critical region or distance is defined from the crack front and a computed damage parameter is compared to a measured critical value to determine whether or not the crack will grow and;

Crack opening displacement (COD) – instead of querying a damage parameter at a distance ahead of the crack, opening is queried at a distance behind the crack tip (conceptually not much different from damage mechanics) and;

Cohesive zone modeling (CZM) – a planar material model is placed at the crack front to account for plastic processes localized there, the defining parameters are commonly chosen because they are numerically advantageous or are the result of experimentation or an inverse technique [3].

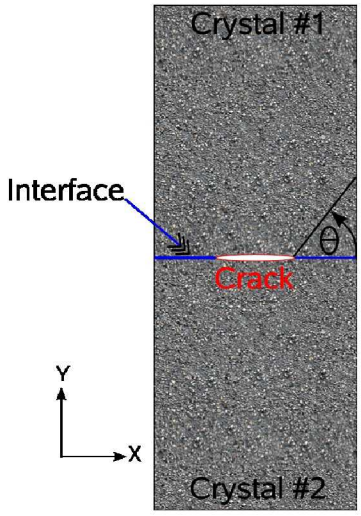

Fig. 4: Idealized bicrystal undergoing intergranular crack growth

Substitution of the bounding values of n into Eqs. 1 reveals some fundamental limitations of state-of-practice methods. First, if $n = 1$, it is found that both stress and strain are proportional to $1/(r)^{1/2}$ (*i.e.* the linear-elastic case). Conversely, as $n \rightarrow \infty$, then strain is proportional to $1/r$ and stress is effectively independent of r (*i.e.* the perfectly-plastic case). At either bound, strain fields are singular, which is directly a result of defining an infinitely sharp crack in the derivation of the HRR fields. This singularity is physically invalid in an elasto-plastic material due to crack tip blunting, which means that the HRR stress and strain fields are not valid at the crack front, $r = 0$. This leads to the motivation for both damage mechanics and COD. Since HRR fields are invalid at the point where they are most important, one can move some distance away and query fields there (or average over some region).

However, these methods inevitably lead to the need for nonphysical parameters, such as a critical distance, and therefore need to be calibrated for each geometrical and loading configuration considered. In addition to the use of nonphysical parameters, a problem exists with mesh convergence. Since strain is singular at the crack tip, and the form of the singularity depends on θ , n, grain orientation, *etc*., a converged solution at the crack front is not possible with mesh refinement. So, another calibration must occur where the finite element size is a fixed ratio of the critical distance, providing a basis for comparison among various finite element models. However, for complicated geometry, (as is the case for microstructural geometry) variations in mesh refinement are needed to obtain

reasonable element shapes and, in some cases, even to make meshing possible. So, although this is a logical approach when comparing idealized models within a well-defined study, it is not a general solution, especially for complicated microstructural geometry.

Crack growth simulation based on CZMs does not produce a singularity at the crack tip as occurs in damage mechanics or COD-based methods. As discussed in Sec. 2, several recent publications detail methods for back-calculation of CZM parameters from far-field displacements. However, in the case shown in Fig. 4, measurement of far-field displacements does not help to distinguish among the various physical processes at each tip and necessarily leads to a CZM for both process zones that does not account for the dominant mechanisms local to the particular crack front. The mechanisms for plasticity within the process zones are, in fact, very different at each tip. Yamakov, *et al.,* [11,12] showed, for an embedded crack growing along a $\Sigma 99$ grain boundary, that one tip will grow in a relatively brittle manner, through void formation, while the other will grow in a more ductile manner, with twin emission blunting the crack tip. This hindrance can be overcome by employing the experimental and measurement methods presented in Sec. 2. By directly measuring the displacement field about each process zone, the back-computed CZMs can be separated and more accurately depict the physical processes occurring at each tip. Not only does the initial MD simulation of such a problem make the understanding of various dominant mechanisms more obvious, it also allows for characterization of process zones through CZMs by the mechanisms that control the local deformation.

4 Conclusions

Given the need for a more physics-based approach to computationally modeling crack growth, there is strong motivation to begin incorporating MD simulation as part of a multiscale analysis. However, current MD simulations are based on unrealistic idealizations; simulations occur over such small length and time scales that they cannot be directly compared with experiment. On the other hand, MD simulation provides useful qualitative insight into the physical processes occurring at a crack. This insight can be used to better predict and understand CZMs modeling the process zone.

Past research has also motivated refinements in experimental observations and measurement. Combining this refinement in measurement techniques with corresponding numerical methods can provide near-crack displacement fields and more accurate models of the process zone through CZMs. In addition, with an understanding of the distinct mechanisms occurring within the process zone from MD simulation, the possibility to validate MD simulation exists. Development of CZMs in this way will improve the existing capability to model the early stages of crack growth.

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