Multi-scale modeling of microstructure dependent intergranular brittle fracture using a quantitative phase-field based method

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Abstract

The fracture behavior of brittle materials is strongly influenced by their underlying microstructure that needs explicit consideration for accurate prediction of fracture properties and the associated scatter. In this work, a hierarchical multi-scale approach is pursued to model microstructure sensitive brittle fracture. A quantitative phase-field based fracture model is utilized to capture the complex crack growth behavior in the microstructure and the related parameters are calibrated from lower length scale atomistic simulations instead of engineering scale experimental data. The workability of this approach is demonstrated by performing porosity dependent intergranular fracture simulations in UO_2 and comparing the predictions with experiments.

1. Introduction

The fracture behavior of brittle materials is strongly influenced by their underlying microstructural features such as pores, second-phase particles, pre-existing micro-cracks, grains, grain boundaries, etc. The shape, size, orientation and spatial distribution of these microstructural features control the initiation of micro-cracks, their propagation, interaction, and the final failure of the material. Hence, the variation of these microstructural features can alter the initiation and propagation behavior of the micro-cracks leading to final failure, which can result in scatter of experimentally measured fracture strength and toughness in a material. Thus, to accurately quantify the fracture properties and their variations in a material, the fracture models should incorporate the effect of microstructural features on the crack propagation behavior.

Probabilistic models at the engineering scale have been proposed to correlate the experimentally observed scatter of fracture properties to the variations in the underlying microstructure. The Weibull distribution function [1] based on the weakest link theory has been widely used to quantify such scatter. The effect of multi-axial stress-state on the probabilistic fracture strength of materials with pre-existing micro-cracks has been addressed in [2] by utilizing the Weibull distribution function. This model has further been extended to consider anisotropy in fracture strength ([3]) and effect of preferential flaw orientations ([4]). In [5], combinations of Weibull distribution function and analytical solutions of stress intensity

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factors of inclined cracks from linear elastic fracture mechanics (LEFM) have been used to relate the effect of flaw density on the probabilistic fracture strength. Similar considerations have been made in [6] to incorporate pore size distribution effect to predict size dependent fracture strength of nuclear-grade graphites. In the weakest link theory, the strength of the material is associated with the failure of the weakest region, and phenomena such as crack arrest or interaction between various micro-cracks are neglected. These limitations have been addressed in fiber-bundle models proposed in [7, 8] where representative regions are assumed connected in parallel or parallel and serial networks. By combining such probabilistic models with LEFM solutions of stress intensity factors, correlations between the scatter of fracture properties and the local variations of microstructural parameters (pore size distribution, etc.) were obtained in [9].

In these probabilistic analytical/semi-analytical models, various assumptions have been made to incorporate the influence of the microstructural features on the fracture strength and toughness, which can introduce uncertainties in their predictions. Additionally, the material parameters utilized in these models are calibrated from engineering scale experiments that can limit the applicability of these models to the calibrated range. Hence, computational modeling of fracture, which can address these deficiencies, has received significant research attention in the last few decades. Over the years several computational methods and models have been developed to investigate microstructure dependent fracture. These methods/models consider the microstructural features explicitly and allows a detailed mechanistic understanding of crack initiation, growth and interaction mechanisms leading to final failure. Though a wide variety of methods/models such as discrete element methods, lattice spring methods, mesh-free methods, peridynamics, etc. have been developed for fracture modeling, the brief overview provided here compares the models/methodologies that are used with conventional/hybrid finite element method (FEM) and can be broadly classified under two categories: (i) sharp crack interface and (ii) diffuse damage.

In the sharp crack interface models, a discontinuity is introduced to represent the cracked boundaries. The Extended FEM (X-FEM), Symmetric-Galerkin Boundary Element Method (SGBEM) alternating with FEM, Voronoi Cell FEM (VCFEM), and Cohesive Zone Model fall under this category. In X-FEM [10], discontinuities in the displacement fields across cracked surfaces are introduced through Heaviside functions and level-set functions are used in conjunction to track the crack front. This method allows the use of conventional displacement-based FEM to model fracture without remeshing. This method has been successfully used in [11] to model brittle fracture in polycrystalline material. The deficiencies in the crack front tracking algorithm in X-FEM has been addressed in [12] and the method has been shown to capture dynamic brittle fracture with crack branching. In the alternating SGBEM-FEM, boundary integral equations of tractions and displacements are formed for sub-domains with cracks, and standard FEM is utilized in the undamaged regions. The principle of superposition, assuming small strain, is then applied to both these fields to model crack propagation [13]. This method has been demonstrated to model complicated micro-crack propagation in composite materials with hard inclusions [14]. In VCFEM, Voronoi cells are constructed surrounding the heterogeneities (pre-existing microcracks/cavities/hard inclusions) and the coefficients of the Airy stress and reciprocal functions are solved to obtain the displacement field [15]. This method has been extended in [16] to simulate the propagation and interaction of multiple cracks in an otherwise homogeneous elastic media. In the

Cohesive Zone Model (CZM), crack propagation is assumed to occur along element interfaces and traction-separation laws are formulated to evolve damage [17, 18]. Since, cohesive elements can only be incorporated at solid-element boundaries in conventional FEM, crack propagation obtained by this method is strongly mesh sensitive. Numerical algorithms with adaptive refinement have thus been developed to overcome this issue and utilized to model dynamic brittle fracture with complicated crack paths [19]. X-FEM with CZM has also been used to model quasi-brittle fracture [20] and micro-crack propagation in dual phase steels [21]. One of the other limitations of CZM is that the effect of stress/strain triaxiality is absent in the traction-separation laws and hence the parameters need to be calibrated for varying triaxialities [22, 23]. In all of these methods, crack propagation direction is determined from the maximum principal stress (local) or energy release rate (global) criteria. Also, pre-existing cracks are assumed and nucleation is enforced externally (not intrinsic). In SGBEM alternating with FEM and VCFEM, significant modification to the conventional FEM formulation is required.

In the diffuse damage models, micro-cracking and damage in a material is considered to happen in a region with finite width. Constitutive equations are developed to degrade the material volume [24] and thus the dependence on triaxiality is intrinsic. The damage models can be implemented as standard non-linear materials models in FEM without any modification to the numerical integration of the equilibrium equations. However, local damage models have been observed to be strongly mesh-sensitive [25], which motivated the development of non-local diffuse damage models. In the non-local models [26], a length parameter (l) is utilized and hence the size of the fracture process zone can be incorporated. In the limit ($l \rightarrow 0$), a sharp crack interface can be obtained from the non-local diffuse damage models. When proper constitutive behaviors are incorporated in the damage laws, these models are suitable for capturing complicated crack propagation behavior [27–29]. More recently, a combination of sharp crack interface and diffuse damage models has been developed in [30] to utilize the advantage of both the approaches. By using the continuum damage mechanics theory for crack initiation and growth, and introducing discontinuities following complete failure of a material volume, appropriate propagation behavior of sharp cracks has been modeled.

The phase-field fracture method, belonging to the category of non-local diffuse damage models, has been used in this work to model intergranular brittle fracture at the microstructure scale. Phase-field methods are widely used to model microstructure evolution, where order parameters, describing the individual phases, and their corresponding concentrations are evolved using relaxation and diffusion equations [31], respectively. The free energy that drives the evolution is constructed from the thermodynamics of the system. A review on the application of the phase-field method to a wide variety of microstructural evolution problems such as solidification, solid-state phase transformation, grain-growth, pattern formation on surfaces, dislocation microstructures, electro-migration and crack propagation has been presented in [32].

In the phase-field fracture models, the relaxation equation in conjunction with the stress equilibrium is solved to evolve the order parameter representing damage. In [33], dynamic brittle crack propagation is modeled using phase-fields where the free energy is related to the hydrostatic strain. The free energy functional used in [33] has been modified by the strain energy density in [34]. Also a critical value of strain energy density is introduced in [34] for

crack initiation. Anisotropy in the interfacial energy of the damage-zone is additionally considered in [35] to model crack kinking under antiplane shear deformation. Comparison of the kink angle has been made with the energy-release rate criterion and force-balance condition in this work. In [36], the strain energy for crack propagation has been modified by considering the effect of compressive volumetric strain. In all these phase-field fracture models, the double well potential has been utilized to represent the influence of damage variable on the free energy. Though these models have been successful in capturing complicated crack propagation events such as branching, merging and fragmentation, the parameters are not directly related to the energy release rate typically used to quantify fracture in engineering nomenclature.

This limitation has been addressed in the free energy functional proposed in [37–44] where the energy release rate has been utilized as the critical parameter for crack propagation. In [37], the evolution of damage is obtained by minimizing the total energy of the system that is comprised of stored elastic energy and dissipated energy associated with the damaged volume. Numerical implementation of the model proposed in [37] has been provided in [38, 39]. An extension of the model in [37] is proposed in [40], where the influence of deviatoric strain components on damage evolution is considered. In [41], the minimization problem in [37] has been modified with a relaxation equation for damage growth. The mobility parameter in the relaxation equation governs the rate of damage growth, and the rate-independent fracture behavior is attained when this parameter value is infinite. In [42, 43] the variational approach to damage evolution proposed in [40] has been preserved. However, contrary to the model proposed in [40], the positive hydrostatic and deviatoric strain components are considered in the free energy definition. Additionally, the total energy of the system has been penalized to prevent crack healing, which yielded a rate-dependent equation for damage evolution. The rate-dependent damage evolution approaches the quasi-static limit when the artificial viscosity parameter tends to zero. This model has been utilized in [44] with higher order gradient terms in an iso-geometric framework. In [45], the free-energy form proposed in [40] has been utilized to investigate anisotropic crack propagation in ferroelectric single crystals under indentation loads.

Extension of the phase-field model to elasto-plastic fracture has been made in [46–49]. In [46], both the elastic and plastic energy has been considered to influence damage evolution in contrary to [47] in which damage evolution is only associated with the elastic energy. Elasto-plastic fracture in heterogeneous microstructure with particles has been analyzed in [48, 49] using a phase-field model with similar free energy and order parameter evolution as in [41]. However, in this model damage evolution under compressive strain state is allowed and is driven by the total strain energy density. Extension of the phase-field model to cohesive fracture has been performed in [50] wherein the total energy of the system is penalized to incorporate the effect of displacement jumps in the cohesive interface. However, this model was found inapplicable to problems with unstructured mesh and complicated crack paths [51]. More recently, the phase-field method has also been applied to analyze the propagation behavior of fluid filled cracks in porous media [52].

Numerical treatment of the phase-field fracture models has been discussed in [38, 42, 43, 47, 53]. Staggered approaches have been pursued in [47] for elasto-plastic fracture and in [42, 43, 53] for brittle fracture, motivated from its robustness proven in gradient-based damage mechanics. A predictor-corrector based mesh adaptivity scheme has been developed

in [54] to overcome the computational difficulties that can arise due to the requirement of small mesh size in phase-field fracture simulations. Numerical investigation on the Γ -convergence has been performed in [51] using one-dimensional representation of the phase-field fracture model proposed in [38]. From the analysis it was concluded that the sharp crack limit is not achievable and a critical length scale exists that provides the minimum deviation from the sharp crack solution. This contradicts the previous analytical work on the Γ -convergence of phase-field models for both the continuous ([55]) and discretized ([56]) representations of damage surfaces.

In the present work, the phase-field model proposed in [42, 43] has been utilized. In this model, the constraint to avoid crack healing has been explicitly imposed, which makes it appealing for this work. Moreover, the strain energy for damage evolution is related to the positive principal strain components that emulate crack face contact condition with an elastic stiffness under compressive strain state. Additionally, the quasi-static limit is achieved from the rate-dependent form of the model by considering near-zero values for the artificial viscosity parameter. In contrast to the staggered approach utilized in [42, 43], the damage evolution and stress equilibrium equations is integrated as a fully coupled system in the present work. Also, the applicability of the phase-field method to model fracture of interfaces is demonstrated in this work. The finitely thick grain-boundaries are modeled as weak interfaces with lower fracture strength than the grain interiors to induce intergranular fracture. Discontinuity in the displacement fields at the interface region is not considered explicitly ([50]) since the variation of properties and states at the interface can capture such jumps in a regularized manner. Finally, the ability of the phase-field fracture method to provide experimentally comparable quantitative estimate of fracture properties from microstructure scale simulations is demonstrated in this work.

In addition to modeling complicated crack paths for microstructure dependent fracture, precise evaluation of model parameters are necessary for accurate, quantitative prediction of engineering scale fracture properties. Atomistic simulations provide natural means for calibrating the parameters of the microstructure dependent fracture models [57–60]. However, the drastic differences in length and time scales between the microstructure and atomistic scales complicate the coupling process. Hence, in recent years several multi-scale methods have been reported to bridge these two scales. Concurrent continuum-atomistic multi-scale methods have been employed by several authors to capture brittle crack propagation [61]. However, the usability of the concurrent multi-scale methods is still restricted to representative volume elements (RVEs) of small size due to significant increase in computational cost. The hierarchical approach to multi-scaling allows much larger RVEs to be considered and has been successfully used in a variety of problems [62–64]. In this approach, the parameters in the microstructure dependent model are evaluated by homogenizing the responses obtained from lower length-scale simulations.

In the present work, the hierarchical multi-scale approach is employed, which utilizes the phase-field fracture model at the microstructure scale with parameters determined from atomistic simulations. The length scale parameter is assigned a physically realistic fracture process zone thickness value obtained from atomistic simulation. The other parameters are calibrated from the stress-strain behavior at the atomistic scale. Additionally, the transferability of the calibrated parameters from the atomistic to the microstructure scale is established. The workability of this approach is demonstrated by investigating the porosity

dependent intergranular brittle fracture strength of UO_2 .

The organization of the paper is as follows. In Section 2, the phase-field fracture model is introduced. Sensitivity studies are performed to obtain a detailed understanding of the model parameters and their transferability across different scales for brittle fracture. The workability of the multi-scale approach is demonstrated in Section 3 by considering porosity dependent intergranular crack propagation in UO_2 . In sub-section 3.1, the calibration of the grain boundary fracture parameters from molecular dynamic (MD) simulations is presented and is followed by the details of the phase-field based finite element (FE) simulations to obtain porosity dependent fracture properties in sub-section 3.2. The paper is concluded in Section 4.

2. Phase-field based fracture model

In this work, the phase-field based fracture model proposed in [42, 43] is utilized. In the model, the order parameter c , describing the damage region in a 1-d scenario, is represented by

$$c = \exp\left(-\frac{|x|}{l}\right) \quad \text{for} \quad -\infty < x < \infty \quad (1)$$

where l is a length parameter that controls the thickness of the damage region and the sharp crack limit is approached as $l \rightarrow 0$. The damage variable (c) varies from 0 to 1, where 0 and 1 represents the undamaged and completely damaged states, respectively. [This concept has been borrowed from diffuse damage models \[24\] and is associated with the loss of area that can sustain applied tractions. Hence, in an isotropic damage formulation, \$c = 0\$ to 1 implies that projected areas in any direction in the material volume evolves from fully intact to completely detached state.](#) A schematic of the damaged profile is shown in Fig. 1 where the crack front is in a direction perpendicular to the plane of the figure.

Figure 1: Spatial distribution of phase-field variable representing damage (c) in 1d.

By using the principle of variations, the area of the damaged surface is obtained as

$$\Gamma_l = \frac{1}{2l} \int_{\Omega} (c^2 + l^2 |\nabla c|^2) d\Omega \quad (2)$$

where Ω is the volume of the domain. Under the application of an external load, the power balance equation of brittle fracture follows

$$\dot{E}_E + \dot{E}_D = P_E \quad (3)$$

where $\dot{E}_E$ is the rate of change of strain energy of the system, $\dot{E}_D$ is the dissipative power due to crack propagation and P_E is the power due to the applied load on the system. The rate of change of strain energy of the system is assumed to have the form

$$\dot{E}_E = \frac{d}{dt} \int_{\Omega} \psi d\Omega \quad \text{where} \quad \psi = [(1-c)^2 + k] \psi_0^+ + \psi_0^- \quad (4)$$

where k is a small value that ensures the positive definiteness of the system after complete damage ($c = 1$) and

$$\psi_0^{\pm} = \lambda \langle \epsilon_1 + \epsilon_2 + \epsilon_3 \rangle_{\pm}^2 / 2 + \mu (\langle \epsilon_1 \rangle_{\pm}^2 + \langle \epsilon_2 \rangle_{\pm}^2 + \langle \epsilon_3 \rangle_{\pm}^2) \quad (5)$$

where ψ_0^+ and ψ_0^- are the specific strain energies associated with the positive and negative components of the principal strains, respectively. In Eq. 5, $\epsilon_1, \epsilon_2, \epsilon_3$ are the principal strains, λ is the Lamé's constant and μ is the shear modulus. The operators $\langle \cdot \rangle_{\pm}$ are defined as $\langle x \rangle_{\pm} = (x \pm |x|) / 2$.

As can be observed from Eqs. 4 and 5, degradation due to damage in this model is only associated with positive principal strains ($\langle \cdot \rangle_+$). Under the action of compressive strains, stresses arising due to the contact of cracked surfaces are considered. The stress tensor is obtained from Eqs. 4 and 5 as

$$\underline{\underline{\sigma}} = \frac{\partial \psi}{\partial \underline{\underline{\epsilon}}} = [(1-c)^2 + k] \frac{\partial \psi_0^+}{\partial \underline{\underline{\epsilon}}} + \frac{\partial \psi_0^-}{\partial \underline{\underline{\epsilon}}} = [(1-c)^2 + k] \underline{\underline{\sigma}}_0^+ - \underline{\underline{\sigma}}_0^- \quad (6a)$$

$$\underline{\underline{\sigma}}_0^{\pm} = \sum_{a=1}^3 [\lambda \langle \epsilon_1 + \epsilon_2 + \epsilon_3 \rangle_{\pm} + 2\mu \langle \epsilon_a \rangle_{\pm}] \underline{n}_a \otimes \underline{n}_a \quad (6b)$$

where $\underline{n}_a$ are the eigen vectors of the strain tensor $\underline{\underline{\epsilon}}$.

The dissipative power in Eq. 3, is described by

$$\dot{E}_D = \int_{\Omega} g_c \dot{\gamma} d\Omega \quad (7)$$

where g_c is a parameter related to the energy release rate and

$$\gamma = c^2 / 2l + l |\nabla c|^2 / 2. \quad (8)$$

To [avoid crack healing](#), i.e.

$$\dot{\gamma}_l(c) = \int_{\Omega} \frac{\partial \gamma}{\partial c} \dot{c} d\Omega \geq 0 \quad (9)$$

the following has been incorporated in the model: (i) appropriate choice of free energy to maintain non-negative $\partial \gamma / \partial c$ and (ii) penalty type constraint on Eq. 7 to enforce $\dot{c} \geq 0$.

Both the rate independent and dependent versions of the fracture model, satisfying the above-stated constraints, are provided in [42, 43]. In the present work, the rate dependent form has been chosen and involves the following coupled system of equations:

$$\nabla \cdot \left([(1-c)^2 + k] \underline{\underline{\sigma_0^+}} - \underline{\underline{\sigma_0^-}} \right) = 0 \quad (10a)$$

$$l\Delta c - \beta = 0 \quad (10b)$$

$$\dot{c} - \frac{1}{\eta} \left\langle \beta + 2(1-c) \frac{\psi_0^+}{g_c} - \frac{c}{l} \right\rangle_+ = 0 \quad (10c)$$

where η is a viscosity parameter. The rate independent limit can be approached as $\eta \rightarrow 0$. To solve the above equations using the Finite Element Method (FEM), they are expressed in weak form as follows:

$$\int_{\Omega} \nabla \delta \underline{u} \cdot \left([(1-c)^2 + k] \underline{\underline{\sigma_0^+}} - \underline{\underline{\sigma_0^-}} \right) d\Omega - \int_{\Gamma} \delta \underline{u} \cdot \underline{t} d\Gamma = 0 \quad (11a)$$

$$\int_{\Omega} \nabla \delta \beta \cdot l \nabla c d\Omega + \int_{\Omega} \delta \beta \beta d\Omega - \int_{\Gamma} \delta \beta l \nabla c \cdot \underline{n} d\Gamma = 0 \quad (11b)$$

$$\int_{\Omega} \delta c \left(\dot{c} - \frac{1}{\eta} \left\langle \beta + 2(1-c) \frac{\psi_0^+}{g_c} - \frac{c}{l} \right\rangle_+ \right) d\Omega = 0 \quad (11c)$$

where $\delta \underline{u}$, $\delta \beta$ and δc are the test functions. The weak form in Eq. 11 is implemented in Idaho National Laboratory's mesoscale MARMOT code based on the MOOSE framework [65] and numerically integrated using the backward Euler scheme.

2.1. Example 1

A 1d strain-controlled problem is considered to explore the behavior of damage evolution obtained from the rate dependent formulation. A cyclic strain, shown in Fig. 2(a), is applied with a strain rate of 1/s. The [contribution of the](#) interfacial terms in Eqs. 10b and 10c is ignored. The parameters used in this simulation are shown in Table 1.

The evolution of stress and damage is shown in Fig. 2(b) and 2(c), respectively. As can be observed from Fig. 2(b), elastic unloading with a damaged stiffness occurs after strain reversals and corroborates with other type of brittle fracture models. The evolution of damage tends to saturate once $c > 0.95$ and is shown in Fig. 2(c).

Table 1: The properties used to perform 1-d simulation.

E (GPa)	g_c (GPa-mm)	l (mm)	η (s/mm)	k (GPa)
210	0.001	0.01	10^{-4}	10^{-6}

Figure 2: The evolution of stress and damage in a 1d cyclically strained problem. (a) Cyclic strain with time; (b) Stress-strain evolution; (c) Stress and damage evolution with time.

The influence of strain rate and viscosity parameter, η , on the damage behavior is shown in Fig. 3. At higher values of η , the stress-strain evolution varies significantly with strain rate. However as $\eta \rightarrow 0$, a strain rate independent behavior can be achieved as shown in Fig. 3.

Figure 3: The effect of viscosity and applied strain rate on the 1d stress-strain behavior.

2.2. Example 2

The single edge notch tension (SENT) specimen shown in Fig. 4(a) is used to demonstrate the workability of the method. The properties used to represent the rate independent sharp crack propagation are shown in Table 2.

Table 2: The properties used to perform phase-field based FE simulation of SENT specimen.

E (GPa)	ν	g_c (GPa-mm)	l (mm)	η (s/mm)	k (GPa)
207	0.3	0.0027	0.0075	10^{-4}	10^{-6}

Figure 4: Simulation of brittle Mode I crack propagation in single edge notch (SENT) specimen using phase-field based fracture model: (a) Specimen geometry and boundary conditions. The displacements u and v are along the directions X and Y respectively; (b) Final configuration; (c) Stress-Strain along the loading direction; (d) Variation of damage variable, c , along line A-B shown in (b).

Based on the length parameter (l), a uniform mesh size $h = 0.0025 \text{ mm}$ can provide a mesh independent solution [42, 43] and is used to discretize the FE model. The final configuration of the specimen and the corresponding stress-strain curve is shown in Figs. 4(b) and 4(c), respectively. As can be observed from Fig. 4(c), the model is able to replicate the brittle fracture behavior, characterized by an immediate unloading beyond a critical load. The variation of the phase-field variable, c , along line A-B on the crack (Fig. 4(b)) is shown in Fig. 4(d) and a comparison between the thickness of the damaged zone and mesh size is also provided.

These examples suggest that the model can capture the rate independent brittle crack propagation behavior satisfactorily. However it is important to determine how the model predictions depend on the mesh size (h), viscosity parameter (η) and crack diffuse width (l). Hence sensitivity studies are performed in the following sub-sections to investigate these dependencies. Further, the difference between the energy release rate (G) used in LEFM and

g_c in the phase field model is established, followed by a study to investigate the sensitivity of fracture stress and energy to g_c .

2.3. Mesh size sensitivity of the fracture model

As stated in [42, 43], the mesh independent behavior of the model is guaranteed only when the interface is sufficiently resolved and the mesh size, h , satisfies $h < l/2$. To verify this behavior, fracture simulations of the SENT specimen are performed using $h = 0.01, 0.005, 0.0037, 0.0025$ and 0.00125 mm for $l = 0.0075$ mm and $\eta = 10^{-3}$ s/mm. The stress-strain curves are compared in Fig. 5(a). The variation of σ_{max} with h is shown in Fig. 5(b). As can be observed from the figure, σ_{max} approaches mesh independency with reduction in h . At $2h/l = 1/3$ and $2/3$, the solutions are completely mesh independent. However, at $2h/l \approx 0.99$, σ_{max} is still observed to be dependent on h . Hence, based on this numerical study, $h = l/3$ can be considered to be an appropriate mesh size to obtain a mesh independent solution.

Figure 5: The effect of mesh size, h , on the fracture behavior obtained from a SENT specimen: (a) Stress-strain evolution; (b) Variation of maximum stress (σ_{max}) with non-dimensionalized h . The parameters used in all the simulations are as follows: $l = 0.0075$ mm, $\eta = 10^{-3}$ s/mm.

2.4. Sensitivity of the brittle fracture behavior to the viscosity parameter

In the phase-field model, the viscosity parameter (η) is used to improve the convergence characteristics by regularizing the fracture behavior through additional dissipation. However, such artificial dissipation can have a strong influence on the predicted fracture properties. For instance, while the use of higher η values allows larger displacement increments, it increases the fracture stress and energy values. To evaluate this influence, Mode-I crack propagation in the SENT specimen described previously is simulated using different η values but the same $l = 0.0075$ mm and $g_c = 2.7$ MPa-mm. A mesh size of 0.0025 mm is used in all the simulations. The stress-strain curves are shown in Fig. 6(a). As can be observed from the figure, though higher viscosities smoothens the unloading behavior, they increase the maximum stress and dissipated energy significantly. A convergence to rate independency can be observed in Fig. 6(b) and 6(c) with decreasing viscosity. Hence, the viscosity parameter needs to be chosen judiciously to obtain computational speed-up in conjunction with a rate independent

solution. The results indicate that a value of η between 10^{-3} and 10^{-4} is able to provide near rate-independent behavior with acceptable computational performance.

Figure 6: Sensitivity of fracture behavior on viscosity (η) obtained from fracture simulations of SENT specimens: (a) Stress-strain along loading direction; (b) Variation of σ_{max} ; (c) Variation of fracture energy calculated from the area under the curves shown in (a).

2.5. Sensitivity of the brittle fracture behavior to the characteristic length parameter

The characteristic length parameter (l) controls the size of the damage region and tends to a sharp crack as $l \rightarrow 0$. Though the use of large l values can cause significant deviation in the fracture properties, small l values require a small mesh size. Thus the minimum possible size of l is determined by the size of the FE problem and computational feasibility. Hence, investigating the influence of l on the brittle fracture behavior and properties is necessary, and is performed by simulating crack propagation in the SENT specimen using different l values but the same $\eta = 10^{-4}$ s/mm and $g_c = 1$ MPa-mm. The simulations are performed with the h -adaptivity feature in MOOSE [65] in which the maximum mesh size (h_{max}) at crack tip is controlled such that $h_{max} = l/3$. In Fig. 7, the automatic mesh adaptivity with the propagating crack is shown.

Figure 7: Adaptive mesh refinement with crack propagation at different stress-strain instances for $l = 0.004$ mm: (a) $\sigma = 276$ MPa, $\epsilon = 0.0033642$; (b) $\sigma = 152$ MPa, $\epsilon = 0.0033665$.

The stress-strain curves for different l values are compared in Fig. 8(a). Since the allowable size of the diffused damage zone increases with l , the stress-strain evolution shows

larger non-linearity prior to unloading for higher values of l . The maximum stress and fracture energy also reduces with increasing l as seen in Fig. 8(b) and 8(c), respectively.

Figure 8: Sensitivity of fracture behavior on l obtained from fracture simulations of SENT specimen: (a) Stress-strain along loading direction; (b) Variation of σ_{max} ; (c) Variation of fracture energy calculated from the area under the curves shown in (a).

As can be observed from the figures, the fracture stress/energy values tend to saturate as the l value is continuously decreased and the model converges towards the sharp crack limit. Choice of the optimal value for l will depend on the dimension of the domain being represented and the smallest element size chosen to obtain a desired computational cost.

2.6. The relationship between energy release rate (G) and g_c

In the phase-field based fracture model, the dissipative power is related to the crack growth rate through the parameter g_c shown in Eq. 7. This parameter is similar to the energy release rate (G) defined as

$$G = -\frac{\partial(U - W)}{\partial A} \quad (12)$$

in LEFM, where U is the strain energy, W is the external work and A is the crack area. Unstable crack propagation in LEFM is considered to happen when a critical energy release rate, G_c , is exceeded, i.e. $G \geq G_c$. Brittle fracture is characterized by a flat G -curve ($G = G_c$), which implies that for rate independency and in the sharp crack limit, g_c should be equal to G_c .

To verify this observation, FE simulation of the SENT specimen shown in subsection 2.2 is performed in ABAQUS [66]. G at every time increment is evaluated from the Mode-I J -integral calculated at the tip of the stationary crack and its evolution with the applied stress is shown in Fig. 9(a). Based on a prescribed value of $G_c = 2.7$ MPa-mm, the applied stress at onset of unstable crack propagation can be obtained and is shown in 9(a). Phase-field based simulation of the SENT specimen is subsequently performed in which $g_c = G_c = 2.7$ MPa-mm is considered. The stress at unstable failure from the phase-field simulation is then compared with the failure stress obtained using the J -integral of the stationary crack and is shown in 9(b). As can be observed from the figure, unstable crack propagation in the phase-field based fracture simulation occurs at a larger stress than that predicted by LEFM. A similar behavior has been reported in [47] where comparisons have been made

with an analytical solution. From this comparison it can be concluded that LEFM G_c values obtained from experiments or lower length scale simulations are not directly usable as the parameter g_c in the phase-field based fracture model and calibration is necessary.

Figure 9: Comparison of critical energy release rate (G_c) for brittle fracture and g_c used in phase-field based fracture model: (a) Evolution of G with stress; (b) Stress at unstable crack propagation for $G_c = 2.7 \text{ MPa-mm}$ and from phase-field based fracture simulation for $g_c = 2.7 \text{ MPa-mm}$ indicating that G_c values cannot be directly used as g_c in the phase-field fracture model.

2.7. Sensitivity of the brittle fracture behavior to the energy release rate type parameter g_c

Phase-field based fracture simulations of the SENT specimen are performed using $l = 0.0075 \text{ mm}$, $\eta = 10^{-4} \text{ s/mm}$ and 3 different g_c values: 0.5, 1 and 2 MPa-mm. The stress-strain evolutions are shown in Fig. 10(a). With larger values of g_c , both the fracture stress and energy increases, as can be observed from the figure. The variation of fracture stress (σ_{max}) with g_c follows $\sigma_{max} \propto \sqrt{g_c}$, as can be observed from the fit in Fig. 10(b). This corroborates the dependence of fracture stress on the critical energy release rate, G_c , in Mode-I linear elastic brittle fracture: $K_{IC} = \sigma_{max} \sqrt{W} f(a/W) = \sqrt{G_c E}$, where K_{IC} , a , W and E are the fracture toughness, crack length, specimen width and Young's modulus, respectively. A sharp unloading in brittle crack propagation implies that the fracture energy is linearly dependent on g_c and is obtained from the fit shown in 10(c). The slope of the linear fit in Fig. 10(c) depends on the geometry of the fracture specimen. This relationship is exploited in sub-section 2.8 to investigate the length-scale invariance of the g_c parameter similar to G_c in LEFM.

Figure 10: Sensitivity of fracture behavior on g_c obtained from fracture simulations of SENT specimens: (a) Stress-strain along loading direction; (b) Variation of σ_{max} ; (c) Variation of fracture energy calculated from the area under the curves shown in (a).

2.8. Transferability of the g_c parameter across different scales for brittle fracture

The length scale of RVEs considered at the microstructural scale is typically much larger than the atomistic scale. Hence, due to the constraint on the mesh size, the minimum l parameter achievable in the microstructure scale fracture analyses is much larger than that used in calibration of g_c from atomistic simulations. Since in brittle materials, crack propagation is not associated with additional crack-tip plastic dissipation, the g_c parameter should be constant irrespective of the length scale.

To establish this, a symmetric center crack problem is considered using two similar geometries, but where one is hundred times larger than the other. The l parameter and mesh size is also scaled accordingly, while the g_c parameter is kept fixed. Very low viscosity values are used in both the cases to ensure rate independent behavior. The stress-strain behavior for both the cases is shown in Fig. 11. Identical $\sigma\sqrt{W}$ can be obtained for both the geometries as seen in Fig. 11(b), which in LEFM implies that

$$K_{IC} = K_{IC-2X} \quad \text{since} \quad K = \sigma\sqrt{W}f(a/W) \quad (13)$$

where K_{IC} and K_{IC-2X} are the fracture toughnesss of the unscaled and scaled geometries, respectively. Hence, under rate independency and sharp crack limit, the fracture toughness and energy release rate is unaltered by scaling the geometry, mesh and length scale parameter. Thus it can be concluded that the g_c parameter used in the phase-field model for brittle fracture is transferable between different length scales as long as the minimum mesh size resolves the defect geometry appropriately.

Figure 11: Comparison of: (a) Stress-strain evolution, and (b) $\sigma\sqrt{W} - \epsilon\sqrt{W}$ between the un-scaled and scaled symmetric center crack geometries.

3. Case Study: Intergranular brittle fracture in UO_2

The porosity dependent intergranular brittle fracture in UO_2 is considered to demonstrate the capability of using atomistically informed parameters in the phase field fracture model. From MD based fracture simulations on bicrystals with different grain boundary structures, it is observed that the $\langle 110 \rangle$ symmetrical tilt $\Sigma 3$ grain boundary exhibits brittle failure [67]. Based on this observation and to simplify the model, it is assumed that all the grain boundaries at the microstructural scale have a $\Sigma 3$ structure and the phase-field parameter, g_c , is calibrated from the corresponding MD simulation (sub-section 3.1). Subsequently, phase-field based simulations of the microstructure with varying porosities are performed to obtain the porosity dependent fracture strength and the predictions are compared with experiments (sub-section 3.2).

3.1. Calibration of the grain boundary fracture parameters

In the MD simulations, a sensitivity study with nine different inter-atomic potentials was performed to obtain the energy release rate for intergranular fracture in UO_2 , and the details are provided in [67]. A schematic of the simulation set-up can be seen in Fig. 12(a). For the MD simulations periodic boundary conditions are applied on the x-faces, where the top and the bottom halves of the simulation cell represent each grain. The two grains are symmetrically tilted with respect to each other about the $\langle 110 \rangle$ axis by about 71° , resulting in two $\langle 110 \rangle$ symmetrical tilt $\Sigma 3$ grain boundaries due to the periodicity, one in the middle and others at the border (top and bottom). The system dimensions are $30.5 \times 36.0 \times 3.2$ nm, with an elliptical hole of size 8×2 nm along the grain boundary in the middle. The loading is applied by adjusting the y coordinate of each atom by 10^{-4} for every 1 ps, corresponding to a nominal engineering strain rate of $10^8/\text{s}$. For the $\Sigma 3$ grain boundary structure, Mode-I brittle fracture is observed as shown in Fig. 12(b). To evaluate the atomistic stresses, the Virial stress formulation is utilized to obtain the stress-strain curve. The nominal stress is represented by the average of the atomistic stresses over the entire volume.

Figure 12: (a) The simulation cell used in MD.(b) Final configuration of the simulation cell.

An identical RVE is considered in the phase-field simulations to calibrate the fracture parameters and is shown in Fig. 13(a). Symmetry boundary condition is applied to the RVE as opposed to periodicity in MD. A numerical sensitivity study is performed where the g_c value is modified and the stress-strain curves from the phase-field based plane stress FE simulations of the RVE are compared with the MD results obtained in [67] using the Yakub potential. From the MD simulation of fracture of the $\Sigma 3$ grain boundary, atomic bond-breaking is observed approximately at a separation distance of 1 nm. Based on this observation, a length scale parameter (l) value of 1 nm is considered in the phase-field simulations. Furthermore, the calibration of the phase-field fracture model parameters is performed assuming rate-independency and hence a viscosity parameter (η) value of 10^{-4} nm/s is considered. After fixing the l and η values, phase-field fracture simulations are performed for different values of g_c and a good agreement is obtained for a value of 0.002 MPa-mm. A comparison of the stress-strain between MD and phase-field for $g_c = 0.002$ MPa-mm is shown in Fig. 13(b). The final configuration of the volume element is shown in Fig. 13(c).

Figure 13: (a) Schematic of the RVE consistent with MD used to calibrate the g_c parameter. (b) Comparison of the stress-strain evolution between the phase-field based plane stress FEM and MD simulation. (c) Final configuration of the volume element.

3.2. Phase-field based intergranular fracture simulation

A numerical study is performed to investigate the impact of porosity on the fracture strength in UO_2 . An average grain size of $8 \mu\text{m}$, which has been typically observed in experiments, is considered. The porosity is varied from 2-5% with a uniform pore diameter of $1 \mu\text{m}$ and the pores are randomly distributed on the grain boundaries. The pores act as crack initiators, and hence to spatially resolve the stress concentrations a length parameter $l = 0.1 \mu\text{m}$ is used. To enforce intergranular crack propagation, the calibrated g_c value of $0.002 \text{ MPa}\cdot\text{mm}$ is used for the grain boundaries while a higher g_c value of $0.01 \text{ MPa}\cdot\text{mm}$ is used for the grain interiors. A uniform Young's modulus, $E = 385 \text{ GPa}$, and Poisson's ratio, $\nu = 0.23$, typical for UO_2 [68] are used in all the simulations.

3.2.1. Effect of randomness of microstructure

A RVE size of $40 \mu\text{m} \times 40 \mu\text{m}$ with ~ 32 grains is considered. Three different random microstructures are generated and are subjected to the boundary conditions shown in Fig. 14. One of the microstructure is displaced along the y-direction rather than the x-direction as shown in Fig. 14 in order to consider any anisotropy effects due to the pore distribution in the microstructure. The fractured configuration of a microstructure and a comparison of the stress-strain evolution are shown in Fig. 15(a) and 15(b), respectively. The variations in the stress-strain evolution observed in Fig. 15(b) suggest that the size of the RVE and the number of grains are reasonable for this study.

Figure 14: Random microstructure of size $40 \mu\text{m} \times 40 \mu\text{m}$ with ~ 32 grains of average grain size $8 \mu\text{m}$ and porosity 2% with randomly distributed pores with a uniform pore diameter of $1 \mu\text{m}$. Symmetric boundary conditions, as shown in the figure, are used to perform the phase-field based fracture simulations.

Figure 15: (a) Final configuration. (b) Stress-strain evolution of random microstructures loaded along X or Y directions. M1, M2 and M3 represents the 3 different microstructures considered.

3.2.2. Effect of strain ratio

One of the microstructures is subjected to different strain ratios and the stress-strain evolution is shown in Fig. 16. The cracked configuration for $\epsilon_2/\epsilon_1 = 0.7$ and $\epsilon_2/\epsilon_1 = 1$ is shown in Fig. 17. A change in crack path due to a difference in strain ratio is evident from the figure.

Figure 16: Comparison of stress-strain evolution along the primary loading direction for different strain ratios (ϵ_2/ϵ_1).

Figure 17: Final configuration for different macroscopic strain ratios: (a) $\epsilon_y/\epsilon_x = 0.7$ (b) $\epsilon_y/\epsilon_x = 1$.

For porosity dependent intergranular brittle fracture, the probable crack initiation sites are at the edge of grain-boundary pores having maximum energy release rate. For uniaxial loading, these regions are expected on grain boundaries aligned perpendicular to the loading direction. In the phase-field simulations, a similar behavior is observed and is elucidated for the uniaxial loading case where displacements are applied on the right face along the x-direction (Fig. 14). Some of the pore-regions on grain boundaries are shown in Fig. 18(a) and their orientations with respect to the loading direction are as follows: A $\approx 16^\circ$, B $\approx 8^\circ$, C $\approx 23^\circ$, D $\approx 8^\circ$, E $\approx 75^\circ$ and F $\approx 85^\circ$. For this loading scenario, the grain boundary regions A, B, C and D are favorably aligned for crack initiation compared to E and F. Thus, a higher value of damage parameter can be observed in these regions (Fig. 18(b)). Though regions B or D have lower deviations from the normal to the loading direction than A, the effect of multiple pores at grain-boundary region A cause crack initiation in this region. Hence, the spatial distribution of pores also have a strongly influence on the location of crack initiation, even for the almost homogeneous distribution considered in this work. The stress-strain state corresponding to the configuration in Fig. 18(b) is shown as (i) in Fig 18(g).

Once the micro-crack is initiated it propagates in the top and bottom directions as shown in Fig. 18(c). A micro-crack is also initiated at the edge of the second pore in region A

that merge with the propagating micro-crack from the first pore (Fig. 18(c)). A continuous micro-crack propagation on top of region A is visible in Fig. 18(d) owing to the favorable orientation of the grain boundaries with respect to the loading direction. At the bottom of region A, crack-bend followed by crack-arrest is observed and is due to the unfavorable orientation of the grain boundaries (Fig. 18(d)). Subsequently, micro-crack initiation at D happens (Fig. 18(e)) that propagates and merges with the arrested micro-crack (Fig. 18(f)) leading to the eventual failure of the microstructure (Fig. 15(a)).

As the loading ratio is modified, the change in the driver for propagation alters the crack path. In the loading scenario $\epsilon_2/\epsilon_1 = 0.7$, micro-crack initiation occurs at the same region (A) as the uniaxial loading. Due to the favorable orientation of grain boundaries at the top of region A, an unobstructed propagation is also observed under this loading case. However, branching of the micro-crack occurs at the bottom of region A that is different from the uniaxial loading case and shown in Fig. 19(a). This difference is due to the contribution of strain component along the y-axis to the driver for crack growth. The overall crack propagation is still governed by the strain component along the x-axis and is shown in Fig. 19(b).

In the biaxial loading condition, all the edges of grain boundary pores have equal probability to initiate a micro-crack since there are two equal maximum principal strain components. Thus, under this loading condition micro-crack initiation is governed by the small variations in the strain-field caused by the spatial distribution of pores. For the microstructure utilized here, the region of micro-crack initiation shifts to F and is shown in Fig. 20(a). As the micro-crack is formed, its propagation is driven by the strain-field at its tip. Hence, the crack is aligned more closely to the x-axis and can be seen in Fig. 20(b).

Figure 18: (a) Initial microstructure. (b) Micro-crack initiation in the weakest region in the microstructure with the legend for damage at right ($c=0$ to 1). (c) Micro-crack initiation at the edge of second pore at A and merging. (d) Micro-crack propagation on top and arrest at the bottom of region A due to favorable and unfavorable orientation of grain boundaries, respectively. (e) Micro-crack initiation at another region D. (f) Merging and propagation of micro-cracks to cause final failure. (g) Macroscopic stress-strain states (i) to (iv) associated with configurations shown in sub-figures 18(b) to 18(e), respectively.

Figure 19: Evolution of micro-crack under strain ratio $\epsilon_2/\epsilon_1=0.7$. (a) Branching is observed after arrest that is different from the propagation mechanism for uniaxial loading 18(f). (b) The crack path in the bottom of region A is significantly influenced by the strain component along y-axis due to the lack of favorably oriented grain boundaries. However, the effective crack path is still governed by the strain component along x-axis.

Figure 20: Evolution of micro-crack under biaxial loading. (a) Micro-crack initiation in region F. (b) Propagation due to the strain field at the tip of the micro-crack.

3.2.3. Effect of porosity

The porosity in one of the microstructure is increased from 2-5% and the stress-strain evolution is compared in Fig. 22. For the same pore-size the number of grain boundary pores increases with porosity, which increase the probability of crack initiation at a lower stress-level and hence lower the fracture strength. A microstructure with a porosity of 4% is shown in Fig. 21(a). As can be seen from the figure, the grain boundaries are significantly more porous than the microstructure with porosity of 2% (Fig. 14). Moreover, an increase in the number of pores can elevate the stress/strain concentration at the edges of grain boundary pores, which can increase the damage in grain boundaries and decrease the fracture strength. The crack path in the microstructure with a porosity of 4% is shown in Fig. 21(b) where the propagation is dominated by the linkage of micro-cracks initiated at the edge of favorably

oriented grain boundary pores. Hence, the crack propagation behavior is largely controlled by initiation for microstructures with higher porosities. The decrease in the effective elastic modulus and fracture stress with increase in porosity is shown in Fig. 22.

Figure 21: (a) Microstructure with a porosity of 4% and pore size $1 \mu m$. (b) Crack path due to uniaxial displacement controlled load.

Figure 22: Comparison of stress-strain evolution along the primary loading direction for different porosities.

The porosity dependent fracture strength and Young's modulus is shown in Fig. 23. A linear fit of the elastic modulus provides $E = E_0(A - Bp)$ where $A = 1.0$, $B=4.0$ and p is the porosity. Similar linear relationship with a lower value of $B=2.32$ has been obtained in [69] using the ultrasonic technique. The variation of fracture stress is fitted with a power-law equation $\sigma_f = \sigma_0 p^{-m}$ where $\sigma_0 = 99.4$ MPa and $m = 0.453$. An exponential functional form obtained from biaxial flexure test has been reported in [70] describing the porosity, average pore and grain size effect on fracture stress. A comparison with the present model by substituting the average grain and pore size of $8 \mu m$ and $1 \mu m$, respectively, in their equation is shown in Fig. 23(b). From the figure it can be observed that the present model overestimates the experimental values by a factor of two-to-three and this difference can be due to the following:

1. The microstructures were not well controlled in the experiments from where the empirical equation has been considered [70]. The variation in the microstructure can impact

the fracture strength and consequently the empirical fit with which the present model has been compared. Hence, in order to perform a rigorous validation of the present model, detailed microstructural information on distribution of defect morphologies and their influence on fracture mechanism is necessary.

2. From fractography experiments at room temperature [70, 71], intergranular fracture was found to be the dominant mechanism though limited transgranular fracture was also observed. The incorporation of transgranular fracture can modify crack path and consequently the predicted strength [11]. Though the phase-field model is able to handle both inter and transgranular micro-crack propagation, the later has been neglected due to the lack of comprehensive experimental information at the microstructure scale.
3. In the simulations only a single grain boundary type has been considered to evaluate the phase-field model parameters. The consideration of other grain boundary types may provide more realistic results.
4. A 2-D approximation of the real microstructure can also affect the fracture stress and energy values obtained from the phase-field simulations. A 3D cubic simulation cell for the same porosity, pore and grain size will introduce more defect on grain boundaries, thus increasing the possibility of earlier crack initiation and causing a lower fracture stress. The workability of this method for complicated 3D crack propagation has been demonstrated in [42, 43]. However, the 3D simulations of these microstructures with uniform mesh have significantly large computational overhead, which restricts the present study to 2D simulations. Mesh adaptivity can reduce the computational bottleneck to perform 3D simulations and is currently being looked into.
5. In the MD simulations, a perfect lattice and a defect free GB (besides the elliptical flaw) has been assumed. However, consideration of atomistic-scale defects can significantly lower the calibrated g_c values and reduce the fracture stress obtained from the phase-field simulations.

Figure 23: Variation of: (a) Effective elastic modulus, and (b) Fracture stress with porosity. The experimental fit in Fig. (b) is obtained from Oguma et.al. [70].

4. Conclusion

In this work, a hierarchical multi-scale approach has been pursued to develop microstructure sensitive brittle fracture model. Attempt has been made to address two important aspects of microstructure dependent modeling of fracture. The first aspect is to develop a method that can capture the propagation of the micro-cracks undergoing complex interactions in a representative domain and a phase-field based method has been utilized for this purpose. The mesh and rate independent nature of the phase-field model has been demonstrated through Mode-I crack propagation in a SENT specimen. Additionally, numerical sensitivity studies have been performed to obtain a quantitative understanding of the influence of model parameters on the fracture stress/energy. The second aspect of incorporating parameter values from lower length scale modeling has been accomplished by calibration of the phase-field model parameters from atomistic scale simulations. The transferability of the calibrated parameters has been established by ensuring that the same energy release rate is achieved at different scales for brittle fracture. Subsequently, the multi-scale approach has been demonstrated by obtaining porosity sensitive brittle fracture properties in UO_2 . Intergranular crack propagation simulations have been performed considering different porosities in representative microstructures. The variation of the elastic modulus and fracture stress with porosity has been then compared with experimental trends. From the comparisons it is evident that though this approach can provide quantitative prediction of fracture properties, it requires detailed microstructure characterization to have a better insight into the mechanisms, create realistic initial conditions and improve the validation.

5. Acknowledgment

This work was funded by the DOE Nuclear Energy Advanced Modeling and Simulation Program.

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