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

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A B S T R A C T

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, and grain boundaries. 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 multiaxial 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 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

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features explicitly and allow 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 evo-