A Phase-field Approach to Model Multi-axial and Microstructure Dependent Fracture in Nuclear Grade Graphite

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Abstract

The fracture behavior of nuclear grade graphites is strongly influenced by underlying microstructural features such as the character of filler particles, and the distribution of pores and voids. These microstructural features influence the crack nucleation and propagation behavior, resulting in quasi-brittle fracture with a tortuous crack path and significant scatter in measured bulk strength. This study uses a phase-field method to model the microstructural and multi-axial fracture in H-451, a historic variant of nuclear graphite that provides the basis for an idealized study on a legacy grade. The representative volume elements are constructed from randomly located pores with random size obtained from experimentally determined log-normal distribution. The representative volume elements are then subjected to simulated multi-axial loading, and a reasonable agreement of the resulting fracture stress with experiments is obtained. Quasi-brittle stress-strain evolution with a tortuous crack path is also observed from the simulations and is consistent with experimental results.

1. Introduction

Nuclear-grade graphites are candidate materials for neutron moderators, reflectors, and structural components in high-temperature gas-cooled reactors. An understanding of the manner by which these components might experience failure from large stresses caused by thermal and irradiation induced deformation during operation is critical to determining appropriate lifetime predictive capabilities and safety-based whole-core modeling. From fracture experiments of unirradiated graphite specimens, quasi-brittle fracture behavior with an associated tortuous crack path is predominantly observed [1,2]. Additionally, large scatter in measured fracture stress and toughness values is obtained for test coupons acquired from the same billet [3,4,5]. It is therefore necessary to develop accurate fracture models for nuclear-grade graphites that address these variabilities in order to optimally design nuclear grade graphite components long-term safe operation in modern reactors.

The nuclear grade graphite microstructure consists of filler particles surrounded by binder matrix and pores produced from the calcination and graphitization process [6]. Under multi-axial stress states, micro-cracks initiate from the pores and propagate through the matrix causing final failure. Hence, porosity and pore size has a significant influence on the failure process and is extensively used in weakest link theory based models to quantify the scatter of fracture strength [3,4]. Grain or particle filler size also influences the fracture behavior for small sized specimens due to the clear size effects on measured strength properties and was considered in fracture models for nuclear grade graphite [7].

Subsequently, more sophisticated models were developed to accurately capture the microstructural influence on the fracture behavior of graphites. For instance, the Weibull distribution function in conjunction with linear elastic fracture mechanics (LEFM) was used in the model developed by Batdorf [8] to capture the effect of multiaxial loading on the fracture strength. In a detailed graphite microstructure-specific model developed by Burchell [9,10], fracture initiation near the pores and propagation along rows of grains is considered to explain the observed statistical variations. A detailed review of probabilistic models of fracture applicable to nuclear grade graphites has been provided in [11]. Though these models have been fairly successful in predicting the scatter in fracture properties under multi-axial stress states, they fail to capture the experimentally observed complicated fracture path.

Over the years, several types of discrete element models (DEM) or lattice models have been developed to investigate brittle and quasi-brittle fracture behavior [12-15]. In these models, spring or beam elements with random properties are linked together based on some ordering typical to a microstructure. Through the progressive failure of these elements, the fracture behavior of a representative microstructural volume can be obtained. These models are able to capture micro-crack formation, growth, merge, and branch as observed in nuclear grade graphites. Specimen size effects, scatter in strength values and quasi-brittle fracture can also be addressed through these models. Though lattice models can capture complicated crack propagation, the random properties of the discrete elements are evaluated through a calibration process and may not have a direct correlation with the microstructure. Also, a discrete assumption of the continuous media at the length scale of the fracture models inappropriately handles the physical mechanisms.

To address the limitations existing in the above modeling techniques, a phase-field based fracture model is used in the present work. Phase-field based fracture models fall under the category of non-local diffused damage models where multi-axial constitutive relationships describe damage at material points [16]. Local diffused damage models, however, have been observed to be strongly mesh sensitive with regard to finite element method (FEM) [17], leading to the development of non-local approaches. In the phase-field model, both the damage variable and its gradient are solved simultaneously, thus removing the sensitivity of mesh on the fracture response. The incorporation of the gradient term introduces a length scale parameter and the sharp crack limit is approached, as this parameter tends to zero. **The phase-field approach has been shown to successfully capture complicated crack propagation under brittle [18-27] and elasto-plastic fracture [26-28].**

In the present work, the phase-field model proposed in [21] is utilized to capture the quasi-brittle fracture under multi-axial loading using properties of the legacy grade of H-451 graphite as the basis for the model system. Two-dimensional representative volume elements (RVEs) are constructed by randomly distributing pores with log-normal size distribution obtained from experiments. Though size and orientation distributions of filler and binder can have a measurable effect on the fracture behavior, they have been neglected in the present work. The quasi-brittle stress-strain response is the outcome solely from the presence of pores of varying size in an otherwise homogeneous matrix that cause micro-crack propagation and arrest. The multi-axial fracture strength obtained from the simulations is subsequently compared with published experimental results.

In this paper, Section 2 describes the phase-field fracture model followed by the details of the microstructure scale simulations in Section 3. Section 4 describes the simulation results and the experimental validation. A summary of research results concludes in Section 5.

2. Phase-field based fracture model

The phase-field model used in this work was proposed in [21], where the damaged region is represented by

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

and c is the damage variable such that $c \in [0,1]$, where 0 and 1 represents the undamaged and completely damaged states, respectively. In Eq. 1, l is the characteristic length parameter that controls the thickness of the damaged zone and the sharp crack limit is approached as $l \rightarrow 0$. Using the definition of the damage variable in Eq. 1, the damaged surface (Γ) can be represented by the integral equation

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

where Ω is the volume of the domain.

The power balance equation for brittle fracture is defined as

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

where E_E is the elastic strain energy, E_D is the energy dissipated due to damage, and P_E is the work done by externally applied tractions. The elastic strain energy is modified to incorporate the effects of damage and is defined as

$$\dot{E}_E = \frac{d}{dt} \int_{\Omega} \psi d\Omega \quad (4.a)$$

$$\psi = [(1-c)^2 + k] \psi_0^+ + \psi_0^- \quad (4.b)$$

where

$$\psi_0^{\pm} = \frac{\lambda}{2} \langle \varepsilon_1 + \varepsilon_2 + \varepsilon_3 \rangle_{\pm}^2 + \mu (\langle \varepsilon_1 \rangle_{\pm}^2 + \langle \varepsilon_2 \rangle_{\pm}^2 + \langle \varepsilon_3 \rangle_{\pm}^2) \quad (5)$$

and k is a small number that ensures positive definiteness of the system after a material point undergoes complete damage. In Eq. 5, λ is the Lamé's constant, μ is the shear modulus, ε_1 , ε_2 , and ε_3 are the principal strains and the operator $\langle x \rangle_{\pm}$ is $(x \pm |x|)/2$. The

definition of strain energy in Eq. 5 ensures that damage is prevented under pure compressive strain states. The stress is derived from Eqs. 4.b and 5 as

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

$$\underline{\sigma}_0^\pm = \sum_{a=1}^3 (\lambda \langle \varepsilon_1 + \varepsilon_2 + \varepsilon_3 \rangle_\pm + 2\mu \langle \varepsilon_a \rangle_\pm) \underline{n}_a \otimes \underline{n}_a \quad (6.b)$$

where $\underline{n}_a$ are the Eigen vectors of the strain tensor $\underline{\varepsilon}$. In Eq. 6.b, $\otimes$ is the outer product operation on the Eigen vectors.

The rate of energy dissipation due to damage evolution is defined as

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

where g_c is an energy release rate type parameter and γ is the damage surface obtained from Eq. 2 as

$$\gamma = \frac{c^2}{2l} + \frac{l}{2} |\nabla c|^2 \quad (8)$$

To prevent crack healing, a weak enforcement of $\dot{c} \geq 0$ in the power balance (Eq. 3) results in a rate dependent form of damage growth

$$\dot{c} = \frac{1}{\eta} \langle l \Delta c + 2(1 - c) \frac{\psi_0^+}{g_c} - \frac{c}{l} \rangle_+ \quad (9)$$

as shown in [21], where η is a viscosity parameter. Rate independent fracture response can be obtained as $\eta \rightarrow 0$. To simulate quasi-static fracture response, Eq. 9 is solved in conjunction with the stress equilibrium

$$\nabla \cdot [\{(1 - c)^2 + k\} \underline{\sigma}_0^+ - \underline{\sigma}_0^-] = 0 \quad (10)$$

The coupled partial differential equations are solved using FEM in the present work and the following weak forms are obtained

$$\int_{\Omega} \nabla \delta \underline{u} \cdot (\{(1 - c)^2 + k\} \underline{\sigma}_0^+ - \underline{\sigma}_0^-) d\Omega - \int_{\Gamma} \delta \underline{u} \cdot \underline{t} d\Gamma = 0 \quad (11.a)$$

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

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

where δu , $\delta \beta$, and $\delta \epsilon$ are the test functions. The weak forms (Eq. 11) are implemented in Idaho National Laboratory's open source FEM code Multiphysics Object Oriented Simulation Environment (MOOSE) [29]. The system of equations is solved monolithically using backward Euler implicit time integration. Instead of using a direct solver based on LU decomposition, the iterative pre-conditioned Jacobian free Newton Krylov method available in MOOSE is utilized. All the simulations are performed in parallel where the additive Schwarz method (ASM) is used to speed up the factorization of the preconditioner. Each of the distributed domains in the parallel environment for ASM is factorized directly using LU decomposition. A relative residual tolerance of 10^{-4} is used for the individual fields to determine convergence at every increment. If convergence is not achieved within the specified number of iterations, the time-step is halved and the system is re-solved for the current increment.

2.1 Demonstration of the phase-field model for brittle fracture

The workability of the phase-field model to capture brittle crack propagation is demonstrated using a single-edge notch tensile (SENT) specimen. The specimen and the corresponding dimensions are shown in Fig. 1(a). The specimen domain is discretized using the bilinear Lagrange finite element shape function. A gradient mesh is utilized such that the damage length-scale is resolved at the crack-tip and along the probable crack-propagation region. A coarser mesh is utilized in regions where material is expected to be undamaged. The properties used in the fracture simulation are tabulated in Table 1.

Table 1. The properties used to perform phase-field based FEM simulation of SENT specimen.

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

As the specimen is displaced on the top face, damage evolution occurs at the tip of the pre-existing crack. As the maximum damage exceeds approximately 0.9–0.95, onset of sharp crack nucleation occurs. The subsequent increase of applied displacements cause unstable crack propagation as seen from the rapid drop in stress in the stress-strain curve (Fig. 1[b]). Complete failure of the specimen could be simulated in 15 mins (wall-time) using 48 processors. The failed configuration is shown in Fig. 1(c). The distribution of damage along a material line A-B across the damage region (Fig. 1[c]) is shown in Fig. 1(d). As observed from Fig. 1(d), the damage curve follows an exponential function described in Eq. 1 with plateauing at the maximum value ($c=1$). The mesh size (h) used in the simulation is compared in Fig. 1(d) with the characteristic length parameter (l) in the damage zone. Consistent with [21], a mesh size $h < l/2$ is able to capture the gradient of damage accurately.

Fig. 1. Simulation of brittle Mode I crack propagation in single-edge notch tensile specimen using phase-field based fracture model: (a) specimen geometry and boundary conditions; (b) stress-strain along loading direction; (c) final configuration; (d) variation of c on along a material line A-B on the crack shown in (c).

This example shows that the phase-field model is able to capture brittle crack propagation behavior that has a linear stress-strain relationship until the fracture strength is exceeded, which is followed by a sharp unloading. The convergence towards a rate-independent sharp crack limit is strongly dependent on the parameters η and l . A detailed discussion that relates to this characteristic is provided in [25]. It is shown **numerically** in [25] that an l value that can resolve the minimum defect dimension in a fracture specimen or RVE is sufficient to provide sharp-crack brittle fracture response. **The influence of the length-scale parameter on crack nucleation has also been discussed analytically in [20, 22, 24].** In [25] the relationship between the g_c parameter used in the phase-field model and the energy release rate, G_c , in LEFM, is also explored. It is shown that though g_c follows the LEFM relationship as

$$g_c \propto \sigma^2 a / E \quad (12)$$

it slightly overestimates the fracture strength when compared to LEFM. In Eq. 12, a is the defect size and E is the adjusted Young's modulus. **Similar relationship has been obtained in [20, 22, 24] from the analytical solution of the damage field.**

3. Microstructure scale phase-field simulation of fracture in H-451

The fracture behavior of H-451 and nuclear-grade graphites in general is affected by the porosity, pore size and shape distributions, filler and binder size, and shape and orientation distributions. In this particular work, the sole effect of pore size distribution is considered in order to evaluate a critical first-order multi-axial fracture response of H-451. The utilization of H-451 as the model system should be considered “idealized” in that the binder and filler matrix is considered as homogeneous and isotropic. The added complexity of these additional microstructural characteristics, which will provide a crucial basis for the differentiation in properties between existing candidate nuclear grades of graphite, will be added in subsequent refinements to the present model. For the pore-based model, the size of the randomly located pores in the two-dimensional RVEs is generated from the log-normal distribution reported in [10]. Also from [10], the aspect ratio of pores within the 50–90% cumulative probability is approximately 0.95. This result suggests that the pores are preferentially circular and has been considered to construct the RVEs. Fig. 2 shows a comparison of the experimentally obtained log-normal pore size distribution and the regenerated distribution from three different microstructural instantiations. A reasonable agreement can be observed from the figure emphasizing that the RVE size of $1 \text{ mm} \times 1 \text{ mm}$ considered in this work is large enough to capture the tail of the distribution (cumulative probability > 0.95).

Fig. 2. Comparison of distribution of pore radii between three representative volume elements. A bin size of $5 \mu\text{m}$ is used to plot the cumulative distribution function (CDF) for the three RVEs. The analytical function $\frac{1}{2} \left(1 + \text{erf} \left[\frac{\log(x) - \mu}{\sqrt{2}\sigma} \right] \right)$ with $\mu = 2.941$ and $\sigma = 0.703$ is obtained from [10].

A typical RVE for H-451 is shown in Fig. 3 in which a minimum geometrical pore radius of $20 \mu\text{m}$ is allowed. The restriction on the minimum pore size ensures that a reasonable FEM problem size is obtained while the effect of the smaller pores on the fracture behavior is still considered. Further, pore radii values between 1 and $20 \mu\text{m}$ are incorporated as effective porosity in a coarser grid with a cell size of $50 \mu\text{m} \times 50 \mu\text{m}$. An effective porosity (f_{eff}) is used to modify the elastic modulus in the coarser grid following $E_{\text{eff}} = (1 - f_{\text{eff}}) E$ and can affect the crack propagation behavior. This treatment prevents damage nucleation from the pores smaller than the geometric resolution, however, which can influence the simulated fracture behavior. Since the bigger pores have higher probability to initiate micro-cracks, explicit representation of pores with size that has

cumulative probability greater than 50% for H-451 (Fig. 2) can reduce the effect of this approximation. A homogenization approach with a porosity-dependent effective flow geometry, or g_c parameter, can address this issue.

The rectangular RVE domain is discretized with a uniform mesh size of $4\text{ }\mu\text{m}$. **The specimen domain is discretized using the bilinear Lagrange finite element shape function.** The pores are incorporated in the microstructure as regions with very low stiffness. Gradient-based mesh adaptivity available in MOOSE is performed to ensure that the pore geometry is sufficiently resolved in the initial microstructure. A length-scale parameter of $l = 10\text{ }\mu\text{m}$ is used to define the damage region. For the minimum geometric pore size allowed in the microstructure, the length scale parameter can ensure a near sharp-crack propagation behavior. To ensure a near rate-independent crack propagation, a viscosity parameter value of $10^{-3}\text{ }\mu\text{m/s}$ is considered based on the numerical studies in [25]. The other material properties are considered from [10] and shown in Table 2. The g_c parameter value is obtained by assuming that it is equal to the critical energy release rate, G_{IC} , and then converting the K_{IC} value reported in [10] to the equivalent G_{IC} value using $G_{IC} = K_{IC}^2/E$. This assumption can lead to slightly over predicted fracture stress as reported in [25].

Fig. 3. A typical representative volume element. The pores are represented as regions with very low stiffness. Gradient-based mesh adaptivity available in MOOSE is performed to generate the initial microstructure to ensure that the pore geometry is sufficiently resolved.

Table 2. Properties of H-451 from [10] utilized in the phase-field fracture simulations.

Young's Modulus (GPa)	Poisson's ratio	$g_c = G_{IC}$ (MPa- μm)	Porosity
7.6	0.18	10.68	0.2

The RVEs are then subjected to uniaxial and multi-axial displacement controlled load with symmetry boundary conditions on the left and bottom faces. Subsequently the effect of randomness in the microstructure and strain-ratios on the fracture strength and crack propagation behavior is compared. **All the simulations took approximately 5-7 hours to complete using 96 processors.**

4. Results and discussion

4.1 Pore dependent fracture behavior

The pore induced micro-crack initiation and growth as obtained from the phase-field simulations is explored using the RVE shown in Fig. 3. The RVE is displaced on the top face along the y-axis with a constant quasi-static rate while the right face is kept traction free. The resulting stress-strain behavior and the corresponding damaged configurations are shown in Figs. 4 and 5, respectively. Significant damage accumulation between pores in Regions I and II shown in Fig. 5(a), results in the onset of unloading depicted by point A in Fig. 4. Damage intensification remains confined within these regions shown in Fig. 5(b), which results in an observed recovery in strength values depicted by Point B in Fig. 4. As the RVE is progressively loaded, micro-cracks initiate and start propagating at other regions shown in Figs. 5(c) and (d), which cause continual unloading (Points C and D in Fig. 4) and the complete failure of the RVE shown in Fig. 5(e).

Fig. 4. The stress-strain response under uniaxial loading of the representative volume element shown in Fig. 3. The inset shows the magnified response at the onset of unloading.

Fig. 5. Damaged configurations of the representative volume element. (a)-(d) corresponds to points A-D shown in the inset of Fig. 4; (e) final configuration after complete failure. The legend in (e) depicts the damage variable, c .

4.2 Effect of randomness of the microstructure

The effect of randomness of the microstructure on the fracture behavior is investigated by comparing the stress-strain response between three different RVEs (shown in Fig. 2) with randomly located pores, and sizes randomly selected from the log-normal distribution. The stress-strain responses under uniaxial loading are compared in Fig. 6. For RVE 1 with loading along y (Case 1) and x (Case 2) and for RVE 3 with loading along y (Case 1), the stress-strain behavior and the fracture strengths are very similar. However, for RVE 2 with loading along y (Case 1), the quasi-brittle response is more prominent and the fracture strength is much lower than the other cases, as can be observed from the stress-strain response.

Fig. 7 shows the final configuration of the three RVEs. As can be seen from the figure, the maximum pore radius in RVE 2 is larger than those in the other RVEs. Thus, comparatively early softening due to micro-crack nucleation from the larger pores can be observed in RVE 2. However, the nucleated micro-cracks are frequently arrested at the smaller pores in RVE 2, which necessitates additional driving force for further propagation. Thus, despite having a less tortuous crack path than RVE 1 and 3, RVE 2 exhibits more quasi-brittle response.

Fig. 6. Comparison of the stress-strain between the three different representative volume elements labeled as RVE 1, 2, and 3. Case 1 and 2 represents two loading scenarios. In Case 1, the representative volume elements are pulled on the top face along the y -axis

and the right face is traction free, whereas in Case 2, the representative volume elements are pulled on the right face along the x-axis and the top face is traction free.

Fig. 7. Final damaged configuration of the three representative volume elements, loaded uniaxially on the top face along y direction. (a)-(c) represents RVE 1–3, respectively. The legend is shown in Fig. 5(e).

4.3 Effect of strain ratio

The effect of strain ratio on the fracture behavior is investigated by considering RVE 1. The top and right faces of the RVE are displaced with different displacement-rates to vary the applied strain ratio. The following loading cases are considered:

Case 1: Positive displacement along y-axis on the top face, traction free right face (uniaxial).

Case 2: Positive displacement along x-axis on the right face, traction free top face (uniaxial).

Case 3: Positive displacements along x and y axes on the right and top faces, respectively. The ratio of displacement rates is +1 (biaxial tensile).

Case 4: Positive y and negative x displacements on the top and right faces, respectively. The ratio of displacement rates along the directions is -1.

Case 5: Positive x and negative y displacements on the right and top faces, respectively. The ratio of displacement rates is -1.

Case 6: Positive x and negative y displacements on the right and top faces, respectively. The ratio of displacement rates between the x and y direction is -0.5.

Fig. 8 compares the stress-strain response between different loading ratios. Under tension-compression loading (Cases 4–6), the fracture strength along the tensile direction reduces as the ratio of tensile to compressive strains decreases. The reduction factor obtained from the simulation can be compared with analytical solution assuming a two-dimensional hole in an infinite media subjected to biaxial strains. A schematic of the geometry and loading is shown in Fig. 9. The stress state at Point A shown in Fig. 9 is related to the remote stresses S_1 and S_2 as

$$\sigma_{rr} = 0 \quad \sigma_{\theta\theta} = 3S_1 - S_2 \quad \text{and} \quad \sigma_{r\theta} = 0 \quad (13)$$

where

$$S_1 = [\lambda(1 + \alpha) + 2\mu]E_1 \quad (14.a)$$

$$S_2 = [\lambda(1 + \alpha) + 2\mu\alpha]E_1 \quad (14.b)$$

and α is the strain ratio E_2/E_1 . As can be observed from Eq. 9, damage growth and the onset of micro-crack initiation is directly dependent on the strain energy. Thus, the ratio of remote stress causing micro-crack initiation between the different loading cases can be obtained by equating the critical strain energy at Point A. Cases 5 and 6 are considered in order to compare the analytical solution of the ratios of failure stress and strain with microstructure scale simulations, since these two Cases experience onset of micro-crack initiation at the same location, as shown in Fig. 10(a). Substituting $\alpha = -1$ and -2 for Cases 5 and 6, respectively, the remote stresses can be expressed as $S_1 = 2\mu E_1$ and $S_2 = -2\mu E_1$ for Case 5, and $S_1 = (2\mu - \lambda)E_1$ and $S_2 = -(4\mu + \lambda)E_1$ for Case 6. The corresponding local circumferential stresses at Point A can be obtained using Eq. 13 as $\sigma_{\theta\theta} = 8\mu E_1$ and $(10\mu - 2\lambda) E_1$ for Cases 5 and 6, respectively. Since all the other stress components are zero at A, attaining the critical strain energy for micro-crack initiation implies that the circumferential stresses are identical. This renders a stress ratio of S_I (Case 5)/ S_I (Case 6) of 1.625 for the elasticity parameters used in this work. Comparing the stresses at Points A and B in the stress-strain curve shown in Fig. 10(b) a similar stress ratio of 1.64 is obtained from the simulations.

A comparison of the micro-crack propagation, between load Cases 5 and 6 is shown in Fig. 11. Though the onset of micro-crack initiation occurs at the same region for both the cases, the subsequent damage mechanism until final failure is drastically different as observed in Fig. 11. For load Case 5, the number of micro-crack initiations is fewer than in Case 6 and the micro-cracks propagate over longer distances causing final failure. For load Case 6, the final failure is caused by the initiation of a larger number of micro-cracks and their propagation over shorter distances. For all of the load cases, Fig. 12 shows the stress ratio at failure and is compared with values experimentally obtained for H-451 [10]. The figure indicates that the proposed approach can capture the shape of the failure surface reasonable well, although the scatter and average values are somewhat under-represented.

Fig. 8. Comparison of stress-strain evolution for RVE 1 between the load cases described in Section 4.3.

Fig. 9. Schematic of a circular hole in an infinite media subjected to remote biaxial strains E_1, E_2 . The remote stress S_1 for crack initiation at Point A is compared with the phase-field fracture simulations for different strain ratios.

(a)

(b)

Fig. 10. (a) Identical micro-crack initiation Region I in RVE 1 for load Cases 5 and 6 described in Section 4.3; (b) stress-strain along tensile direction at initiation, A for Case 5 and B for Case 6.

(a)

(b)

Fig. 11. Final damaged configuration of RVE 1 under: (a) load Case 4 and (b) load Case 6 described in Section 4.3.

Fig. 12. Comparison of traction components x-y at failure between phase-field model and experiments for the different loading scenarios,

5. Summary and Conclusions

The pore size dependent microstructure-scale fracture in nuclear grade graphite represented by an idealized version of H-451 was investigated using a phase-field based approach. The initial microstructure was generated using the experimentally obtained log-normal pore size distribution. A comparison of the pore radii used in the RVEs was made with experiments to confirm that a sufficiently large RVE size has been chosen to incorporate the tail of the distribution. Phase-field fracture simulations of different RVEs under uniaxial loading were performed to investigate the effect of microstructural variations on the stress strain response and the associated scatter. The simulations indicate that crack path tortuosity, quasi-brittle stress-strain behavior, and scatter in fracture stress could be obtained, which highlight the ability of this approach to model fracture in nuclear grade graphite. Further, multi-axial simulations were performed and the resulting fracture stress ratios were compared with experiments. The model is observed to represent the shape of the multi-axial fracture surface reasonably well, although the average fracture strength and the associated scatter were under predicted.

The phase-field model used in this study provides a viable pathway to link atomistic to engineering scale models to predict multi-axial fracture strength and the associated scatter in nuclear grade graphites. The results presented demonstrate the ability of the approach to accurately model fracture in nuclear grade graphite through explicit consideration of microstructural features. This modeling approach is also more predictive, since the changes in the microstructure and underlying mechanism can be incorporated in a physical manner rather than relying upon ad hoc changes in parameters. The additional complexity exhibited by graphite filler size and character, forming conditions, bulk isotropy, and pore/void distributions are all elements that can be added in subsequent models in order to provide higher resolution to different candidate grades being considered for deployment in nuclear structural applications.

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