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A stochastic XFEM model for the tensile strength prediction of heterogeneous graphite based on microstructural observations

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A B S T R A C T

A stochastic XFEM model based on microstructural observations has been developed to evaluate the tensile strength of NBG-18 nuclear graphite. The nuclear graphite consists of pitch matrix, filler particles, pores and micro-cracks. The numerical simulations are performed at two length scales due to large difference in average size of filler particles and pores. Both deterministic and stochastic approaches have been implemented. The study intends to illustrate the variation in tensile strength due to heterogeneities modeled stochastically. The properties of pitch matrix and filler particles are assumed to be known at the constituent level. The material models for both pitch and fillers are assumed to be linear elastic. The stochastic size and spatial distribution of the pores and filler particles has been modeled during the micro and macro analysis respectively. The strength of equivalent porous pitch matrix evaluated at micro level has been distributed stochastically in the elemental domain along with filler particles for macro analysis. The effect of micro-cracks has been incorporated indirectly by considering fracture plane in each filler particle. Tensile strength of nuclear graphite is obtained by performing the simulations at macro-level. Statistical parameters evaluated using numerical tensile strength data agree well with experimentally obtained statistical parameters available in the literature.

1. Introduction

Graphite is a key material for high temperature gas reactor (HTGR) and pebble bed modular reactor (PBMR). Graphite serves as moderator, reflector, core and core support structures [29]. Nuclear graphite is an efficient neutron moderator with low neutron absorption properties under the influence of fast neutron irradiation [54]. Depending upon the manufacturing process, behavior of nuclear graphite can be brittle or quasi-brittle [30]. A large scatter has been observed in the elastic and strength properties of NGB-18 grade nuclear graphite. It is polycrystalline in nature and possesses inherent heterogeneities such as coke particles (filler particles), micro-cracks and porosity lying in the pitch matrix [53]. NBG-18 nuclear grade graphite shows an effect of specimen volume on the tensile strength [50]. Starting experimental testing [18–20,22] provided the basic foundation to understand the material behavior of nuclear graphite. The strength prediction models of nuclear graphite are initially classified into deterministic models [37,42,49] and probabilistic models [10]. From Ref. [48], it was concluded that Weibull model was inferior as compared to fracture mechanics and Rose/Trucker model [37]. Considering the microstructural aspects of the nuclear graphite strength, Burchell fracture model [7] is found quite successful for several nuclear grades. Later, various FEM based model were presented for predicting the reliability of nuclear graphite components subjected to service conditions such as prestresses [33], irradiation damage [13,14,24] and fast neutron irradiation with radiolytic oxidation [47]. The limitations and issues related with the reliability of nuclear graphite components were listed by Ref. [43]. In order to improve the accuracy of strength prediction model for graphite components, various failure criteria [2,8,55,56] were proposed including multi-axial aspect with damage mechanics. Further, various FEM models based on X-ray tomography images [4,6] and micromechanics techniques [5,23] were presented for the evaluation of variation in bulk mechanical properties of nuclear graphite. The conservative failure prediction of NBG-18 were presented using weak link theory [16,17]. With the advancement of computational power, efficient multi-scale modeling approach has been proposed such as 3-D cellular

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automata model [52], site-bond lattice model [28] and lattice model [38] for the prediction of variation in the strength. Although, the documented work presented on numerical modeling provides an immense understanding of nuclear graphite behavior but numerical prediction for reliability and variation of strength is still missing. Thus, the present study intends to cover the statistical aspect of NBG-18 tensile strength through proposed stochastic XFEM model based on its available microstructural information [21].

NBG-18 nuclear grade graphite composed of heterogeneities such as filler particles (reinforced particles), pores, micro-cracks and pitch matrix. The prediction of scatter in strength of nuclear graphite is possible through stochastic modeling of the heterogeneities. The various FEM based stochastic models have been proposed which are categorized into possibilistic [15,35,25,51] and probabilistic [9,12,36,39,45] approaches. Various stochastic models in conjunction with probabilistic and possibilistic approaches have been proposed [32,40].

The main aim of this study is to predict the variation in tensile strength of NBG-18 nuclear graphite in terms of assumed properties of pitch matrix and coke filler particles. Thus, a probabilistic stochastic XFEM model has been proposed to account the effect of porosity and filler particles on the tensile strength of NBG-18 under plane stress condition. The probabilistic stochastic model (as the size/spatial distribution of heterogeneities) follows a specific probability function. The other input parameters such as fracture plane orientation are assigned to filler particles and porous pitch strength is assigned to macro analysis obtained from micro simulations. Based on the microstructural characterization of the NBG-18 nuclear grade graphite [21], the volume fraction of the pores and the filler particles have been taken as 14% and 25% respectively. Pore size is assumed to vary from 4 μm to 36 μm whereas the filler particles size varies from 200 μm to 600 μm with average size of 380 μm. The aspect ratio of both pores and filler particles is assumed as one. Material model for both pitch and fillers is assumed to be linear elastic with modulus degradation after threshold stress value. XFEM simulations have been performed at two different length scales. The analysis at smaller length scale (micro analysis) models stochastic size/spatial distribution of pores in the matrix material. The macro analysis models the domain with stochastic size/spatial distribution of filler particles (assigned with stochastic fracture plane orientation) in the equivalent porous pitch matrix (porous pitch strength obtained by micro analysis has been assigned stochastically). Numerical tensile strength data is obtained from the macro analysis. Statistical parameters evaluated using numerical tensile strength data are compared with experimental statistical parameters available in the literature [16]. Specifically, the objectives of the present work are as follows.

- A stochastic XFEM framework has been proposed for the numerical evaluation of tensile strength probability.
- The effect of microstructural features has been evaluated on the tensile strength of NBG-18 nuclear grade graphite.
- The proposed scheme for modeling microstructural features at micro and macro scales is very specific and unique due to large difference in average size of pore and filler particles.
- The proposed model uses both deterministic and stochastic approaches. The properties of pitch matrix, filler particles, and fracture stress on a fracture plane are assumed to be fixed at the constituent level. The pore size variation and pores distribution leads to variation in matrix strength, and random fracture plane orientation leads to variation in load bearing capacity of the filler particles. Thus, the variation in tensile strength is obtained entirely due to the microstructural features modeled stochastically.

This paper is organized as: in section 2 a brief discussion and presentation of the governing equations, XFEM formulation and failure criterion have been done. Section 3 illustrates the numerical implementation of stochastic processes (size/spatial distribution of fillers, etc.), equilibrium iterative scheme and tensile strength procedure. In section 4, the numerical results obtained by micro and macro analysis have been discussed along with statistical observations. Finally, concluding remarks based on the macro analysis of tensile strength are presented in section 5.

2. Numerical formulation

This section presents the displacement approximation, governing equations, level set functions for holes and inclusions and failure criterion for filler particles and pitch matrix.

2.1. Displacement approximation for inclusions and holes

At a particular node of interest $\mathbf{x}_i$, the displacement approximation i.e. trial function, $\mathbf{u}^h(\mathbf{x})$ for a 2-D body in presence of inclusions and holes can be written as [46,11,27,41].

$$\mathbf{u}^h(\mathbf{x}) = \sum_{i=1}^{n} N_i(\mathbf{x}) \left[\bar{\mathbf{u}}_i + \underbrace{\varphi(\mathbf{x})\,\mathbf{a}_i}_{i\in n_i} + \underbrace{[\psi(\mathbf{x}) - \psi(\mathbf{x}_i)]\,\mathbf{b}_i}_{i\in n_h} \right] \tag{1}$$

where, $\bar{\mathbf{u}}_i$ is the nodal displacement vector associated with the continuous part of the finite element solution; $\mathbf{a}_i$ and $\mathbf{b}_i$ are unknown additional enriched degree of freedom; n is a set of all nodes in the mesh; n_i and n_h are the set of nodes belonging to those elements which are cut by the inclusions and holes respectively; $\varphi(\mathbf{x})$ and $\psi(\mathbf{x})$ are the level set and Heaviside functions respectively.

2.2. Governing equations

Strong form of equilibrium equations in terms of Cauchy stress tensor can be expressed as,

$$\nabla.\bar{\boldsymbol{\sigma}} + \mathbf{b} = 0 \ \text{ in } \ \Omega \tag{2}$$

where, $\bar{\boldsymbol{\sigma}}$ is Cauchy stress tensor and $\mathbf{b}$ is body force vector per unit volume.

The weak form of the equilibrium equation can be written as,

$$\int_{\Omega} \boldsymbol{\sigma} : \ \delta\boldsymbol{\varepsilon} d\Omega = \int_{\Omega} \mathbf{b}.\delta\mathbf{u} d\Omega + \int_{\Gamma_t} \bar{\mathbf{t}}\,.\delta\mathbf{u} d\Gamma \tag{3}$$

where, $\mathbf{u}$ is the displacement field vector over the domain Ω and $\bar{\mathbf{t}}$ represents the traction force field vector acting on the boundary Γ_t as shown in Fig. 1.

Substituting trial and test functions and using arbitrariness of nodal variations, the following system of discrete equations are obtained,

$$[\mathbf{K}]\{\Delta\mathbf{U}\} = \{\Delta\mathbf{F}\} = \{\mathbf{F}_{\text{ext}}\} - \{\mathbf{F}_{\text{int}}\} \tag{4}$$

where, $\Delta\mathbf{U}$ is the incremental nodal displacement vector. $\Delta\mathbf{F}$, $\mathbf{F}_{\text{ext}}$ and $\mathbf{F}_{\text{int}}$ represent the incremental, external and internal force vectors respectively for a particular load step. $[\mathbf{K}]$ is the global stiffness matrix.

The elemental stiffness matrix $[\mathbf{K}^e]$ in $[\mathbf{K}]$ and elemental external force vector $\{\mathbf{F}^e_{\text{ext}}\}$ in $\{\mathbf{F}_{\text{ext}}\}$ over the elemental domain Ω^e are defined as [3,26],