Phase field model for irradiation-induced crack propagation in outer coating layers of TRISO particle fuel in space reactor applications

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Abstract

As an advanced fuel form, TRISO particle fuel exhibits relatively high reliability due to the excellent fission product containment capability of its thin coating layers; however, it remains susceptible to cracks or pores in the coatings during production, transportation, and service. These irregular geometric features can significantly compromise structural integrity. Therefore, to facilitate the application of TRISO particles in space reactors, analyzing and predicting crack propagation in their coatings is essential. This study presents the material properties, irradiation behavior, and fission gas release model for TRISO particles, and establishes a phase field model to investigate crack propagation characteristics in the outer three coating layers. Model accuracy for TRISO particle performance is verified through an IAEA benchmark problem and comparison with BISON program results. The reliability of the phase field model for crack simulation is validated via analysis of a notched tensile plate and the Kalthoff experiment. The effects of a crack in the IPyC layer, a residual pore in the SiC layer, a crack on the outer side of the OPyC layer, and the simultaneous presence of a crack in the IPyC layer with a residual pore in the SiC layer are investigated sequentially. Calculation results reveal that cracks in the IPyC layer induce debonding between IPyC and SiC layers, but are insufficient to propagate into the SiC layer during early burnup stages. Residual pores in the SiC layer lead to complete fracture of the coating layers, primarily attributable to excessive gas pressure from the inner IPyC layer rather than structural weakening by the pores. Cracks in the OPyC layer generate concentrated tensile stress on the outer side of the SiC layer during early burnup stages, which subsequently alters crack propagation paths in the coating layers during later burnup stages. Therefore, in addition to employing material detection techniques to screen out

TRISO particles with excessive defects prior to FCM pellet fabrication, it is crucial to enhance the structural integrity maintenance capability of coating layers and implement fundamental measures such as expelling accumulated gases from the particles. These actions are vital for safe and stable operation of TRISO particle fuel in space reactors.

Full Text

Phase Field Model for Irradiation-Induced Crack Propagation in Outer Coating Layers of TRISO Particle Fuel for Space Reactor Applications

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Abstract

As an advanced fuel form, TRISO particle fuel exhibits relatively high reliability due to the excellent capability of its thin coating layers to contain fission products. However, these coatings remain prone to cracks or pores during production, transportation, and usage, which can significantly impact their structural integrity. To advance the application of TRISO particles in space reactors, analyzing and predicting crack propagation in their coatings is crucial. This study introduces material properties, irradiation behavior, and fission gas release models for TRISO particles, and establishes a phase field model to investigate crack propagation characteristics in the outer three coating layers. The model' s accuracy for TRISO particle performance was verified through an IAEA benchmark problem and comparison with BISON program results. The reliability of the phase field model for crack simulation was validated by analyzing a notched tensile plate and the Kalthoff experiment. The effects of four scenarios were investigated in sequence: a crack in the IPyC layer, a residual pore in the SiC layer, a crack on the outer side of OPyC, and the simultaneous presence of a crack in the IPyC layer and a residual pore in the SiC layer. The results reveal that cracks in the IPyC layer cause debonding between IPyC and SiC layers but are insufficient to propagate into the SiC layer during early burnup stages. Residual pores in the SiC layer lead to complete fracture of the coating layers, primarily due to excessive gas pressure from the inner IPyC layer rather than structural weakening by the pores. Cracks in the OPyC layer cause concentrated

tensile stress on the outer side of the SiC layer during early burnup, altering the crack propagation path during later stages. Therefore, in addition to using material detection techniques to screen out TRISO particles with excessive defects before FCM pellet production, it is essential to enhance the structural integrity of coating layers and implement fundamental measures such as expelling accumulated gases from the particles. These actions are crucial for the safe and stable operation of TRISO particle fuel in space reactors.

Keywords: TRISO particle, Phase field, Fracture mechanics, Nuclear engineering, Space reactor

1. Introduction

Based on stringent requirements for reactor stability and safety, several Accident Tolerant Fuels (ATFs) have been developed and partially implemented [1-2], aiming to maintain fuel structural integrity and ensure reactor safety under both normal and accident conditions. Among these, Fully Ceramic Microencapsulated (FCM) fuel represents a promising candidate, consisting of TRistructural-ISOtropic (TRISO) coated fuel particles dispersed within a Nano-Infiltration and Transient Eutectic-phase SiC (NITE-SiC) matrix. To ensure the stability of the entire fuel pellet, it is crucial to investigate its fundamental unit—the TRISO particle.

A TRISO particle consists of a kernel surrounded by four consecutive coating layers, as illustrated in Fig. 1 [Figure 1: see original paper]. The kernel serves as the reactor' s heat source through nuclear reactions and can be made of UO_2, UN, or UCO. The first coating layer, known as the Buffer layer, is composed of low-density pyrocarbon (PyC). It acts as a cushion, providing space for gaseous fission products while alleviating stresses caused by kernel expansion on the outer coating layers [4]. The second layer is the Inner Pyrolytic Carbon (IPyC) layer, made of dense PyC, which protects the SiC layer from corrosion during manufacturing and shields it from damage caused by gaseous and solid fission products [5-6]. The third layer, deposited on the IPyC using Chemical Vapor Deposition (CVD), is referred to as CVD-SiC (to distinguish it from NITE-SiC). The SiC layer not only contains fission products but also serves as the main pressure vessel to maintain the structural integrity of the TRISO particle [7-10]. Finally, the outermost layer is the Outer PyC (OPyC) layer, which acts as the final barrier for fission products and protects the CVD-SiC layer during manufacturing [5]. Owing to this multi-layered coating structure, TRISO particles can effectively contain fission products and maintain structural integrity, exhibiting excellent irradiation stability and thermo-mechanical performance [11-12].

Experimental and numerical studies of TRISO particles have established a solid foundation. Irradiation experiments have shown that the buffer layer' s porosity causes its volume to shrink under neutron irradiation [13]. J. L. Hales et

al. simulated TRISO particles using the BISON code [14], demonstrating the feasibility of numerical simulation and validating the program' s effectiveness. C. Zhang et al. employed COMSOL to develop simulation methods for TRISO particles and FCM pellets [15-16], concluding that TRISO particles are relatively reliable under normal HTGR conditions. However, with increasing demands for space exploration and deep-sea missions, research and development of space reactors have become increasingly urgent [17-19]. Previous studies [20] revealed that space reactor requirements for higher fuel temperatures, greater fission rates, and longer operational lifetimes cause the internal gas pressure on the inner side of the IPyC layer to increase significantly during mid-to-late burnup stages. This results in higher tensile stresses in the SiC layer, greatly increasing its probability of failure. Cracks may even develop in the outer coating layers, potentially leading to TRISO particle collapse, as shown in Fig. 2 [Figure 2: see original paper] [21]. The stability of nuclear fuels, cladding, and other structural components plays a critical role in reactor operation [22-23]. Therefore, studying crack propagation characteristics in the outer coating layers of TRISO particles is of paramount importance. Only by exploring and predicting the mechanisms and influencing factors of crack initiation and propagation can the safe and stable application of TRISO particles and FCM fuel in space reactors be advanced.

In engineering problems where crack phenomena are difficult to investigate experimentally, researchers must rely on numerical simulation methods to predict complex crack paths [24], especially under the intricate operating conditions of TRISO particles. Consequently, numerical simulation methods for crack propagation have seen significant development. The discrete crack model introduces new boundaries for crack surfaces through adaptive mesh reconstruction [25]. The eXtended Finite Element Method (XFEM) enhances cracked elements by integrating discontinuous shape functions into the conventional Finite Element Method (FEM) framework [26-27]. Similarly, the Cohesive Zone Model (CZM) simulates crack propagation by allowing displacement jumps along element boundaries, effectively modeling debonding and interfacial fractures, with cracks confined to predefined paths such as element edges [28-31]. The phantom-node method models cracks independently of the mesh by overlapping elements at the crack location, allowing for discontinuous displacement without enrichment functions [32]. Furthermore, element-erosion methods address fracture surfaces by setting stresses of elements meeting the fracture criterion to zero, providing an alternative approach for simulating crack growth [33]. However, these complex crack simulation methods are challenging to apply to practical engineering problems.

In contrast, the Phase-Field Method (PFM), which has gained significant attention recently, offers a more convenient approach for fracture simulation. It represents discrete cracks using a scalar field that smoothly transitions between intact and fully fractured material without treating cracks as physical discontinuities. This eliminates the need for explicit tracking of fracture surfaces, simplifying simulation of crack propagation, branching, and merging in complex

geometrical models. Moreover, by directly solving Partial Differential Equations (PDEs) to determine the phase-field distribution, PFM adopts a numerical solution process similar to other physical fields, making crack simulation more convenient and accessible, including for multi-physics coupling. Currently, several phase-field approaches have been developed based on software platforms such as ABAQUS [34], MOOSE [35], FEniCS [36], and COMSOL [37-39]. The phase field method has been applied to analyze multiphysics-coupled crack propagation [40-42] and engineering problems such as hydraulic fracturing [43], concrete cracking [44], coal seam fracturing [45], and hydrogen-induced cracking in pipelines [46]. However, studies on crack propagation in TRISO fuel particles remain limited. The microstructure of SiC in TRISO particles [47-48] and its oxidation behavior [49] have been experimentally studied, and the fracture strength of SiC has been investigated [50]. A. M. Recuero et al. employed an interaction integral approach to calculate stress intensity factors for cracks in the inner pyrolytic carbon layer perpendicular to the silicon carbide layer [51]. Y. Li simulated micro-defect-induced cracking in the IPyC layer using XFEM [52]. J. Tan et al. simulated cracks within the IPyC layer and at the IPyC-SiC interface through phase field modeling, concluding that combined effects of shrinkage and creep-induced stress relaxation play a crucial role in determining crack evolution and subsequently impact stress distribution in the SiC layer [53]. Overall, crack propagation characteristics in TRISO particle coating layers and their influencing factors still require further investigation.

This paper develops a phase-field model to simulate crack propagation characteristics in the outer three coating layers of TRISO particles. A 2D axisymmetric geometry model of the IPyC, CVD-SiC, and OPyC layers is constructed, incorporating material properties, irradiation behaviors, and fission gas pressure to simulate TRISO particle operating conditions. The mechanical model was validated against the IAEA Coordinated Research Program (CRP-6) Case 8 benchmark, and the accuracy of the complete TRISO particle model was confirmed through comparison with BISON simulation results, detailed in our previous study [20]. Subsequently, crack propagation characteristics in the outer three layers are investigated. First, the influence of prefabricated crack depth in the IPyC layer on crack propagation and maximum tensile stress in the SiC layer is analyzed. Then, the effect of residual pores of different sizes in the SiC layer is studied. The impact of prefabricated cracks in the OPyC layer is also examined. Finally, the study explores crack propagation characteristics caused by residual pores in the SiC layer following interface damage between IPyC and SiC layers due to prefabricated cracks in the IPyC layer during early burnup. Recommendations for limitations on crack and pore sizes and their impact on TRISO particle stability are provided as part of the conclusions.

2. Model Description

Fig. 3 [Figure 3: see original paper] illustrates the model components and their interactions, providing a basis for the subsequent explanation of specific steps involved in model construction.

2.1 Mechanical Governing Equations and Material Properties

The mechanical calculation model, built with the "Solid Mechanics" module in COMSOL, is formulated based on Cauchy' s equation:

$$\nabla \cdot \sigma + F_v = 0$$

where σ is the Cauchy stress tensor and F_v represents the body force per unit volume. The stress is calculated using a linear elastic constitutive model:

$$\sigma = C : \varepsilon_e$$

where C is the material matrix associated with Young' s modulus and Poisson' s ratio, and ε_e represents the elastic strain vector. The elastic strain is derived by subtracting inelastic strain from total strain, while the strain field is obtained from the displacement vector:

$$\varepsilon = \frac{1}{2}(\nabla u + \nabla u^T)$$

$$\varepsilon_e = \varepsilon - \varepsilon_{in}$$

where ε denotes total strain, u is the displacement vector, and ε_{in} corresponds to inelastic strain, which includes initial strain, external strain, and creep strain.

Experiments [13] and previous studies [20] have shown that during early burnup stages, the IPyC layer and buffer layer separate, forming a gap that eliminates significant interaction and stress transfer between the two layers. Consequently, this study focuses on constructing the geometric model for only the outer three coating layers. Moreover, previous studies demonstrated that temperature within the outer three layers is nearly uniform [20], eliminating the need for a heat transfer model. Additionally, due to high mesh refinement requirements for crack simulation, a 2D axisymmetric model was developed to reduce computational costs, as shown in Fig. 4 [Figure 4: see original paper].

The relationship between base vectors of local spherical coordinates (r, θ, ϕ) and global cylindrical coordinates (ρ, z, ϕ) is given by:

$$r = \sqrt{\rho^2 + z^2}, \quad \theta = \arctan\left(\frac{\rho}{z}\right)$$

Regarding mechanical properties, Young' s modulus of PyC is expressed by the following equations [54]:

$$E = E_0 \left[1 - 0.01 \cdot BAF_0 \cdot \ln\left(\frac{L_c}{45}\right)\right] \cdot \left(\frac{\rho}{1.9}\right) \cdot (1 - 0.01 \cdot \Phi \cdot T)$$

where E_0 is 25.5 GPa, BAF_0 represents the initial degree of anisotropy (reasonable value: 1.03), L_c is crystallite diameter size (45 Å), and ρ, Φ, and T denote density (10^6 g/m^3), neutron flux (10^{25} n/m^2), and temperature (°C), respectively.

Poisson' s ratio of IPyC is 0.21 [55], and its density is 1900 kg/m^3 [14].

Young' s modulus of CVD-SiC is obtained experimentally [56]:

$$E = E_0 - B(T - T_0)$$

where E_0 is 460 GPa, B is 0.04 GPa/K, and T_0 is 962 K. Poisson' s ratio and density of SiC are set to 0.21 and 3210 kg/m^3, respectively [56].

2.2 Irradiation Behavior

Under neutron irradiation, PyC undergoes irradiation creep and irradiation-induced dimensional change, while SiC experiences creep and swelling. This section explains the corresponding strain models.

2.2.1 Burnup Burnup calculation in TRISO particles follows the model proposed by Olander [57], where burnup is defined as the ratio of fissions to initial uranium atoms:

$$\beta = \frac{\int_0^t \dot{F} dt}{N_U^0}$$

where $\dot{F}$ and N_U^0 represent fission rate per unit volume (fissions/m^3/s) and initial uranium atom density (atoms/m^3), respectively. These quantities are calculated as:

$$\dot{F} = N_f \cdot \sigma_f \cdot \Phi$$

$$N_f = \frac{D \cdot TD \cdot N_A}{M_U}$$

where q is enrichment (ratio of fissile atoms to total uranium atoms), σ_f is effective fission cross-section in the relevant neutron energy spectrum (barns),

N_f is total uranium atoms per unit volume, Φ is neutron fluence (n/m^2), D is theoretical density ratio, TD is theoretical density (g/cm^3), N_A is Avogadro' s constant, and M_U is uranium dioxide molar mass (g/mol). The relationship between burnup Bu (MWd/kgU) and β (%FIMA) is:

$$Bu = 0.01 \cdot \beta \cdot 949.2$$

Fast neutron flux is calculated using the BISON formula [58]:

$$\dot{\Phi}_f = c \cdot P$$

where $\dot{\Phi}_f$ is fast neutron flux, c is a conversion factor (typically 3×10^{13} n/(m^2 · s)/(W/m)), and P is linear heat rate (W/m).

2.2.2 Irradiation-Induced Dimensional Change, Creep, and Swelling During irradiation, both porous and dense PyC layers experience fast neutron fluence causing irradiation-induced dimensional changes. The irradiation strain rate for IPyC differs in radial and tangential directions, described by German' s formulas [59]:

$$\dot{\varepsilon}_r = A_r \cdot \Phi_f, \quad \dot{\varepsilon}_t = A_t \cdot \Phi_f$$

where $\dot{\varepsilon}$ and Φ_f denote irradiation strain rate (1/(10^{25}n/m^2)/s) and fast neutron fluence (10^{25}n/m^2), respectively.

With prolonged neutron irradiation, radiation effects on IPyC microstructure result in creep. The irradiation-induced creep rate is described by [59]:

$$\dot{\varepsilon}_{cr} = K \cdot \Phi_f \cdot \sigma_{eff}$$

where $\dot{\varepsilon}_{cr}$ is creep rate (1/s), K is creep constant (m^2/n/MPa), ρ_0 is initial PyC density (g/cm^3), σ_i are principal stresses, ν_{cr} is Poisson' s ratio for creep (0.5), and T is temperature.

Silicon carbide is also subject to irradiation creep:

$$\dot{\varepsilon}_{cr,SiC} = K_{SiC} \cdot \Phi_f \cdot \sigma_{eff}$$

where $K_{SiC} = 0.4 \times 10^{-31}$ m^2/n/MPa.

SiC also undergoes irradiation swelling, with neutron-induced swelling between 1250°C and 1500°C expressed by [59]:

$$V_{sw} = V_0 \cdot \left(1 - e^{-\Phi_f/\Phi_0}\right)$$

where V_{sw} is volumetric strain from swelling and $\Phi_0 = 0.3396 \times 10^{25}$ n/m^2.

At neutron flux 5×10^{17} n/m^2 and temperature 1500K, irradiation-induced dimensional change (IIDC), swelling, and creep constants are shown in Fig. 5 [Figure 5: see original paper]. As burnup progresses, PyC undergoes radial contraction followed by expansion, while tangential direction continuously contracts. SiC swelling and creep are relatively small compared to PyC behavior.

2.2.3 Fission Gas Behavior In nuclear fuels, fission gas atoms are generated within uranium dioxide grains through nuclear fission. These atoms form intragranular bubbles or diffuse to grain boundaries, coalescing into intergranular bubbles. When concentration exceeds a critical threshold influenced by temperature and other factors, gases release into free volume—this process is Fission Gas Release (FGR) [60-63]. After release, fission gases interact with layers beyond the kernel and generate internal pressure on the IPyC layer. Accurately modeling fission gas release is critical because gases do not immediately release into free space and can dramatically affect TRISO particle coatings, significantly influencing simulation accuracy for fuel performance and failure assessment.

The fission gas model incorporates several key effects: gas dissolution, atom diffusion, bubble growth, boundary concentration saturation, and influences of grain growth and external pressure. These factors are modeled using equations and conditions to account for gas atom coalescence, migration, and resulting internal pressures on the IPyC inner side. This model was validated and refined in previous studies [20]. Since previous calculations are comprehensive and sufficient, this study directly uses gas pressure values calculated under typical HTGR and more stringent space reactor conditions from prior research, as shown in Fig. 6 [Figure 6: see original paper].

2.3 Phase Field Model for Brittle Fracture

2.3.1 Brittle Fracture Theory Consider a domain Ω with pre-existing crack Γ, where Dirichlet and Neumann boundary conditions are applied. For instance, one side has fixed constraint while the other applies given traction f or displacement u, as shown in Fig. 7 [Figure 7: see original paper].

According to Griffith' s theory [64], the energy required to create a fracture surface per unit area equals the critical fracture energy density G_c, also called critical energy release rate. The total potential energy is:

$$\Pi = \int_{\Omega} \psi_e d\Omega - \int_{\Omega} F_v \cdot u d\Omega - \int_{\partial\Omega} f \cdot u dS$$

where terms represent elastic energy, fracture energy, body force energy, and external force energy. The linear strain tensor is:

$$\epsilon = \frac{1}{2}(\nabla u + \nabla u^T)$$

Assuming isotropic linear elasticity, the elastic energy density function is defined by Miehe et al. [65]:

$$\psi_e = \frac{\lambda}{2}\text{tr}[\epsilon]^2 + \mu\text{tr}[\epsilon^2]$$

where λ and μ are Lamé constants derived from Young' s modulus and Poisson' s ratio, and $\text{tr}[A]$ represents matrix trace.

Theoretically, crack distribution can be obtained by solving Eq. (19) through energy conservation. However, approximations and field concepts must be introduced to solve for crack distribution.

2.3.2 Phase Field Approach to Fracture Energy By introducing a scalar phase field $p(x,t) \in [0,1]$, brittle fracture can be successfully simulated [39]. The phase field approximates the fracture surface Γ, where $p = 1$ denotes cracked material and $p = 0$ indicates intact material (as shown in Fig. 7).

The crack surface density per unit volume is given by Miehe et al. [65]:

$$\gamma(p, \nabla p) = \frac{1}{2l_0}p^2 + \frac{l_0}{2}|\nabla p|^2$$

where l_0 is the length scale parameter governing the transition region of the phase field and representing crack width. Applying this approximation transforms the complex surface integral into a domain integral, facilitating phase field model construction:

$$\int_\Gamma G_c d\Gamma \approx \int_\Omega G_c \gamma(p, \nabla p) d\Omega$$

Crack surface energy is driven by elastic energy, controlling phase field evolution. To ensure crack propagation is only influenced by tensile loading, elastic energy must be decomposed, with the compressive component having no contribution [39]. The spectral decomposition method is:

$$\epsilon = \sum_{i=1}^{3} \lambda_i n_i \otimes n_i$$

$$\epsilon^+ = \sum_{i=1}^{3} \langle \lambda_i \rangle_+ n_i \otimes n_i, \quad \epsilon^- = \sum_{i=1}^{3} \langle \lambda_i \rangle_- n_i \otimes n_i$$

where λ_i are principal strains, n_i are direction vectors, and $\langle\cdot\rangle_\pm$ are Macaulay brackets.

In Eq. (19), ψ_e represents energy stored per unit volume. Applying the decomposed strain tensor, the reference energy function for undamaged elastic solid ψ_0 is similarly decomposed:

$$\psi_0(\epsilon) = \psi_0^+(\epsilon) + \psi_0^-(\epsilon)$$

Considering crack propagation and assuming only the tensile part is influenced by phase field, energy degradation is incorporated:

$$\psi_e(p, \epsilon) = g(p)\psi_0^+(\epsilon) + \psi_0^-(\epsilon)$$

The monotonically decreasing degradation function $g(p)$ describes stiffness reduction, satisfying $g(0) = 1$, $g(1) = 0$, and $g'(1) = 0$. A common power function form is:

$$g(p) = (1-p)^2$$

For a domain with kinetic energy, it is expressed as:

$$K = \int_\Omega \frac{1}{2}\rho\dot{u}^2 d\Omega$$

The total Lagrange energy function combines fracture energy, elastic energy, kinetic energy, and external potential energy:

$$L = \int_\Omega \left[\frac{1}{2}\rho\dot{u}^2 + g(p)\psi_0^+ + \psi_0^- + G_c\gamma(p, \nabla p)\right] d\Omega - \int_\Omega F_v \cdot u d\Omega - \int_{\partial\Omega} f \cdot u dS$$

Applying variational principle ($\delta L = 0$) yields governing equations:

$$\nabla \cdot \sigma + F_v = \rho\ddot{u}$$

$$\frac{G_c}{l_0}(p - l_0^2\nabla^2 p) = 2(1-p)H(x,t)$$

where σ is the Cauchy stress tensor, decomposed as:

$$\sigma = g(p)\frac{\partial\psi_0^+}{\partial\epsilon} + \frac{\partial\psi_0^-}{\partial\epsilon}$$

If applied directly, the phase field would recover after load removal, contradicting crack irreversibility. To ensure monotonic increase, a strain-history field $H(x,t)$ records maximum elastic energy density:

$$H(x,t) = \max_{\tau\in[0,t]} \psi_0^+(\epsilon(x,\tau))$$

Replacing ψ_0^+ with $H(x,t)$ yields the strong form PDE:

$$\frac{G_c}{l_0}(p - l_0^2\nabla^2 p) = 2(1-p)H$$

2.3.3 Weak Form for FEM and Solution Strategy Phase-field modeling involves a coupled multi-physics problem with displacement and phase field as primary fields, plus strain-history variable H. The displacement field is solved using COMSOL' s "Solid Mechanics" module, while the phase field is governed by energy conservation. For finite element implementation, governing equations are reformulated into weak form [39,41]:

$$\int_\Omega \sigma : \delta\epsilon d\Omega = \int_\Omega F_v \cdot \delta u d\Omega + \int_{\partial\Omega} f \cdot \delta u dS$$

$$\int_\Omega \left[\frac{G_c}{l_0} p\delta p + G_c l_0 \nabla p \cdot \nabla\delta p\right] d\Omega = \int_\Omega 2(1-p)H\delta p d\Omega$$

To avoid prohibitive computational cost of fully coupled calculations, this study adopts a decoupled solver to sequentially solve for displacement field, history strain field, and phase field (as shown in Fig. 3), enabling reasonable crack simulation.

Phase-field parameters for the outer three coatings assume length scale parameters $l_1 = 3$ μm for PyC and $l_2 = 1$ μm for SiC. The critical energy release rate G_c is derived using Borden et al.' s formula [66]:

$$G_c = \frac{\sigma_c^2 l_0}{E}$$

where σ_c is tensile strength (200 MPa for PyC [68] and 667 MPa for SiC [59]), and E is Young' s modulus dynamically calculated from Eq. (6) and Eq. (7). Anisotropic PyC' s E is represented by the average value in three directions.

3. Verification

The code was validated against the IAEA HTGR benchmark, specifically Case-8 from the IAEA Coordinated Research Program (CRP-6) [69]. This case verified computational accuracy by modeling the outer three coatings subjected to ten 100-day cycles. In each cycle, fuel temperature increased linearly from 873 K to 1273 K, then dropped back to 873 K, while gas pressure on the IPyC inner side varied linearly. Maximum tangential stresses at IPyC and SiC inner surfaces compared well with results from other codes, demonstrating accurate mechanical performance simulation. Thermomechanical properties of the complete TRISO particle were also compared with BISON results, validating simulation reliability. Detailed results are available in our previous study [20].

To validate the phase-field calculation method, two typical test cases were selected.

3.1 Notched Tensile Plate

A square plate with an initial notch under static tension is shown in Fig. 8 [Figure 8: see original paper]. Vertical displacement u_y is applied to the upper boundary with u_x fixed. Material parameters are: $E = 210$ GPa, $\nu = 0.3$, $G_c = 2700$ J/m^2, and length scale $l_0 = 1.5 \times 10^{-2}$ mm. Maximum element size h is $l_0/2$. Displacement increment $\Delta u = 1 \times 10^{-5}$ mm is applied for initial 450 time steps, followed by $\Delta u = 1 \times 10^{-6}$ mm until complete fracture.

Results in Fig. 9 [Figure 9: see original paper] show stress concentration at the notch with gradual crack formation and propagation, showing excellent agreement with S. Zhou et al. [39].

3.2 Kalthoff Dynamic Fracture Experiment

To verify transient calculations and phase-field modeling under shear, the Kalthoff dynamic fracture experiment was selected [70]. In this experiment, a steel plate with pre-existing cracks is impacted, generating stress waves that cause brittle fracture. The computational problem is constructed as shown in Fig. 10 [Figure 10: see original paper].

Specified velocity v is:

$$v = v_0 \exp\left(-\frac{t}{t_0}\right)$$

where $v_0 = 16.5$ m/s and $t_0 = 1$ µs. Material properties are: $\rho = 8000$ kg/m^3, $E = 190$ GPa, $\nu = 0.3$, $G_c = 22130$ J/m^2, and $l_0 = 3.9 \times 10^{-4}$ m. Simulation runs to 90 µs, with phase field results at several times shown in Fig. 11 [Figure 11: see original paper]. Crack appears at 24.84 µs and extends upward at approximately 65° to the horizontal axis, consistent with [39] (63°-67°) and experimental results [70]. Cracks simulated using XFEM [71] and phantom nodes

method [72] in Fig. 12 [Figure 12: see original paper] show similar patterns, demonstrating the reliability of our phase field approach for brittle fracture.

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4. Demonstration Problems

Cracks may form during manufacturing or use in PyC layers [40,73], while residual pores commonly exist in SiC layers [74,75]. These irregular geometries cause stress concentration, significantly affecting TRISO particles and potentially causing coating fracture. This study analyzes four scenarios: (1) crack on IPyC inner side, (2) residual pore in SiC layer, (3) crack on OPyC outer side, and (4) combined crack in IPyC and residual pore in SiC. Since IPyC and SiC are not monolithic, debonding may occur at their interface. When a crack reaches the interface, it tends to deflect in both directions [76]. Therefore, a thin 0.8 μm layer is defined on IPyC' s outer side and OPyC' s inner side, with critical energy release rate set to 0.8 times that of PyC to simulate interfacial damage. Geometric models are shown in Fig. 13 [Figure 13: see original paper].

Irradiation behavior is incorporated, with IPyC layer subjected to fission gas pressure. To ensure accuracy and convergence, pressure is linearly removed once the crack reaches OPyC's outer side; otherwise, separated materials would move too far apart.

To investigate sensitivity to geometric parameters and provide recommendations for pre-existing crack size limitations in engineering applications, this study parameterized crack depth and pore radius in scenarios 1 and 2 (Table 1). Since SiC is highly reliable under normal conditions, scenarios 1 and 3 use typical HTGR conditions [14,77], while scenarios 2 and 4 use more stringent space reactor conditions [20] (Table 2).

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5. Results and Discussion

5.1 Effect of a Crack in the IPyC Layer

Irradiation behavior is most active before 1.5×10^7 s (Fig. 5), when maximum tangential stress in IPyC occurs. After this point, stress gradually relaxes with burnup progression [20]. Therefore, crack formation and propagation primarily occur during early burnup. If no cracks form by this time, none will appear subsequently. Maximum calculation time is set to 1.5×10^7 s.

Figs. 14-16 show phase fields at selected times for pre-existing cracks of 1 μm, 6 μm, and 10 μm depth in IPyC inner side. With 1 μm depth, stress distribution remains uniform with no significant crack effect, and maximum phase field value at calculation end is only 0.17, indicating no propagation. With 6 μm depth, crack begins propagating toward SiC at 0.80×10^7 s, deflecting at the interface and causing IPyC-SiC debonding. With 10 μm depth, propagation starts earlier

at 0.43×10^7 s, expanding more rapidly after reaching the interface, with most of IPyC' s outer region separated from SiC by 1.50×10^7 s.

Fig. 17 [Figure 17: see original paper] shows maximum phase field values at 1.5×10^7 s and crack initiation times for different pre-crack depths. No propagation occurs for depths <5.8 μm. When propagation occurs, initiation time becomes earlier as pre-crack depth increases.

Fig. 18 [Figure 18: see original paper] presents tangential stress distribution at 1.5×10^7 s for 5 μm, 6 μm, and 10 μm pre-cracks. Without propagation, the notch induces significant tensile stress in IPyC while SiC remains compressive. For 6 μm pre-crack, local debonding causes strong compressive stress concentration in SiC beyond the crack tip due to IPyC constraint, while the crack front region experiences tensile stress. Fortunately, this tensile concentration is confined within IPyC and insufficient to fracture SiC.

Fig. 19 [Figure 19: see original paper] shows debonded area proportions and maximum tangential stress in SiC at calculation end for different pre-crack depths. IPyC cracks increase SiC tensile stress. Without propagation, SiC remains compressive at burnup end. Once cracking occurs, stress concentration from interface debonding and crack tip causes SiC tensile stress. Deeper pre-cracks cause more interface separation, which alleviates SiC tensile stress but remains significantly higher than without propagation.

For a 10 μm pre-crack simulated through fuel lifetime, Fig. 20 [Figure 20: see original paper] compares maximum tangential stress on SiC inner surface with and without pre-existing crack. As the crack approaches SiC inner side, it induces sudden tensile stress increase. Since SiC strength is much higher than pyrolytic carbon and stress concentration is localized, no immediate cracking occurs in early burnup. However, at 7.6×10^7 s, maximum tangential stress becomes significantly higher than without initial IPyC crack, which could considerably impact long-lifetime applications like space nuclear reactors.

5.2 Effect of a Residual Pore in the SiC Layer

SiC with residual pores of 0.1 μm and 1 μm radii at different times are shown in Figs. 21-22. With 0.1 μm pore, no significant stress concentration occurs; instead, excessive IPyC internal pressure pulls the SiC layer apart, causing coating failure. With 1 μm pore, the geometric defect' s impact is more pronounced, causing cracks to form on both sides and propagate inward and outward, eventually fracturing all three coatings.

Fig. 23 [Figure 23: see original paper] shows complete fracture time of outer three coatings and gas pressure at fracture for different residual pore sizes. Larger pore radius causes slightly earlier fracture. When pore radius exceeds 0.2 μm, it begins impacting SiC structure. However, residual pore effects on structural strength are not very significant—even with 1 μm pore, coatings fracture after more than five and a half years. SiC fracture is primarily due to excessive

fission gas pressure rather than residual pores. In this model, TRISO particles cannot withstand gas pressures exceeding 139 MPa.

5.3 Effect of a Crack in the OPyC Layer

HTGR conditions were first applied to simulate this crack type. Figs. 24-25 show phase field and tangential stress at 7.6×10^7 s for 10 µm pre-crack on OPyC outer side, plus SiC inner surface stress comparison. Although this pre-crack induces stress concentration, maximum phase field value remains only 0.28 at fuel lifetime end. SiC inner surface tangential stress is higher than without crack throughout lifetime, but impact is weaker than IPyC inner side pre-cracks. However, due to pyrolytic carbon' s radial shrinkage under irradiation, tensile stress transmitted to SiC outer surface may initiate fracture from outside.

Therefore, potential impacts under space reactor conditions were further investigated. Fig. 26 [Figure 26: see original paper] shows phase field with OPyC outer side pre-crack under space reactor conditions. Unlike IPyC inner cracks, this type remains highly stable through early and mid-burnup. Although slight expansion occurs, OPyC inward shrinkage is supported by SiC, preventing propagation until 18×10^7 s. At 18.155×10^7 s, tensile stress concentration at two SiC outer surface locations causes corresponding cracks to initiate and propagate inward. This path is similar to ceramic laminate crack patterns [78]. By 18.200×10^7 s, both cracks fully penetrate SiC and IPyC layers, causing complete fracture of TRISO particle outer coatings—earlier than with 1 µm SiC residual pore, but both scenarios result in complete failure only at burnup end.

5.4 Combined Effect of Crack in IPyC Layer and Residual Pore in SiC Layer

Simulated crack propagation results for combined IPyC crack and SiC residual pore are shown in Fig. 27 [Figure 27: see original paper]. During early burnup, the IPyC crack extends and causes IPyC-SiC interface debonding. Stress from this main crack causes SiC tensile stress, leading to complete outer coating fracture earlier than with only SiC residual pore. Therefore, engineering applications should particularly avoid and limit IPyC crack sizes. Complete fracture occurs at 18.18×10^7 s, the earliest among all studied scenarios.

Overall, these defects provide geometric conditions for stress concentration and crack propagation. In early burnup, IPyC crack propagation from irradiation only causes IPyC-SiC debonding rather than complete coating failure. The primary cause of complete fracture is excessive IPyC internal gas pressure from high temperature and fission gas accumulation during later burnup stages. Therefore, before deploying TRISO particles in space reactors, it is crucial to screen for minimal defects and implement measures to maintain coating structural integrity.

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6. Conclusions

This paper developed a phase field model for analyzing TRISO particle outer three coatings using COMSOL Multiphysics. Fuel behavior was thoroughly considered, including condition-dependent material properties, burnup, irradiation effects, fission gas release, and gas pressure formation.

Model accuracy for TRISO particle behavior was validated against IAEA CRP-6 Case 8 benchmark stress calculations and BISON code results for complete TRISO particles, clearly demonstrating simulation accuracy [20]. The phase field model was validated through notched tensile plate and Kalthoff experiment simulations, confirming reliable crack propagation simulation for brittle fracture.

This study analyzed common TRISO particle defects: pre-existing cracks on IPyC inner side, residual pores in SiC layer, pre-existing cracks on OPyC outer side, and combined IPyC crack with SiC residual pore. Results show:

1. Pre-cracks deeper than 5.8 μm on IPyC inner side propagate outward toward SiC, deflecting at the interface and causing layer debonding. This increases tensile stress near the crack tip but is insufficient to fracture SiC. Deeper pre-cracks cause earlier propagation and faster separation.
2. SiC pores with radius >0.2 μm cause cracks to form at burnup end, propagating inward and outward and eventually fracturing all outer coatings. Even perfect materials cannot withstand gas pressures exceeding 139 MPa.
3. OPyC outer side pre-cracks have small impact during early/mid-burnup but cause concentrated tensile stress at two SiC outer surface locations at burnup end, changing crack paths and causing two cracks to propagate inward, leading to complete coating fracture.
4. Combined IPyC crack and SiC residual pore cause complete fracture earlier than SiC pore alone.

In conclusion, defects create conditions for stress concentration and crack propagation. For space reactor deployment, material detection techniques (e.g., X-ray radiographs [79]) should avoid IPyC cracks >5.8 μm and SiC pore radii >0.2 μm, while minimizing OPyC cracks. Even perfect coatings cannot withstand >139 MPa gas pressure, necessitating fundamental measures: modifying SiC structure to enhance strength, replacing SiC with stronger materials, or expelling fission gases. Future work should develop methods like PF-CZM [78,80-82] for analyzing IPyC-SiC debonding and TRISO-FCM matrix separation, and employ topology optimization [83] and multi-objective optimization [84] to improve fuel performance. Finally, pellet and fuel rod cracks must be simulated to promote FCM fuel application in space reactors.

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Note: Figure translations are in progress. See original paper for figures.