FEM Simulation of Interfacial Fracture and its Effect on Fission Gas Release under Irradiation in UN-U3Si2 Composite Fuel

Authors: Tan, Miss Peiyin, Liu, Prof. Guisen, Zhao, Mr. Chenlong, Zhang, Mr. Zikang, Sun, Dr. Zhipeng, Xin, Dr. Yong, Chen, Dr. Ping, Zhang, Prof. Lei, Shen, Prof. Yao, Shen, Prof. Yao

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Abstract

The UN-U3Si2 composite is a promising candidate for accident tolerant fuel (ATF); however, its interfacial mechanical response, fracture mechanisms, and the role of fission gas bubbles under various service environments remain incompletely understood. To address this issue, we developed a unified damage model implemented via a user-defined material subroutine (UMAT) in ABAQUS. This model uses a modified cohesive zone model (CZM) that explicitly incorporates interfacial bubbles and accounts for irradiation creep and swelling effects in the matrix. Employing this model, we investigated interfacial damage behavior and its impact on fission gas release (FGR) and fuel fragment in UN-U3Si2 fuel. Simulations of polycrystalline UN-U3Si2 under various loading conditions reveal rate-dependent mechanisms at the interface: rapid-loading (e.g., loss of coolant accident) triggers brittle fracture due to fast crack propagation, whereas slow-loading (e.g., long-term steady-state operation) suppresses cracking via creep-induced stress relaxation. Further analysis of the rapid-loading scenario demonstrates that, the presence of bubbles fundamentally alters the fracture mechanism by shifting crack initiation site from triple junctions to bubble edges due to stress concentrations. In systems with high bubble densities, local microcracks initiate between adjacent bubbles and rapidly link up to form complex networks, which increase the risk of fuel fragmentation. This study elucidates these complex failure mechanisms, providing a reliable computational framework for predicting fracture behavior and optimizing UN-U3Si2 performance in advanced reactors.

Full Text

Preamble

FEM Simulation of Interfacial Fracture and its Effect on Fission Gas Release under Irradiation in UN-U3Si2 Composite Fuel Peiyin Tan 1, Guisen Liu 1,, *Chenlong Zhao 1, Zikang Zhang 1, Zhipeng Sun 2, Yong Xin 2, Ping Chen 2,*, Lei Zhang 3 ,Yao Shen 1,* 1State Key Lab of Metal Matrix Composites, School of Materials Science and Engineering, Shanghai Jiao Tong University, Shanghai 200240, China 2State Key Laboratory of Advanced Nuclear Energy Technology, Nuclear Power Institute of China, Chengdu 610213, China 3School of Mathematical Sciences, MOE-LSC and Institute of Natural Sciences, Shanghai Jiao Tong University, Shanghai 200240, P.R. China Abstract: The UN-U3Si2 composite is a promising candidate for accident tolerant fuel (ATF); however, its interfacial mechanical response, fracture mechanisms, and the role of fission gas bubbles under various service environments remain incompletely understood. To address this issue, we developed a unified damage model implemented via a user-defined material subroutine (UMAT) in ABAQUS. This model uses a modified cohesive zone model (CZM) that explicitly incorporates interfacial bubbles and accounts for irradiation creep and swelling effects in the matrix. Employing this model, we investigated interfacial damage behavior and its impact on fission gas release (FGR) and fuel fragment in UN-U3Si2 fuel. Simulations of polycrystalline UN-U3Si2 under various loading conditions reveal rate-dependent mechanisms at the interface: rapid-loading (e.g., loss of coolant accident) triggers brittle fracture due to fast crack propagation, whereas slow-loading (e.g., long-term steady-state operation) suppresses cracking via creep-induced stress relaxation. Further analysis of the rapid-loading scenario demonstrates that, the presence of bubbles fundamentally alters the fracture mechanism by shifting crack initiation site from triple junctions to bubble edges due to stress concentrations. In systems with high bubble densities, local microcracks initiate between adjacent bubbles and rapidly link up to form complex networks, which increase the risk of fuel fragmentation. This study elucidates these complex failure mechanisms, providing a reliable computational framework for predicting fracture behavior and optimizing UN-U3Si2 performance in advanced reactors.

Keywords: Cohesive zone model; Fission gas bubbles; Interfacial fracture; UN-U3Si2 composite fuel; FEM simulation

1 Introduction

- Corresponding author. E-mail addresses: liuguisen@sjtu.edu.cn (G. Liu), chenping_{npic}@163.com (P. Cheng), yaoshen@sjtu.edu.cn (Y. Shen).

Since the Fukushima Daiichi nuclear accident, the development of fuels with enhanced safety margins has been a primary focus within the nuclear field. Accident tolerant fuel (ATF) concepts are introduced to improve reactor safety under severe accident scenarios while simultaneously maintaining or enhancing

performance under normal operating conditions [1].

Compared to traditional UO2 fuel, non-oxide ceramic fuels have attracted considerable interest owing to their superior thermal conductivity, higher uranium density, and broader potential for various reactor types. Among the candidates, Uranium Mononitride (UN), Uranium Silicide (U3Si2), and their composite (UN-U3Si2) are considered critical options for next-generation advanced fuels because of their excellent properties [2,3]. While UN possesses high thermal conductivity, high uranium density, and low irradiation swelling, its susceptibility to oxidation upon contact with air, water, or steam limits its direct application in light water reactors (LWRs) [4]. Conversely, U3Si2 displays good chemical compatibility with water but exhibits higher irradiation swelling rates [5,6]. By combining the strengths of both materials, the UN-U3Si2 composite fuel is expected to maintain high uranium density and thermal conductivity while improving environmental stability and irradiation performance, rendering it a highly promising ATF candidate [7,8]. Recent years have seen significant progress in research regarding UN-U3Si2 composite fuels across several fronts. In terms of fabrication, advanced powder metallurgy techniques, such as spark plasma sintering (SPS) [9] and liquid-phase sintering [10], have been developed to successfully fabricate composite fuel pellets with high density, controllable microstructure, and excellent performance. Through both experimental characterization [11] and computational simulation [12,13], researchers have investigated thermophysical properties (e.g., thermal conductivity, thermal expansion) and mechanical properties (e.g., hardness, fracture toughness), and their connections to microstructure (e.g., phase distribution, grain size). Regarding irradiation performance, studies have been conducted on post-irradiation microstructure performance characterization [14], with recent attempts to utilize artificial intelligence for performance optimization [15].

Extensive post-irradiation examinations (PIE) and microstructural characterizations [16,17] have confirmed that mechanical failure of nuclear fuel under both service and accident conditions is predominantly characterized by intergranular fracture or phase boundary separation. Consequently, the interfacial response is a critical factor governing fuel 2 / 34 integrity and safety limits.

Notably, fuel pellets are subjected to mechanical loading rates that vary widely between normal operation and accident scenarios. During transient events such as rapid power ramps or loss of coolant accidents (LOCA) [18,19], pellets experience rapid-loading. Normal operational transients like reactor startup and shutdown also involve relatively high and fluctuating loading rates, which remain below the intensities of accident scenarios. Finally, during long-term steady-state operation, the loading rate decreases to an extremely low, quasi-static level [20]. Regarding microstructural evolution, inert fission gas atoms (e.g., Xe and Kr) exhibit a strong propensity to precipitate due to their negligible solubility in the fuel matrix. Driven by high temperatures and assisted by irradiation-induced supersaturated vacancies, these gas atoms diffuse to and are trapped by defects such as dislocations and grain boundaries, subsequently nucleating into fission

gas bubbles [21].

Therefore, in the extreme irradiation environment of a reactor, fuel pellets undergo not only thermomechanical loading but also complex evolution, including fission gas bubble evolution and fracture, all of which collectively dictate the mechanical response at material interfaces. When crack initiation and subsequent propagation occur at these interfaces, forming macroscopic cracks, the negative impact on fuel performance is multifaceted.

Interfacial cracking degrades heat transfer capability and reduces the effective thermal conductivity, thereby diminishing the advantage over traditional UO2 [22,23]. Furthermore, this can lead to elevated pellet temperatures and steeper temperature gradients, resulting in increased internal thermal stress [24]. Furthermore, interfacial cracking compromises the structural integrity of the fuel, potentially inducing fragmentation under vibration or thermal shock. This affects the fuel-cladding interaction and may exacerbate fission gas release. If a large volume of fission gas is rapidly released into the pellet-cladding gap, it accelerates stress corrosion cracking (SCC) of the cladding, potentially leading to cladding failure, thus affecting service life and reactor safety [21,25].

Given the limited availability of experimental data, numerical simulation has become an indispensable tool investigating interfacial fracture behavior in nuclear materials.

Regarding numerical methodology, existing research largely employs multi-scale simulation techniques, including the finite element method (FEM) [26,27], phase field modeling (PFM) [28,29], and molecular dynamics (MD) [30]. While MD reveals intrinsic fracture mechanisms 3 / 34 the atomic scale, spatiotemporal limitations make it difficult to simulate engineering-scale crack propagation. Although PFM is capable of simulating complex crack evolution naturally, methods like CZM are often preferred for known fracture paths (e.g., interfaces) for their superior computational efficiency. Specifically, the FEM approach combined with CZM embeds cohesive elements at potential fracture sites (e.g., phase boundaries, inter-laminar interfaces, weak zones) described by a traction-separation law, naturally unifying crack initiation and propagation. This method avoids the numerical instability caused by stress singularities at crack tips in traditional fracture mechanics, features clear physical parameters, offers high computational efficiency, and is easily adaptable for engineering applications. For the study of UN-U3Si2 interfacial fracture mechanisms at the micrometer scale, the FEM-CZM framework is highly efficient, effectively compensating for the limitations of nuclear material experiments while predicting grain/phase boundary behavior. Furthermore, when introducing fission gas bubbles into the composite system, the FEM-CZM approach provides a direct and flexible means to visualize and regulate the effects of bubble evolution.

Despite recent achievements in the fabrication and characterization of UN-U3Si2 composite fuels, the mechanical response mechanisms of UN-U3Si2 interfaces under different loading rates and burn-up level remain unclear. Additionally, the

fracture mechanisms at various boundaries within this system (UN-U3Si2 phase boundaries, UN-UN grain boundaries, and U3Si2-U3Si2 grain boundaries) and their interaction with fission gas bubbles are not fully understood. Under the influence of fission gas bubbles, the fracture mechanisms of these three interfacial types become complex. The crack evolution behavior at these interfaces directly governs in-service performance of the fuel and the safety of reactor operations.

Therefore, revealing the interfacial damage mechanism under multi-field coupling and elucidating the mechanical behavior under different loading rates is of great scientific significance and engineering value for assessing service reliability.

To address these issues, our study employs a coupled FEM-CZM approach to construct a three-dimensional (3D) damage model for UN-U3Si2 composite fuel containing fission gas bubbles, irradiation swelling and creep effects. In detail, a constitutive model accounting for irradiation swelling and creep effects is applied to the matrix phases, while modified cohesive elements characterizing the dynamic evolution of fission gas bubbles are embedded at the 4 / 34 interfaces. This enables, for the first time, a 3D multi-physics coupling of irradiation creep, swelling, and bubble dynamics. The developed model is implemented via a user defined material (UMAT) subroutine in ABAQUS. This study addresses two primary issues: the mechanical response and state of interfaces under different loading rates and the interaction between fission gas bubbles and interfacial crack evolution. Using this model, this study systematically investigates the mechanical response of interfaces under different loading rates and the impact of fission gas bubbles on interfacial crack evolution, and elucidates the influence of loading conditions on interfacial fracture mechanisms by performing uniaxial tensile simulations of irradiated UN-U3Si2 composite fuels at various loading rates. The results demonstrate that rapid loading modes and the presence of phase boundary bubbles significantly affect the evolution behavior of interfacial cracks, thereby directly dictating the macroscopic in-pile performance and dimensional stability of the fuel.

The structure of the paper is as follows: Section 2 details the material models and computational framework employed. Section 3 systematically explores the interfacial mechanical response the UN-U3 Si2 composite under slow-loading, medium-loading, and rapid-loading, elucidating the dominant fracture mechanisms across these mode regimes. We further analyze the interactions between fission bubble and crack evolution, delineate the initiation and propagation of interfacial cracks in bubble-free conditions, assess the effects of bubble location and density on crack evolution, and assess the influence of fracture behavior on FGR and pellet dimensional changes. Finally, Section 4 summarizes the study and presents the main conclusions.

2 Models

Our study develops a three-dimensional (3D) damage model containing fission gas bubbles, irradiation swelling and creep effects, which can effectively simulate

the fracture of interface under multi-field coupling. In section 2, the numerical models, material constitutive relations, and the computational framework employed in this study are detailed. The theoretical formulation of the cohesive zone model (CZM) for simulating interfacial fracture is introduced, along with the specific model parameters in section 2.1. The constitutive models for the composite fuel and the detailed finite element implementation algorithms are presented in section 2.2. 5 / 34

2.1 Cohesive Zone Model (CZM)

Classical elastic fracture mechanics predicts an infinite stress singularity at the crack tip, a premise that is physically inconsistent with reality. To address this limitation, Dugdale [31] and Barenblatt [32] proposed the cohesive zone model (CZM). This model categorizes a crack into two distinct regions: a traction-free region located far from the crack tip and a region in the vicinity of the crack tip that sustains cohesive forces.

The finite element method based on cohesive zone modeling has since emerged as a powerful tool for simulating interfacial debonding and crack propagation. Its core principle involves pre-inserting zero-thickness cohesive elements along potential fracture paths, with the traction-separation constitutive relation defining these interfaces to characterize the progressive damage and failure processes of materials. Commonly used damage initiation criteria include the maximum nominal stress criterion, maximum nominal strain criterion, quadratic nominal stress criterion, and quadratic nominal strain criterion [33]. Among these, the quadratic nominal stress criterion is more widely adopted due to its closer approximation to the actual stress states experienced by materials. For modeling damage evolution, the energy-based approach is more widely adopted in both practical engineering simulations and scientific research. Energy-based damage evolution models include the Power-Law[34] and the Benzeggagh-Kenane (B-K) criterion [35]. The Power-Law is primarily suited for scenarios dominated by a single fracture mode or where mixed-mode effects are negligible, whereas the B-K criterion is designed for mixed-mode fracture. Given the brittle nature of UN-U3Si2 composite fuel and the complexity of its internal grain structure, the quadratic nominal stress criterion (Eq. (1)) was selected as the damage initiation criterion, where denotes the stress component at the crack, the subscripts n, s and t refer to the normal and the two shear directions; max, max, max represent the stress peaks in the normal, first shear and second shear directions, respectively.

The symbol '< >' denotes Macaulay brackets, which are commonly used to address cracking and closure phenomena in materials. The B-K criterion (Eq. (2)) was employed for damage evolution, 6 / 34 + 훧훧 − 훧훧 + 훧훧 + 훧훧훧 + 훧훧훧 where , 훧훧 release rate; denotes mode I and mode II critical strain energy represent the effective strain energy , 훧훧, 훧훧훧 release rate at the current state of mode I, mode II and mode III; is a semi-empirical criterion exponent applied to crack initiation and growth.

Common forms of traction-separation (T-S) laws for cohesive elements primarily include exponential, bilinear, constant, and trapezoidal constitutive models [36]. Given the brittle fracture nature of the UN-U3Si2 composite fuel, a bilinear T-S law is adopted in this study, as illustrated in Fig. 1 [Figure 1: see original paper]. In the linear softening stage described by this bilinear law, the stress decreases linearly with damage evolution, as expressed by the following equation: = 1 − represents the stress calculated based on the undamaged elastic modulus, and denotes the scalar damage variable, calculated as follows: here, where denotes the effective displacement at the current state (corresponds to that at the onset of damage. represents that at complete failure, and 7 / 34 Fig. 1. Schematic diagram of bilinear T-S law.

The material investigated in this study is UN-U3Si2 composite fuel, which comprises three distinct types of interfaces: UN-U3Si2 phase boundaries, UN-UN grain boundaries, and U3Si2-U3Si2 grain boundaries. To simplify calculations, the mechanical properties of the UN and U3Si2 grain boundaries were approximated as equivalent, employing a unified set of cohesive element parameters. Consequently, two sets of cohesive parameters were implemented in the model to characterize the grain boundaries and phase boundaries, respectively.

The significant lattice mismatch between the tetragonal U3Si2 and FCC UN structures inhibits the formation of coherent or semi-coherent interfaces, resulting in weak interfacial bonding. Consequently, the phase boundary may demonstrate the lowest fracture resistance under load. The key parameters governing these interfaces, specifically the maximum separation stress and fracture energy, are listed in Table 1 .

Table 1 Related parameters of cohesive elements. Interface type Parameter Nominal stress in normal direction Nominal stress in the first shear direction Phase boundary Nominal stress in the second shear direction Fracture energy Grain boundary Nominal stress in normal direction 8 / 34 Value

100 MPa

Nominal stress in the first shear direction Nominal stress in the second shear direction Fracture energy

10 J/m2

The UN-U3Si2 composite fuel is composed of two polycrystalline materials of UN and U3Si2. Accurate numerical simulation of this composite needs to incorporate the elastic property, irradiation creep, and irradiation swelling behaviors of each phase, as well as the evolution of interfacial fission gas bubbles. Consequently, the constitutive material models and their corresponding parameters are detailed sequentially below. 2.2.1.1 Elastic property The elastic modulus ( ) and Poisson' s ratio ( ) of UN depend on the theoretical density ratio and temperature given by [37]: . The specific expressions are = 0.258 1 − 2.375

= 1.26 In this study, a density ratio of 95% is assumed, with the simulation temperature of 800 K. The calculated elastic modulus ( ) and the Poisson' s ratio ( ) of the UN are 219.0 GPa and 0.264, respectively.

The elastic modulus ( ) and Poisson' s ratio ( ) of U3Si2 [38] are 120.0 GPa and 0.177, respectively. 픧 3 픧 3 9 / 34 2.2.1.2 Creep model UN and U3Si2 are polycrystalline materials, with their creep deformations mainly dominated by two mechanisms. One is the diffusion mechanism and the other is the dislocation motion mechanism. At low-to-intermediate temperatures, the creep regime is primarily dominated by diffusion mechanisms, encompassing both irradiation and thermal diffusion creep. The contribution of the dislocation creep mechanism becomes pronounced only at temperatures above 1000 K [39]. Under the specific condition of 800 K considered in this study, the creep model for UN and U3Si2 [39] is described by the following equation: + 2 exp − is the macroscopic creep rate (where constant (8.314 픧 the stress (adopt is the grain size (= 1 is the fission rate is the ideal gas $^{-1}$);); T is the temperature ( ). The coefficients for U3Si2 1 = 6.5926 × 10 for U3Si2 the coefficients are 20 퓗, 2 = 1.6138 × 10 114007 / 픧 2.2.1.3. Irradiation swelling model , 2 = 4.792, = 172647 / 픧 1 = 6.5248 × Irradiation swelling is primarily attributed to the accumulation of fission products within the fuel. Among the fission products, the noble gases Kr and Xe account for a substantial fraction, within a cumulative fission yield of ~ 26%. The formation of Kr and Xe bubbles contributes significantly to volumetric swelling. The irradiation-induced swelling of UN and U3Si2 is described using the following empirical model [40,41]: 10 / 34 = 2.15 픧 3 = 3.88008 퐵 where + 0.79811 퐵 is the theoretical density ratio (%, set to 95 in this work); the fuel burnup, with the unit of fissions per initial heavy metal atoms (represents). The is calculated as: 퐵 × 푀 × × where × 100 are the molar mass and density of the fuel phase, respectively; is the molar fraction of uranium; is the Avogadro constant; and represents the fission density, given by The irradiation swelling strain rate is calculated by converting the data according to the 퐵 = following equation: 풔 where ( ) represents irradiation-induced swelling; is the identity tensor. 2.2.1.4 Bubble self-growth model To simulate fission bubble growth under realistic irradiation conditions, the evolution of the bubble radius with irradiation time is described by the following empirical model [42]: 11 / 34 픦퐵 = 820 − 315 × 0.93 where is the time (− 1.025

2.2.2 Computational Model

The finite element model and algorithms employed for the composite fuel simulation are detailed in this subsection, as well as the method used to introduce fission gas bubbles at the interface. 2.2.2.1 FEM analysis model Currently, UN-U3Si2 composite fuel pellets are primarily fabricated by co-sintering U3Si2 and UN powders. The SEM morphology [2] of the pellets is shown in Fig. 2 [Figure 2: see original paper]. The microstructure of UN-U3Si2 composite fuel consists of U3Si2 phase dispersed within UN matrix phase; it can be also characterized as that the UN phase encapsulates the U3Si2 phase.

Fig. 2. SEM image of UN-U3Si2 composite fuel [2]. Based on the microstructural characteristics and phase distribution of the composite fuel, representative volume element (RVE) model with dimensions was constructed using the commercial 100 휇 software ABAQUS for finite element analysis. The model comprises the UN matrix, the × 100 휇 × 20 휇 U3Si2 phase, and the interface (Fig. 3 [Figure 3: see original paper]). The bulk regions were meshed using C3D6 elements, while COH3D8 elements were employed at the interface. The meshed RVE model consists of a total of 139,113 elements, including 6,097 cohesive elements. 12 / 34 Fig. 3. FEM model of UN-U3Si2 composite fuel: (a) The 3D representative volume element (RVE), with the UN matrix and U3Si2 phase are rendered in blue and red, respectively; (b) Three types of interface distribution: UN grain boundary, U3Si2 grain boundary and UN/U3Si2 phase boundary. 2.2.2.2 Interfacial Bubble Model In the treatment of interfacial bubbles, this study premises that the primary focus is the impact of pre-existing bubbles on interfacial fracture under irradiation. Consequently, the kinetics of bubble nucleation are not explicitly modeled. Bubbles of specific dimensions are randomly distributed across three types of interfaces: the UN-U3Si2 phase boundary, the UN-UN and the U3Si2-U3Si2 grain boundaries. In the numerical framework, a finite width is introduced to the bubble boundary to prevent numerical convergence problems. This regularization enables a continuous transition of properties (stiffness, stress, damage) between the bubble and the matrix, resulting in a robust and stable numerical solution.

Therefore, the interface is spatially subdivided into three zones: (A) intact material; (B) the bubble boundary; and (C) the bubble core, as illustrated in Fig. 4 [Figure 4: see original paper].

This study assumes that bubbles represent regions where lattice atoms are replaced by gas atoms or vacancy clusters. Consequently, these regions lose their load-bearing capacity, resulting in a localized discontinuity similar to cracking. The specific damage assignment rules for bubbles with finite-width interface are as follows:

Zone A (Intact material): For point located in this zone, the interface is regarded as intact, and the damage ( ) is set to 0. 13 / 34 Zone B (Bubble boundary): As we characterize bubble boundary as finite-width interface, the damage within this region B change from 1 (bubble) to 0 (intact matrix). In detail, if the point falls within bubble boundary, the damage is linear interpolated as a function of the distance from the center of bubbles according to Eq. (13):) = ‖ ‖ − 풭 (− 0 represents the width of bubble boundary, in Eq. (12). where can be calculated based Zone C (Bubble core): If the point is located in this zone, interface is assumed to be fully damaged, with of 1. 2.2.2.3 Algorithm Fig. 4. Schematic diagram of the interface region.

Finite element simulations of the uniaxial tensile behavior of UN-U3Si2 composite fuel at an irradiation temperature of 800 K were conducted in ABAQUS via UMAT subroutine.

The computational workflow of the UMAT developed for this study is shown in Fig.5. The program identifies the materials (interface/matrix) and runs the corresponding module.

For matrix element, the program invokes the bulk constitutive module. The routine begins by reading the current strain and initializing the stress. It then enters a constitutive iteration loop: based on the current stress state, the irradiation creep strain rate (14 / 34 and irradiation swelling strain rate ( ) are calculated to determine the total inelastic strain increment ( ). Then stress is updated via constitutive laws using the current strain, followed by a check to determine if the inter-iteration stress residual fails within the prescribed convergence tolerance. If convergence is not achieved, the iteration repeats using the updated stress until the criterion is met. Finally, the stress and inelastic strain for the current increment are updated.

For cohesive element, the program invokes the cohesive module. First, the mechanical driven damage ( ) are computed using the current displacement according to the traction-separation law, and the bubble growth-induced damage ( ) are calculated.

Then, the final damage is defined as the maximum of these two values ( ). Specifically, is determined by first calculating the max (current radius of fission gas bubbles using the growth kinetics from Eq. (4), and then ,) applying the rules in Eq. (13). It is noted that, for fully damaged elements, the stiffness is assigned a small positive value to enhance numerical stability. At the end of this module, the stress and damage state of the element are output. 15 / 34 Fig. 5 [Figure 5: see original paper]. Computational flowchart of the UMAT subroutine developed for the FEM simulation.

3 Results and Discussions

In this section, we detail the numerical simulation results concerning the interfacial mechanical response and microstructural evolution of UN-U3Si2 composite fuels. In section the mechanisms of interfacial damage are systematically explored. Through a comparative analysis of slow, medium, and rapid loading modes, it elucidates the interfacial failure behavior and uncovers the intrinsic relationship between strain rate and damage modes.

In section 3.2, we focus on the rapid-loading scenario, investigating the impact of fission gas bubbles on interfacial crack evolution. Finally, in section 3.3, we conclude with comprehensive discussions of these findings and critically assess the capabilities and constraints of the developed numerical model.

3.1 Interfacial Damage Mechanisms of UN-U3Si2 Composite Fuels

From the perspective of nuclear fuel engineering, the mechanical loading on a reactor core varies significantly between normal operational scenarios and tran-

sient accident 16 / 34 conditions. Consequently, investigating interfacial damage under different loading rates is essential, as it provides the critical theoretical foundation and data support necessary for assessing the structural integrity of fuel elements throughout their entire lifecycle, ranging from steady-state operation to anticipated transients. This section focuses on the dominant influence of loading rate on the interfacial behavior of composite fuels and elucidates the underlying competing mechanisms. Regarding boundary conditions, the bottom surface of the model was fully fixed ( ), while a uniform displacement was applied to the top surface along the y-direction. To represent different operating scenarios, the loading rates Ux = Uy = Uz = 0 were categorized as slow-loading ( ), medium-loading ( ) and rapid-loading (

3.1.1 Slow-loading mode

5× 10 . Final loading strain is set to 10% for all three cases.

As shown in Fig. 6 Figure 6: see original paper, under the slow-loading condition ( ), plastic strain constitutes a significant proportion of the total strain. Further analysis of the damage area (Fig. 6(b)) indicates that the macroscopic crack area remains zero or negligible, implying the absence of visible cracking or damage. This phenomenon can be attributed to the synergistic dominance of the extremely slow loading rate and the irradiation creep mechanism. Due to the extremely low loading rate, the internal stress accumulation is relatively slow. This allows sufficient time for irradiation creep to continuously relax the loading-induced stress.

Consequently, further stress buildup is effectively suppressed, maintaining the stress at a consistently low level. Consequently, interfacial stresses remain consistently below the crack initiation threshold, preventing the material from reaching critical damage conditions. Under these conditions, irradiation creep completely dominates the mechanical response of the material. Furthermore, the evolution of bubbles over time leads to an increase in the 'total damage area,' a trend that is highly consistent with the growth of the bubble area. After deducting the contribution of bubbles, the actual crack area is negligible, indicating that no significant crack nucleation or propagation occurred during this process. 17 / 34 Fig. 6. Temporal evolution of strain response and interfacial damage in slow-loading mode : (a) Evolution of total strain (ϵtot), elastic strain (ϵe)， plastic strain (ϵp), and total damaged area ( ); (b) Decomposition of the damaged area into bubble-induced (displays the interfacial damage ( ) distribution at the final time step ( ) contributions. The inset), and crack-induced (Scrack In summary, under this loading regime, the material accommodates external deformation t = tf demands primarily through plastic flow. The synergy between the plastic strains induced by irradiation creep and swelling and the slow loading rate establishes a "damage-safe" mechanism: stress is continuously dissipated before it can accumulate to levels capable of causing destructive failure. Therefore, the structural integrity of the material is maintained even as it undergoes significant plastic deformation. In this process, irradiation creep

plays a critical role in stress buffering and relaxation, effectively preventing the occurrence of mechanical failure.

3.1.2 Medium-loading mode

As illustrated in Figs. 7(a) and (b), during the initial phase of medium-rate loading), the contribution of plastic strain is relatively low. Consequently, stress rises rapidly, reaching the interfacial damage threshold at approximately 35 s, which triggers crack initiation and subsequent propagation. As loading progresses, the proportion of plastic strain gradually increases, leading to a deceleration in stress accumulation and a corresponding reduction in the crack propagation rate. Ultimately, a stable crack of finite length is formed along the interface.

In this regime, the damage evolution process is governed by two competing mechanisms:

External loading generates the driving force for crack initiation and propagation, whereas plastic flow (dominated by irradiation creep) continuously relaxes local stresses. The creep process effectively relaxes local stresses at the crack tip, continuously dissipating strain 18 / 34 energy and thereby inhibiting the driving force for propagation. Macroscopically, although the crack continues to extend under the driving stress, the continuous dissipation of strain energy by creep suppresses stress buildup at the crack front, resulting in a significant deceleration of the propagation rate. Consequently, variations in loading rate have a significant impact on this damage process. Further decreasing the loading rate delays crack initiation, reduces propagation speed, and potentially limits the final crack length; sufficiently slow, the behavior transitions to the previously described slow-loading (creep-dominated) mode. Conversely, increasing the loading rate causes interfacial stresses to reach the damage threshold in a shorter time, leading to earlier initiation and faster propagation, which may eventually evolve into a through-crack. If the rate is sufficiently high, the system shifts to the rapid-loading mode (detailed in the subsequent section).

Fig. 7 [Figure 7: see original paper]. Temporal evolution of strain response and interfacial damage in medium-loading mode: (a) evolution of total strain (ϵtot), elastic strain (ϵe), plastic strain (ϵp), and total damaged area (decomposition of the damaged area into bubble-induced (The inset displays the interfacial damage ( ) distribution at the final time step ( ), and crack-induced (Scrack); (b)) contributions.

In summary, under medium loading rates, the UN-U3Si2 composite fuel exhibits a t = tf transitional deformation mode between the rapid and extremely slow loading regimes. Its mechanical behavior is neither purely damage-dominated brittle failure nor purely creep-dominated safe deformation. The dynamic balance between stress accumulation and time-dependent relaxation, determined by the loading rate, plays a pivotal role in regulating the failure path of the composite fuel.

3.1.3 Rapid-loading mode

Under rapid-loading conditions (exhibits typical stress-driven quasi-brittle fracture behavior. As shown in Fig. 8 Figure 8: see original paper, the 5× 10 the UN-U3Si2 composite fuel 19 / 34 proportion of plastic strain is negligible, indicating that the material undergoes almost no significant plastic deformation. Simultaneously, as shown in Fig. 8(b), the crack area increases rapidly, leading to the formation of a continuous crack across the domain within a short timeframe, which indicates severe interfacial failure. The fundamental reason for this behavior lies in the excessively high loading rate, which results in an insufficient time window for the activation of time-dependent deformation mechanisms such as irradiation creep. Consequently, the material is unable to effectively relax local stresses through the creep process. Instead, the work done by external loads is primarily converted into elastic strain energy and interfacial fracture energy, causing stress to accumulate sharply at the interface and rapidly exceed the strength threshold. Once damage initiates, cracks propagate swiftly along the weakened interface and rapidly coalesce with defects such as pre-existing bubbles, ultimately forming a network of macroscopic through-cracks. This process is essentially a stress-driven, quasi-brittle fracture event: macroscopic cracks initiate and extend rapidly while simultaneously connecting with or engulfing existing microscopic defects (e.g., fission gas bubbles). This establishes a through-thickness macroscopic crack path in a short time, leading to global material failure.

In summary, under the rapid-loading mode, stress-driven crack initiation and propagation constitute the dominant mechanism, while time-dependent deformation and damage processes are significantly suppressed. These results indicate that under high-rate transient conditions (such as accidents or power ramps), the failure behavior of UN-U3Si2 composite fuel is highly sensitive to interfacial strength and defect distribution (particularly fission gas bubbles). This insight provides critical engineering implications for assessment of safety margins. The specific mechanisms regarding the impact of interfacial strength and defect distribution on interfacial failure under rapid-loading will be investigated in detail in section 3.2. 20 / 34 Fig. 8. Temporal evolution of strain response and interfacial damage in rapid-loading mode: (a) evolution of total strain (ϵtot), elastic strain (ϵe), plastic strain (ϵp), and total damaged area ( ); (b) decomposition of the damaged area into bubble-induced (displays the interfacial damage ( ) distribution at the final time step ( ) contributions. The inset), and crack-induced (Scrack t = tf

3.1.4 Theoretical analysis of rate-dependent constitutive relation

Although the simulation results in sections 3.1.1 ~ 3.1.3 have demonstrated the significant impact of loading rate on interfacial damage modes, the critical conditions under which the competition between loading rate and creep quantitatively

governs stress accumulation and relaxation remain unclear. To mechanistically explain the distinct behaviors observed, where cracking is fully suppressed at slow-loading condition (propagates almost instantaneously at rapid-loading condition ( ). This section derives an analytical solution for steady-state stress within a unified framework. By 5× 10 establishing the quantitative relationship among loading rate, irradiation creep, and bubble-induced damage, this analysis provides a theoretical benchmark for the investigation of bubble-crack interactions in section 3.2.

In the present constitutive framework, the plastic strain rate is formulated to capture irradiation-induced inelastic behaviors as follows: = + where σ denotes the current Cauchy stress (MPa). The parameter represents the effects of irradiation creep according to Eqs. (7) and (8). represents the effect of irradiation swelling, as given by Eqs. (11) and (12).

Within a single time increment, the stress increment is expressed as: 21 / 34 denotes the elastic stiffness tensor of the material, and represents the where, total strain increment within the current step. By substituting Eq. (14) into Eq. (15), the differential form of the stress evolution is obtained as: − This equation is reformulated as a first-order ODE with respect to time , given by:

Since characterizes the effect of irradiation swelling, its evolution depends only on irradiation time, exhibiting a monotonic increase as time extends. Among the three loading modes studied, the slow-loading mode exhibits the lowest loading rate and requires the longest duration to reach the prescribed strain. Under this condition, the deviation between and the loading rate is minimized. Even under this extreme condition, estimations indicate an order-of-magnitude relationship of approximately , using the experimental data with Eqs. (8-11). Conversely, in the rapid and medium loading modes, the significantly shortened loading duration leads to a reduced , while increases. This renders the relative influence of 22 / 34 more negligible. So, within the scope of this study, the contribution of to the total deformation is minor. Consequently, the general solution of Eq. (17) can be estimated from the general solution of the simplified equation: , the solution to Eq. (18) approaches:

It follows that under irradiation, the steady-state stress in the material is governed by the ratio of the external loading rate ( ) to the irradiation creep effect ( ) within the timeframe of this study. Here, serves as a constant input parameter consistent with the applied loading conditions.

In the slow-loading mode (section 3.1.1), the formula predicts that a smaller leads to a stabilized, lower stress level after a long duration. This theoretical behavior is perfectly captured by the simulation, where irradiation creep-induced relaxation effectively counteracts the stress accumulation from external loading. Conversely, for rapid-loading scenarios (section 3.1.3), Eq. (19) implies that a larger results in significant stress buildup. This corresponds to the numerical observation where stress rapidly accumulates and exceeds the critical limit, thereby triggering damage evolution.

In summary, the evolution of interfacial stress is collectively governed by the loading rate, irradiation creep, and irradiation swelling. Specifically, the loading rate directly dictates the rate of stress accumulation. Irradiation creep characterizes the material' s capacity to relax and dissipate stress; a higher creep rate results in a lower steady-state stress level under identical external loading conditions. Irradiation swelling, while introducing an additional strain rate via volumetric expansion, contributes minimally to the interfacial stress due to its relatively small magnitude. Consequently, interfacial stress is primarily dominated by the 23 / 34 loading rate and irradiation creep. Since irradiation creep is an intrinsic material property defined by Eqs. (7) and (8), which cannot be directly adjusted, the loading rate serves as the key variable that can be prescribed in operational scenarios or numerical simulations. Varying the loading rate fundamentally alters the interfacial evolution mechanism in UN-U3Si2 composite fuel. This study reveals a significant loading rate sensitivity in the interfacial damage evolution of the material: a mere 50-fold increase in loading rate is sufficient to induce a transition from a state of structural integrity to a rapid failure mode. This occurs because steady-state stress correlates linearly with loading rate when the swelling rate is much lower than the strain rate. At slow-loading mode, creep dominates stress relaxation, keeping stresses low and suppressing damage nucleation. Conversely, under the rapid-loading mode, insufficient relaxation causes the steady-state stress to exceed the fracture threshold.

We identify this transition as a fundamental mechanism relevant to in-pile service conditions, particularly during transients like reactivity-initiated accident (RIA) or thermal shocks from emergency shutdowns. Understanding this mechanism is vital for predicting fuel integrity and optimizing safety margins under accident conditions.

3.2 Interfacial Bubble-Crack Interactions

In this model, fission bubbles are treated as defects that act as stress concentrators, particularly under rapid-loading where creep relaxation is insufficient to mitigate their impact.

Consequently, this section focuses on the rapid-loading mode. We systematically investigate the influence of bubble location and density on interfacial crack evolution within the UN-U3Si2 composite fuel by comparing scenarios with bubbles distributed along grain or phase boundaries against a bubble-free baseline. The loading rate and magnitude for all cases in this section are consistent with those in section 3.1.3.

3.2.1 Crack Evolution without Bubbles

In the microstructure of UN-U3Si2 composite nuclear fuel, the interfaces are critical regions that affect its mechanical properties and integrity. Among them,

the triple junction interface of UN-U3Si2, due to geometric features, becomes a significant area of stress concentration.

Finite element simulations of uniaxial tension were first performed on the bubble-free model, with the results presented in Fig. 9 [Figure 9: see original paper]. The stress distribution at the onset of crack 24 / 34 initiation is shown in Fig. 9(a). It reveals significantly higher stresses in the side regions (the yellow regions). This is attributed to the higher stiffness of the UN material located in these regions and the specific boundary conditions. The magnified inset (red box) reveals that the local stress at the phase boundary has reached 50 MPa, satisfying the critical damage threshold. The damage state index, defined as $\Phi =$ max 2 , quantitatively characterizes the current interfacial state by comparing the local stress with the critical damage stress, where signifies the onset of interfacial failure.

As shown in Fig. 9(b), the maximum value of damage state index is localized at the $\Phi \geq 1$ heterogeneous triple junctions. These junctions act as primary stress concentrators, rendering them preferential sites for crack initiation, as evidenced by Fig. 9(c). Subsequently, the damage evolution depicted in Figs. 9(d) ~ (f) demonstrates that cracks propagate predominantly through the phase boundaries, favoring interfaces oriented perpendicular to the applied load.

Crack initiation occurs primarily at heterogeneous triple junctions due to significant stress concentrations and lower fracture strength thresholds in these regions. Specifically, the stress concentration stems from special geometric feature and the mismatch in elastic constants between the two phases. Coupled with the lower fracture strength thresholds, these factors render heterogeneous triple junctions as the preferential sites for crack nucleation under local stress concentration. Following initiation, damage evolution is driven by the external load, with cracks tending to propagate along interfaces perpendicular to the loading direction. Regarding microscopic path selection, propagation is predominantly confined to the phase boundaries. This is attributed to the lower fracture toughness of phase boundaries compared to grain boundaries, which reduces the energy barrier for propagation and provides an energetically favorable path for crack extension. Consequently, heterogeneous triple junctions serve as the primary initiation sites, while crack propagation proceeds predominantly along phase boundaries oriented perpendicular to the external load. 25 / 34 Fig. 9. Simulation of crack initiation and propagation in the interface with no bubble : (a) distribution of interfacial stress ($ $1) at crack initiation ( ), with the inset highlighting stress concentration at the triple junction; (b) contour of the damage state index (t = 6.5 s at crack initiation (the damage at crack initiation (t = 6.5 s) ,where regions with $\Phi \geq 1$ indicate the onset of failure; (c) distribution of $\Phi =$ max); (d) ~ (f) temporal evolution of damage propagation at t = 6.5 s 10.73 s, 11.33 s, 15.18 s

3.2.2 Fission Bubble Effects on Interfacial Fracture

The behavior of fission gas bubbles is a critical factor governing the performance and safety of nuclear fuels under irradiation. From a micromechanical perspective, these bubbles act as significant porosity defects that drastically alter the mechanical response of the fuel material. Consequently, a fundamental understanding of how bubbles influence fuel interfacial behavior is essential. This section systematically elucidates the impact of bubble location and density on interfacial crack evolution. In section 3.2.2.1, the specific roles of bubbles at phase boundaries and grain boundaries in crack initiation and propagation are investigated. Subsequently, in section 3.2.2.2, the effects of bubble concentration are detailed by comparing crack evolution scenarios under varying bubble densities, providing an in-depth analysis of how dense bubble clusters affect fracture behavior and fuel pellet integrity. To facilitate comparison, the loading conditions in all scenarios within this section are identical to the simulation conditions of the bubble-free system. 26 / 34 3.2.2.1 The Role of Fission Bubble Positions This section systematically elucidates the influence of fission gas bubble positions on interfacial fracture behavior. The results demonstrate that phase-boundary bubbles shift the crack nucleation sites from the heterogeneous triple junctions to the edge of the nearest bubble, and lead to premature failure, whereas bubbles at grain boundaries contribute minimally to this initiation process. Furthermore, regardless of whether bubbles are located at phase or grain boundaries, cracks exhibit a strong tendency to propagate towards bubble-rich regions. This confirms that bubble distribution is the governing factor determining the fracture path.

When bubbles are present at phase boundaries, the contour of the damage state index is presented in Fig. 10 [Figure 10: see original paper]. A crack is clearly observed initiating at the bubble edge, propagating initially toward the triple junction (indicated in red). In this figure, the blue regions correspond to the pre-existing bubbles, whereas other colored gradients represent the damage evolved under the current stress state. Furthermore, compared to the bubble-free system, the onset of cracking in this model is advanced to t = 5.95 s. This corresponds to an 8.46% reduction in initiation time relative to the bubble-free baseline, a result directly attributable to the presence of phase-boundary bubbles.

Fig. 10. Simulation of crack initiation with bubbles in phase boundaries: contour of the damage state index () at crack initiation ( ), where regions with $\Phi = \max \Phi \geq 1$ indicate the onset of failure. t = 5.95 s A comparison of the crack locations in Fig. 9(b) and Fig.10 reveals that the presence of phase-boundary bubbles alters the site of initial crack nucleation. Under identical external conditions, the initiation site shifts from the heterogeneous triple junctions to the edge of the 27 / 34 nearest bubble, with the initial propagation direction oriented toward the triple junction. This shift is primarily attributed to the higher stress concentration at the bubble edge compared to the heterogeneous triple junction. Furthermore, the stress threshold for initiation at phase boundaries is

inherently lower than that at grain boundaries. Additionally, local stress concentrations at triple junctions near bubbles promote crack initiation in neighboring areas.

Consequently, the bubble edge nearest the triple junction emerges as the preferential site for crack nucleation.

As damage evolves, the crack extends toward new interfaces. As shown in Fig. 11 Figure 11: see original paper, the final propagation trajectory follows path 1. This path reveals a strong tendency for crack propagation to coalesce with bubbles, specifically those located at phase boundaries. The primary reasons are twofold: first, the lower interfacial energy at phase boundaries; and second, the stress concentration induced by fission bubbles. These factors facilitate crack propagation, prompting the crack to select this energetically favorable path. Distinct cracks continuously coalesce, ultimately forming a transverse crack across the domain. However, since this specific path coincides with the trajectory observed in the bubble-free scenario, a supplementary simulation was conducted to determine if the propagation path changes when bubble positions are altered, thereby verifying the tendency for cracks to select bubble-rich paths. Even after altering the bubble positions, the crack continues to propagate along the direction of high bubble density. As shown in Fig. 11(b), the crack preferentially propagates along path 2, which corresponds to a trajectory with relatively higher bubble density.

In conclusion, phase-boundary bubbles fundamentally alter the fracture mechanism by shifting the crack initiation site from the heterogeneous triple junction to the edge of the nearest bubble. During crack propagation, the spatial distribution of bubbles significantly influences the fracture trajectory. Cracks exhibit a strong tendency to coalesce with bubbles, making bubble-rich zones the preferential pathways for crack extension. 28 / 34 Fig. 11. Comparison of damage evolution patterns under different bubble spatial configurations in phase boundaries: (a) damage propagation at damage evolution sequence (for the initial configuration; (b) t = 9.11, 11.08) after changing the bubbles positions. 12.24 s However, the presence of grain-boundary bubbles does not shift the crack initiation site, t = 8.41, 10.96, 13.21 s as the local stress rise is insufficient to overcome the inherent strength disparity between grain and phase boundaries. As evidenced by Fig. 12 Figure 12: see original paper, initiation remains localized at the heterogeneous triple junction, occurring at the same timestep as in the bubble-free system. To analyze the local stress state, stress was monitored at four key locations defined in Fig. 12(a).

Location A is situated at the phase boundary, while Location B lies on a bubble-free UN grain boundary. Locations C and D are located on a bubble-containing UN grain boundary, with C positioned remote from the bubble and D in the vicinity of the bubble. Although Location B exhibits higher absolute stress (64.6 MPa) than Location A (46.6 MPa), its higher damage threshold maintains a 35% safety margin, whereas Location A operates within a critical 7% of failure. Even with bubble-induced stress concentrations elevating Location D (69.2 MPa)

above Location C (66.1 MPa), the stress remains below the threshold. Instead, heterogeneous triple junction near A (phase boundary) reaches its initiation limit (50 MPa) 29 / 34 first.

The crack propagation behavior is shown in Figs. 12(c) ~ (e). Based on the final fracture morphology, The crack preferentially propagates along a path simultaneously satisfying three conditions: perpendicular orientation, a high fraction of phase boundaries, and high bubble density. As indicated, the path marked by the red solid line corresponds to high bubble density and a perpendicular orientation, whereas the red dashed line aligns with a high fraction of phase boundaries and the perpendicular direction. However, neither pathway satisfies all three conditions simultaneously. Consequently, the actual crack propagation deviates from these two trajectories. Instead, the final route shown in Fig. 12(e) follows a path that successfully integrates all three factors. This indicates that crack propagation induced by grain-boundary bubbles is consistent with that at phase -boundary bubbles system.

Through a comprehensive analysis of grain boundary bubbles, it was found that the presence of fission gas bubbles at grain boundaries has a negligible impact on crack initiation under the current model and loading conditions. Regarding crack propagation, corroborates the conclusions drawn in the phase-boundary system, which propagates along bubble-rich phase boundaries oriented perpendicular to the external load. 30 / 34 Fig. 12. Simulation of crack initiation and propagation with bubbles in grain boundaries : (a) distribution of interfacial stress ($ $1) at crack initiation ( ), with marked stress at phase boundary (Location A), UN grain boundary without bubbles (Location B), away from bubbles edge (Location C), bubble edge (Location D) and heterogeneous triple junctions; the damage state index ((b) contour of t = 5.95 s 2) at crack initiation ( ), where regions with $\Phi \geq 1$ indicate the onset of failure; (c) ~ (e) temporal evolution of damage propagation at t = 5.95 s 9.18 s, 11.00 s, 3.2.2.2 The Role of Fission Bubble Density 13.60 s Based on the preceding analysis, the role of fission bubbles is non-negligible. The presence of fission bubbles fundamentally influences the initiation and propagation of interfacial cracks in nuclear fuel composites. To investigate the impact of bubble density, this subsection examines crack evolution in high-density bubble regimes, by modeling 40 bubbles randomly distributed along phase and grain boundaries, and comparing the results with a 10-bubble system. The analysis indicates that high bubble density drives localized microcracking and network formation, resulting in fine-scale fuel fragmentation and accelerated fission gas release via crack-assisted venting. 31 / 34 The temporal evolution of the damaged area for the 10 and 40 bubble systems is compared in Fig. 13 Figure 13: see original paper, with the inset highlighting the initial damage stage, which reveals a distinct disparity between the dense and sparse systems during the initial stages. This disparity is ascribed to the rapid formation of inter-bubble microcracks within the dense system, which triggers an accelerated accumulation of damage. The evolution process in the dense system can be categorized into three primary regimes: crack initiation around bubbles (stage), crack nucleation at phase boundaries (stage

) and subsequent crack propagation (stage). These correspond to stages in the sparse system, respectively.

III40 III10 In the dense system, during first regimes, it exhibits a rapid surge in damage area (stage ,), followed by a deceleration in the growth rate (stage). The abrupt rise in stage I40 is attributed to the reduced inter-bubble spacing and significant stress concentration effects.

These factors facilitate strong bubble-bubble interactions, inducing the rapid formation of local microcracks. The subsequent deceleration occurs because the initiation of these local cracks partially relieves the local stress, thereby reducing the driving force. Here, coalesced bubbles effectively behave as a single large void, exhibiting a growth rate comparable to the sparse system. As loading progresses to stage , multi-site crack nucleation along phase boundaries triggers a steep rise in the damaged area, followed by stable crack propagation in stage . In contrast, the first stage of the sparse system (stage) is a slow and steady accumulation of damage. Despite crack initiation at bubble edges, III40 the large inter-bubble spacing prevents microcrack coalescence. The subsequent evolution in stages closely parallels that of the dense system (stage corresponding to crack nucleation at phase boundaries and subsequent propagation, III10 III40 respectively. This similarity in the stage is attributed to a multi-site crack nucleation mechanism at phase boundaries, which is primarily governed by the interfacial fracture strength and external loading, independent of bubble density. Notably, the higher total damage area in the dense system stems from the more microcrack accumulation during the early initiation stage.

Comparing Figs. 13(b) with (c) and (d) reveals that the fundamental failure mechanism remains consistent regardless of bubble density. In both systems, bubbles at phase boundaries shift crack initiation to their edges and guide propagation through bubble-rich regions, 32 / 34 confirming the universality of this failure mode. However, in the dense scenario, reduced inter-bubble spacing causes high stress concentrations, leading to many localized cracks (indicated in black). The presence of localized cracks effectively establishes a weakening path traversing the bubbles (Fig. 13(c)). Unlike the isolated damage zones observed in the sparse system, these dense clusters facilitate rapid crack coalescence along the weakened paths, ultimately leading to more complex cracks network. Furthermore, the dense distribution of bubbles promotes the intersection of cracks, leading to the breakdown of the continuous fuel matrix into small, isolated fragments. Fuel cracking and pulverization during a LOCA has been observed, however, the mechanism driving the phenomenon is still not clear [43]. The present simulations demonstrate that inter-bubble microcracking facilitates the formation of complex fracture networks, offering a plausible explanation for this fine-scale fragmentation. This fragmented structure poses a significant challenge for reactor safety: in the event of cladding rupture, fine fuel fragments are highly susceptible to coolant washout and subsequent release into the primary circuit, significantly exacerbating the severity of accident consequences.

Crucially, the formation of such interconnected fracture networks not only com-

promises the structural integrity of the fuel, but also establishes direct physical pathways for fission gas release (FGR). Fission gas release (FGR) refers to the migration and escape of gaseous fission products (primarily Xe and Kr) from the fuel matrix into the free volume of the fuel rod. It critically degrades fuel performance by reducing gap thermal conductivity, increasing internal pressure, and accelerating cladding corrosion. In actual reactor environments, complex mechanical stresses driven by thermal expansion mismatches, differential swelling, and power ramps are inherent. Under these conditions, the localized crack-dominated bubble interlinkage observed in Figs. 13(b) and (d) becomes inevitable. Consequently, connectivity is expected to significantly contribute to the overall FGR. 33 / 34 Fig. 13. Damage evolution under different bubble density: (a) comparison of total damage accumulation) over time between 10 and 40 bubbles. The inset details a magnified view of the early loading stage, identifying distinct stages of damage progression; (b) final damage morphology for the 10-bubble case; (c) crack evolution occurs along a path weakened by extensive local micro-cracking for the 40-bubble case; (d) final damage morphology for the 40-bubble case, with local microcracks marked by black circles.

Under steady-state conditions without macroscopic damage, FGR is generally governed by diffusion-controlled mechanisms, relying on the slow migration and coalescence of bubbles to form release pathways. However, based on the analyzed above, cracks can interconnect bubbles prior to significant growth, establishing a route for gas venting to the fuel rod free volume, thereby further influencing the FGR behavior. The release network induced by cracking significantly differs from that formed by traditional diffusion, stemming from the fundamental disparity in their underlying physical mechanisms. Specifically, the diffusion-based network is governed by the diffusion of gas atoms and vacancies, whereas the crack-based network is primarily driven by fuel deformation and stress distribution. 34 / 34 Consequently, these distinct release pathways may lead to divergent FGR kinetics, ultimately impacting fuel service life and safety. Therefore, accurately capturing crack evolution is indispensable for a comprehensive understanding of in-pile fuel behavior.

In this subsection, the failure mechanism identified in sparse bubbles systems extends to dense systems, confirming its applicability across varying burnup levels (different bubble densities). Specifically, high bubble density promotes localized microcracking between adjacent bubbles, forming preferential fracture paths. This drives the development of complex crack networks that cause fine-scale fuel fragmentation. Such fine fragmentation significantly increases the risk of fuel dispersal upon cladding rupture, underscoring the critical need to incorporate bubble-density-dependent fracture models into high-burnup safety assessments.

Furthermore, the crack fundamentally alters FGR kinetics by interconnecting bubbles prior to significant growth. This crack-assisted mechanism accelerates gas venting compared to traditional diffusion, making the accurate capture of crack evolution indispensable for predicting fuel performance and safety.

3.3 Discussions

The 3D damage model developed in this study enables, for the first time, a fully coupled simulation of irradiation creep, swelling, and fission gas bubble dynamics at a three-dimensional scale. Unlike previous models confined to single operating conditions, our framework accommodates complex and high bubble densities configurations, demonstrating the universality of bubble-induced failure mechanisms. Beyond elucidating the interfacial behavior of UN-U3Si2 composite fuels, the established model possesses significant extensibility to other nuclear fuels where interfacial fracture is the dominant failure mode and the explicit consideration of interfacial bubbles is necessary.

Based on the theoretical framework established in section 3.1.4, the approximate constitutive equation (Eq. 19) quantifies the intrinsic dependence of interfacial stress on the loading rate . This relationship demonstrates that stress is linearly proportional to the loading rate, when the contribution of irradiation swelling is negligible compared to that of the mechanical loading. While specific variations in irradiation creep and swelling compliance may induce fluctuations, the model remains valid at the order-of-magnitude level.

Crucially, higher loading rates directly amplify interfacial stress. This surge, approaching an 35 / 34 order of magnitude, is typically sufficient to overcome the critical fracture strength. This precipitates the shift from structural integrity to crack initiation and propagation, fundamentally altering the service state of the entire fuel pellet. Consequently, this work provides a robust foundation for the damage prediction and safety assessment of diverse accident tolerant fuel (ATF) systems.

However, there are some limitations and assumptions in the current model that should be noted. We only explicitly modeled bubbles located at the grain and phase boundaries, without explicitly modeling the intragranular bubbles. This simplification is based on the following considerations: intragranular bubbles (bubbles inside the grains) are extremely small and numerous [44], and modeling all of them explicitly would result in an excessive computational cost. Therefore, their effect was simplified and included through the irradiation swelling model by capturing volume change due to small intragranular bubbles. Since this study focuses on interfacial fracture, this simplification is acceptable.

Furthermore, the shape of the bubbles in interface was assumed to be perfectly circular.

In reality, bubbles can have irregular shapes, like ellipse, lenticular or other complex contours.

However, modeling the evolution of such complex bubble shapes requires knowing how their boundaries change over time. Although this is theoretically possible in the current model, experimental data are lacking. Considering that this work focuses on the effect of bubbles on crack evolution, and using different convex shapes would not fundamentally change the mechanism, circular bubbles

are used as a typical case for this study. Due to the lack of specific data for bubble growth in UN-U3Si2, we used empirical formulas based on UO2 data.

Future work will aim to update these parameters as more experimental data becomes available.

Regarding material interface parameters, some material properties (fracture parameters) for the interface were estimated because experimental data for UN-U3Si2 is limited. It is important to emphasize that the main goal of this study was to reveal the failure mechanisms and qualitative trends, rather than to provide exact quantitative predictions. However, the calibration of material parameters can be conducted for more accurate predictions.

4 Conclusions

To address the interfacial mechanical response, fracture mechanisms, and the role of 36 / 34 fission gas bubbles of UN-U3Si2 ATF under different service environments, this study developed a 3D damage model incorporating fission bubble evolution. Using this model, we deeply explore the complex damage mechanisms of the interface and reveal the role of fission bubbles on interfacial fracture behavior. The key conclusions gained from this study are summarized as follows:

A three-dimensional (3D) damage model coupling the finite element method (FEM) with a cohesive zone model (CZM) was developed. In this model, a constitutive model incorporating irradiation creep and swelling is applied to the matrix, while modified CZM explicitly capturing the dynamic evolution of fission gas bubbles are embedded at the interface.

The interfacial fracture behavior is strongly dependent on the loading rate. While slow loading allows creep relaxation to suppress cracking, rapid loading drives stress-induced failure. Theoretical modeling confirms stress scales linearly with strain rate; consequently, rapid loading induces stress surges that exceed the critical threshold, triggering damage initiation.

Fission gas bubbles in the phase boundaries significantly change the crack evolution process. In the absence of bubbles, heterogeneous triple junctions are the primary nucleation sites due to stress concentration. Conversely, the presence of bubbles at phase boundaries changes the crack initiation sites and significantly accelerating interfacial failure. Moreover, by simulating bubbles at grain and phase boundaries, the cracks preferentially propagate along bubble-rich phase boundaries oriented perpendicular to the external load.

Comparative simulations of low and high bubble densities reveal that high bubble density promotes local inter-bubble microcracking, which interconnects to exacerbate fuel fragmentation. These macroscopic cracks create rapid pathways for FGR, shifting the release mechanism from diffusion-controlled to crack-induced. Identified as a novel FGR mechanism distinct from bubble coalescence, cracking not only modulates FGR kinetics but also profoundly impacts the fuel's

thermal profile, operational lifetime, and pellet-cladding mechanical interaction.

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