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Peridynamic investigation on thermal fracturing behavior of ceramic nuclear fuel pellets under power cycles

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ABSTRACT

A coupled thermo-mechanical bond-based peridynamic model is developed to investigate thermal fracturing behaviors, including random initiation and subsequent propagation of interacting thermal cracks, in ceramic nuclear pellets under power cycles. To go beyond the differences of typical time scales between thermal and mechanical systems, a multi-rate time integration scheme is introduced to the numerical model. A penalty method for contact between the fuel pellets and cladding is also incorporated into the coupled model. Two benchmark examples are provided to prove the correctness and accuracy of the proposed numerical model. Thermo-mechanical fracturing behaviors of fuel pellets under power cycles are then investigated using the coupled bond-based peridynamics, that can accurately predict realistic thermal crack patterns, including both radial and circumferential cracks. From the numerical results, it is found that radial cracks occur during power rises, but circumferential cracks initiate when the power is ramped down. The numerical results are in good agreement with previous experimental observations. In addition, the influence of cyclic power amplitude, cyclic power rate, cyclic power types, and convective heat transfer between fuel pellets and cladding on thermal fracturing behaviors of fuel pellets are studied. The numerical results can provide references for the design of nuclear fuel pellets.

1. Introduction

Thermo-mechanical behaviors of light water reactor fuel rods are significantly affected by failures of ceramic fuel pellets, both at the engineering scale and at the mesoscale [1–3]. Uranium dioxide (UO_2) is typically the primary component of the ceramic nuclear fuel pellets [2]. Researchers discovered that the thermal conductivity of UO_2 decreases with increasing temperature and non-stoichiometry [4]. In addition, the ceramic fuel pellets are placed in cladding, and there exist gaps between the fuel pellets and the cladding, that leads to further complexity of this problem. In the early life of fuel pellets, large thermal gradients result in the initiation and propagation of radial cracks at microscopic, mesoscopic, and macroscopic scales during the initial power ramp because of the fission process. On the one hand, significant microscopic structural changes and deterioration of the fuel pellets become the limiting factors for long term and transient reactor performance [5]. On the other hand, the formation of thermal cracks at multiple scales decreases the thermal conductivity within the fuel, and they are important contributors to the decrease in bulk thermal conductivity over the whole life of the fuel as the burnup increases [3]. Moreover, thermal cracking behaviors in fuel pellets play critical roles in cladding failures caused by pellet-clad mechanical interaction (PCMI) [5,6]. Therefore, it is essential to understand the thermal and thermo-mechanical behaviors of ceramic nuclear fuel pellets for the evaluation of fuel performance, and for preventing potential nuclear accidents.

In the past decades, nuclear fuel modeling was conducted in support of fuel management in numerous reactor systems. The bulk of previous numerical simulations were focused on the standard finite element methods (FEM). A number of researchers applied FEM to simulate the mechanical behaviors of fuel pellets in the radial direction, under axisymmetric assumptions, by disregarding the coupling of multiple physical system and crack propagation in fuel pellets [7,8]. To model fuel pellets in a multiple physical system, i.e., coupled thermo-mechanical conditions, Ramirez et al. [9] applied FEM to couple heat conduction and mechanical deformation in UO_2 fuel rods in a one-dimensional (1-D) configuration, using COMSOL Multiphysics®. Newman et al. [10] developed a coupled thermo-mechanical model with heat and oxygen diffusion in UO_2 fuel rods to investigate the opening of a pre-existing crack in a fuel rod caused by thermal expansion.

A number of previous attempts were conducted to simulate crack

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initiation and propagation in fuel pellets under power cycles. Jankus and Week [11] implemented the modification of pellet material properties, such as Young's modulus, Poisson's ratio, and creep parameters, into FEM to represent pellet damage. Marchal et al. [12] incorporated smeared cracking models into FEM to study thermal fracturing behaviors of fuel pellets. Williamson and Knoll [13] simulated fuel pellet cracking using interface elements to model cracks as discrete entities with cohesive zone models at pre-defined locations in FEM meshes. Williamson et al. [14] performed a multi-dimensional multi-physics finite element analysis of nuclear fuel pellets by including fracture via relocation and smeared crack models. Although the abovementioned numerical models were applied to study the thermo-mechanical behaviors of fuel pellets, certain limitations of stress singularities at crack tips, crack initiation, and propagation still existed within the framework of FEM. Huang et al. [3] tried to eliminate the limitations within FEM, and simulated thermally driven randomly initiated cracks in fuel pellets using the discrete element method (DEM). However, in a previous numerical study [3], re-meshing techniques are required in the conventional FEM and crack growth paths in different hierarchical forms could not be captured. To improve the capacity of dealing with fracture problems in conventional FEM, some scholars proposed strain softening elements [15] and efficient re-meshing techniques [16–18], which are important contributions in the development of FEM. Moreover, some meshfree numerical methods, such as 'cracking particle model' (CPM) [19,20] and screened poisson equation approaches [21], were proposed to capture crack initiation and propagation, spontaneously.

As an alternative continuum model in solid mechanics, peridynamics was formulated in terms of integro-differential equations, rather than partial differential equations, by Silling [22]. One of the advantages of peridynamics is that the governing equations of motion naturally support the presence of discontinuities in the deformation field [23]. A further advantage of the peridynamic theory is that the resulting equations of motion are naturally discretized using particle-based methods [24]. A number of scholars applied different peridynamic theories to study fracturing behaviors in different materials, including glass [25,26], PMMA [27–34], composite materials [35,36], ceramic [37–39], concretes [40,41], and rocks [42–48].

In addition, the bond-based peridynamic (BB-PD) model was developed to solve thermal diffusion, thermo-elastic, and thermodynamic problems. The 1-D and two-dimensional (2-D) thermal transfer models were formulated by Bobaru and Duangpanya [49,50] to solve temperature distribution problems with discontinuities. Oterkus et al. [51] also extended the fully coupled thermo-mechanical model to solve 1-D, 2-D, and three-dimensional (3-D) thermodynamic problems based on the BB-PD theory. Xu et al. [52] applied the BB-PD model to investigate the elastic vortices and instabilities of thermally-driven cracks in brittle materials. For the thermal fracturing behaviors of fuel pellets, Mella and Wenman [53] predicted the fracture behavior of a pellet for specified (pre-computed) temperature profiles using BB-PD. Oterkus and Madenci [4] employed BB-PD to predict cracking in a fuel pellet under a simple power ramp and power down. However, fuel pellets were in simple thermal conditions, and contacts between cladding and fuels were not considered in the previous study [4].

In this study, a coupled thermo-mechanical bond-based peridynamics (TM-BB-PD) model, with a new multi-rate explicit time integration scheme, is developed to investigate thermal fracturing behaviors in ceramic nuclear fuel pellets under different power cycles. The coupled TM-BB-PD model can be separated into two parts that are used to handle the heat transfer problems, mechanical deformation, and fracture problems. As the typical scales of thermal-mechanical systems may differ by several orders of magnitude, a new multi-rate explicit time integration scheme is implemented. In addition, a penalty method for contact between fuel pellets and cladding is incorporated into the coupled TM-BB-PD. Two benchmark examples are presented to validate the correctness and accuracy of the proposed coupled TM-BB-PD model in terms of solving thermo-mechanical deformation and thermal fracture problems, from not only a qualitative point of view, but also a quantitative point of view. The thermo-mechanical fracturing behaviors of fuel pellets under power cycles are then simulated to predict realistic thermal crack patterns, including both radial and circumferential cracks. It is found from numerical results that the radial cracks occur during the power rise, but circumferential cracks form when the power is ramped down. The present numerical results are in good agreement with previous experimental observations. The effects of cyclic heating amplitude, cyclic heating rate, cyclic power types, and convective heat transfer coefficients between fuel pellets and cladding on thermal fracturing behaviors of fuel pellets are also investigated.

This paper is organized as follows. The coupled thermo-mechanical bond-based peridynamic theory is described in Section 2. Two benchmark examples to verify the correctness and accuracy of the proposed numerical model are presented in Section 3. Thermal fracturing behaviors in ceramic nuclear fuel pellets are simulated in Section 4. Effects of cyclic heating amplitude, cyclic heating rates, cyclic power types, and convective heat transfer coefficients are discussed in Section 5. Conclusions are drawn in Section 6.

2. Coupled thermo-mechanical peridynamic methodology

2.1. Governing equations

2.1.1. Mechanical deformation

In the BB-PD theory [22,23], it is assumed that a spatial region $\Re_0$ in the reference configuration, as shown in Fig. 1(a), is occupied by material points. A material point $\mathbf{X}$ is related to other material points $\hat{\mathbf{X}}$ within the neighboring regions of $\mathbf{X}$, that can be assumed as a circular disk in 2-D models. The neighboring region of $\mathbf{X}$ is mathematically defined as:

$$\mathscr{H}_{\mathbf{X}} = \{\hat{\mathbf{X}} \| \hat{\mathbf{X}} - \mathbf{X} \| \leq \delta\} \tag{1}$$

where δ is the radius of a circular region centered at $\mathbf{X}$, defined as the horizon.

In contrast to classical continuum mechanics, the governing equation of peridynamics is formulated as an integro-differential instead of a partial differential equation, that is given as [22,23]:

$$\rho(\mathbf{X}, t)\frac{\partial^2 \boldsymbol{u}(\mathbf{X}, t)}{\partial t^2} = \int_{\mathscr{H}_{\mathbf{X}}} \boldsymbol{f}(\hat{\mathbf{X}} - \mathbf{X}, \quad \hat{\boldsymbol{u}}(\hat{\mathbf{X}}, t) - \boldsymbol{u}(\mathbf{X}, t), t) dV_{\hat{\mathbf{X}}} + \boldsymbol{b}(\mathbf{X}, t) \tag{2}$$

where ρ is the mass density, $\boldsymbol{u}$ is the displacement vector, $\boldsymbol{b}$ is the body force density, that is the external force applied unit reference volume, and $\boldsymbol{f}$ is the pairwise force density between two interacting material points $\mathbf{X}$ and $\hat{\mathbf{X}}$ with units $\mathrm{N/m^6}$.

The magnitude and orientation of the pairwise force density $\boldsymbol{f}$ are dependent on both the reference and deformed locations of two interacting material points. To conveniently express the pairwise force density $\boldsymbol{f}$, two relative variables are defined in the following forms:

$$\boldsymbol{\xi} = \hat{\mathbf{X}} - \mathbf{X} \tag{3}$$

$$\boldsymbol{\eta} = \hat{\boldsymbol{u}}(\hat{\mathbf{X}}, t) - \boldsymbol{u}(\mathbf{X}, t) = (\hat{\boldsymbol{x}} - \hat{\mathbf{X}}) - (\boldsymbol{x} - \mathbf{X}) \tag{4}$$

where $\boldsymbol{\xi}$ is the relative position vector in the reference configuration in Fig. 1(a), and $\boldsymbol{\eta}$ represents the relative displacement vector in the deformed configuration, as shown in Fig. 1(b).

At the instant t, the pairwise constitutive force density function between two material points $\mathbf{X}$ and $\hat{\mathbf{X}}$, within the interacting region $\mathscr{H}_{\mathbf{X}}$, can be characterized by the following general form:

$$\boldsymbol{f}(\boldsymbol{\xi}, \boldsymbol{\eta}, t) = f(s(\boldsymbol{\xi}, \boldsymbol{\eta}), \theta, t)\frac{\boldsymbol{\xi} + \boldsymbol{\eta}}{\|\boldsymbol{\xi} + \boldsymbol{\eta}\|} \|\boldsymbol{\xi}\| \leq \delta \tag{5}$$

where f is a scalar-valued function of the distance between material points in the reference and deformed configurations shown in Fig. 1(a)