Journal of the European Ceramic Society 38 (2018) 3037–3048

Contents lists available at ScienceDirect

Journal of the European Ceramic Society

journal homepage: www.elsevier.com/locate/jeurceramsoc

Original Article

Simulation of thermal shock cracking in ceramics using bond-based peridynamics and FEM

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ARTICLE INFO

Keywords:
Thermal shock cracking
Refractory ceramics
Bond-based peridynamics
Nonlinear heat transfer
Fracture

ABSTRACT

The effects of moderate intensity 'hot' or 'cold' shock in brittle solids have been extensively studied, while much less is known about thermal shock response during large temperature variations. In this study, a combined finite element – peridynamics numerical procedure is proposed for the simulation of cracking in ceramic materials, undergoing severe thermal shock. Initially, Finite Element nonlinear heat transfer analysis is conducted. The effects of surface convection and radiation heat exchange are also included. Subsequently, the interpolated temperature field is used to formulate a varying temperature induced action for a bond-based peridynamics model. The present model, which is weakly coupled, is found to reproduce accurately previous numerical and experimental results regarding the case of a 'cold' shock. Through several numerical experiments it is established that 'cold' and 'hot' shock conditions give rise to different failure modes and that large temperature variations lead to intensified damage evolution.

1. Introduction

Ceramics and refractories are an extremely diverse family of materials that have met wide applicability across many industries. They exhibit high compressive strength, hardness and melting point, low thermal and electrical conductivity as well as the ability to maintain their properties at elevated temperatures. Due to their excellent performance under elevated temperatures, typical applications include: dies for metal forming, liquid steel technologies, thermal barrier coatings and others [1,2]. Aluminum oxide (Al_2O_3) and zirconia (ZrO_2) are two commonly used engineering oxide ceramics [3]. However, the inherent brittle nature of ceramic materials makes them prone to cracking when subjected to sudden temperature variations. Due to its paramount importance, thermal shock induced cracking in ceramic materials has been studied by many researchers over the last decades. Plentiful studies in the literature, both numerical and experimental, aim to investigate the maximum temperature change a brittle material can withstand prior to cracking, thus estimating its thermal shock resistance [4–9]. Furthermore, thermal fatigue due to repeated temperature fluctuations is of high academic and industrial interest [10,11].

Investigations on the thermal induced stress field, have illustrated that specimens undergoing cold shock develop tensile stresses near the boundary and compressive stresses in the interior [7,8]. The reversed effect is observed during heating of the specimen where tensile stresses develop in the interior. Lu and Fleck [7] presented a systematical classification of solids based on their thermal resistance. Cracking of the material was investigated assuming a pre-existing crack embedded in the area under tension and the resulting stresses were compared with the maximum allowed. Bahr et al. [12] investigated the emerging crack patterns after water quenching of pre-heated quartz and glass plates and simulated the crack evolution using multiple-crack models [8].

Early investigations were carried out assuming pre-existing crack or cracks in the medium. More recent studies on thermal shock employ elaborate lattice [13], nonlocal ([14,15]) and gradient ([5,16]) models to simulate the initiation and propagation of cracks as well as approaches for the incorporation of microstructural characteristics [17,18]. Additionally, studies on the induced thermal stresses have illustrated that it is crucial to account for temperature dependent material parameters in the simulations [6,19]. Usually, materials tend to exhibit a softening behaviour as the temperature increases due to decrease of Young's modulus. As reported in [6], not considering the temperature dependency of the material properties tends to lead to underestimation of the actual thermal shock resistance. In their work, Papathanasiou et al. [19] carried out a detailed investigation on the thermomechanical response of ceramic refractories under extreme temperature changes. The nonlinear heat equation was solved using FEM for a 2D problem, taking into consideration radiation heat exchange and temperature dependant thermal and elastic material

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https://doi.org/10.1016/j.jeurceramsoc.2017.12.039
Received 17 October 2017; Received in revised form 12 December 2017; Accepted 20 December 2017
Available online 23 December 2017
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properties. The calculated temperature field was subsequently used to determine the induced stress field and the results were compared with those arising from linear models for different values of the Biot number.

In this study, the bond-based peridynamic theory is used for the simulation of fracture in brick-like alumina specimens during a sudden, extreme temperature change. The experimental and numerical results of cold shocked alumina, reported in [15], are compared with the results of the proposed method for validation purposes. Numerical results for cold shock of specimens with temperature dependent properties are derived as well. The model is also used to simulate the fracture of a hot shocked specimen. To the best of the authors' knowledge, numerical simulations for hot shock related analysis are scarcer, while some experimental procedures have been reported to yield results that are not easily reproducible [20].

The present study is organized as follows: Section 2 defines the problem considered and the temperature dependence of alumina's thermal and mechanical properties. In Section 3 the FE scheme employed for the solution of the nonlinear heat transfer problem is presented. The uncoupled peridynamic model and the nondimensional parameters employed are introduced in Section 4. Section 5 is devoted to the validation of the new solution methodology. This is achieved through comparison with the numerical and experimental results reported in [15]. The effect of including radiative heat transfer and temperature dependent thermal and mechanical material properties is also studied. In Section 6, the hot shock phenomenon is studied and the results are compared with observations from the relevant literature. Concluding remarks and suggestions for future work are included in Section 7.

2. Geometry and materials

Thermal shock is divided into two distinct categories: 'hot' shock and 'cold' shock. During a hot shock, the temperature of the material is rapidly increased, while in cold shock the temperature is decreased. Both cases are crucial for the identification of the maximum temperature variations a material can withstand prior to failure. In this study, thin rectangular alumina (Al_2O_3) specimens, subjected to sudden and extreme temperature variations, will be simulated numerically. For the cold shock case the pre-heated (to a specified temperature T_0) brick is assumed to undergo sudden heat exchange with a surrounding fluid of temperature $T_\infty = 293.15\,\mathrm{K} \ll T_0$. In the hot shock case, the specimen is assumed initially at room temperature $T_0 = 293.15\,\mathrm{K}$ and then heated due to exposure at an ambient with temperature $T_\infty \gg T_0$. Various values of T_0 for the cold shock and T_∞ for the hot shock will be considered during the simulations.

In all cases heat transfer is assumed to take place only in the xy plane. Fig. 1, illustrates the physical and numerical model under investigation. The specimen's half-length and thickness are $L = 5H$ and $W = 0.2H$ respectively where H is half the height. Taking advantage of the system's symmetry along y and x axes, only one quadrant of the initial domain is simulated. Adiabatic conditions apply to the edges that coincide with lines of symmetry. Convection and radiation loses occur on the other two edges, as shown in Fig. 1. Initially the specimen is assumed to be at a uniform temperature T_0 and stress free. The material is linear, isotropic, homogeneous and in pristine condition at the initial configuration.

Due to the severe temperature variations refractories experience throughout their lifetime, it is imperative to include the temperature dependency of the thermal and elastic properties. This need is reflected by the vast scientific effort to accurately capture the variation of these parameters in a wide range of temperatures [21–24]. Based on experimental data for polycrystalline alumina, the temperature dependency of the specific heat capacity c_p and thermal conductivity k can be approximated with adequate accuracy by inverse power laws [19]:

$$k(T) = k_0 + k_1 T^{-1},\ \mathrm{Wm^{-1}K^{-1}} \tag{1a}$$

$$c_p(T) = c_0 + c_1 T^{-1},\ \mathrm{Jkg^{-1}K^{-1}} \tag{1b}$$

where, T is the absolute temperature, k_0, k_1, c_0 and c_1 are constants with values -4.5536, 12227, 1429.4 and -197620, respectively. Although more elaborate and accurate functions have been described in [21], Eqs. (1a) and (1b) are adopted here due to their simple form. It is obvious that as temperature increases, the specific heat capacity increases while the thermal conductivity decreases. This is expected, as materials at higher temperatures tend to store heat instead of conducting it [19,23].

The temperature field is determined considering thermal convection and radiation/irradiation between the material and its environment. Heat exchange can be estimated through the implementation of the Newton cooling law and Stefan-Boltzmann law. To fully characterize heat transfer, two additional parameters must be defined: the emissivity $\varepsilon \in [0,1]$ and the heat transfer coefficient h. Heat exchange can then be written as:

$$q_{\mathrm{surf}} = q_{\mathrm{conv}} + q_{\mathrm{rad}} = h(T - T_\infty) + \varepsilon\sigma(T^4 - T_s^4), \tag{2}$$

where, $\sigma = 5.67\,10^{-8}\,\mathrm{W^{-2}K^{-4}}$, is the Stefan-Boltzmann constant and T_s is the temperature at the surface of the solid. Following [19], heat loss due to radiation is taken as $\varepsilon = 0.80$.

Estimation of the convective heat transfer coefficient h, is crucial for the accurate simulation of the heat transfer between alumina and the surrounding medium. Various experimental configurations have been proposed in the literature (e.g. [25,26]) but as reported in [1], results exhibit high dispersion. Following [15], the value $h = 50{,}000\,\mathrm{Wm^{-2}K^{-1}}$ is employed, as representative of the heat transfer between a liquid and a solid (water quenching for cold shock or molten steel for hot shock).

The temperature dependence of alumina's mechanical properties needs also to be accounted for. The elastic modulus E and fracture toughness K_{IC}, decrease as the temperature increases while, the thermal expansion coefficient α and Poisson's ratio ν, increase. In the subsequent analyses, the use of the Bond-based peridynamic model

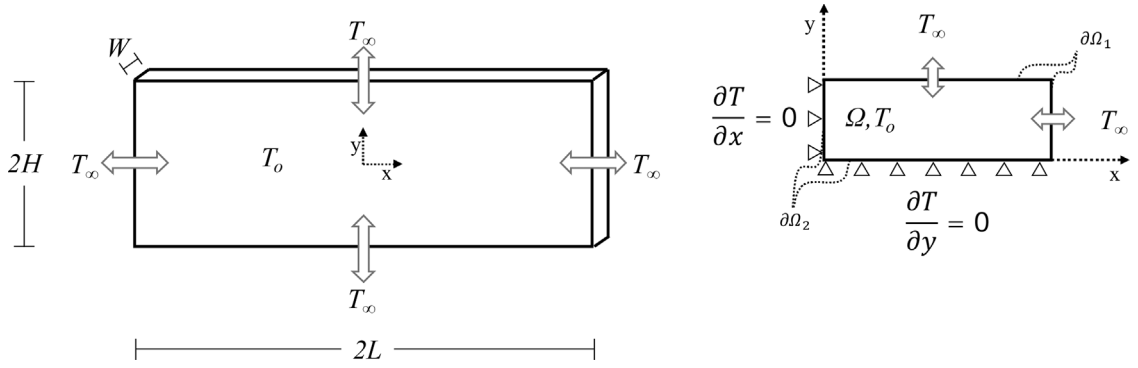

Fig. 1. Physical (left) and numerical (right) model of the alumina specimen subjected to 2D heat transfer.

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