Thermal shock residual strength of ultra-high temperature ceramics with the consideration of temperature

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Abstract When suffered from severe thermal shock ultra-high temperature ceramics for high-temperature applications will present to strength reduction or fracture due to microcrack and macrocrack propagation induced by the shocks. And the thermal shock residual strength is one of the most important indexes that evaluate the ceramic material for further use after thermal shock. This paper established a temperature dependent thermo-fracture mechanics model to predict the residual strength of ultra-temperature ceramics after thermal shock. And the critical thermal shock temperature that causes the material strength drop is determined and show differences from the one without temperature-dependent material properties. Also these studies demonstrate the significance of incorporating temperature-dependent material properties on the prediction of thermal shock residual strength of ultra-high temperature ceramic materials.

Keywords Ultra-high temperature ceramics, Thermal shock, Fracture, Residual strength.

1. Introduction

Ultra-high temperature ceramics (UHTCs) are a family of ceramic based composites mainly consisted of transition metal compounds, particularly refractory borides and carbides composites of Zr, Hf and Ta, such as ZrB_2, TaC, HfN and HfB_2, which have melting points higher than 3000^{o}C. Essentially, these UHTCs possess an excellent and unique set of bulk properties including unusually high melting points, high thermal conductivity, high elastic modulus and retain strength at high temperatures. And they can be potentially used at temperatures above 2000^{o}C in an oxidizing environment [1-2]. This combination of properties make these materials potential candidates for a variety of high-temperature structural applications, including engines, thermal protection system such as leading edges and nose-cones for a new generation of hypersonic vehicles, plasma arc electrodes, furnace elements, and high temperature shielding [3-5]. In these applications, UHTCs usually experience severe thermal shock. And it is known that cracking and other forms of damages are induced in UHTCs or ceramic composites when subjected to severe thermal shocks. As a result, the strength of thermally shocked UHTCs can be significantly degraded. Therefore, it is necessary to investigate thermal shock fracture resistance behavior of UHTCs of these advanced materials.

Significant progress has been made in the understanding of thermal shock fracture behavior of ceramic materials with great efforts of theories and experiments done by many researchers. At present, the research of thermal shock resistance mostly focuses on the effects of surface defects, temperature, indentation crack length [7,8,9], particle reinforced [10,11] or whisker reinforced [12] on thermal shock resistance performance to explain the mechanisms of thermal shock failure in experimental way. Theoretical researches of the effect of surface heat transfer coefficient on thermal shock resistance had been made [13], and several evaluation theories of thermal shock resistance had been reported [6,14,15,16].

In many experiment research works of thermal shock fracture behavior, residual strength is usually used to evaluate thermal shock resistance behavior of UHTCs [5,8,9,15]. Because the microcracks exist in ceramics, when a ceramic specimen is subjected to sufficiently severe thermal shocks, some of the pre-existing micro-cracks will initiate and grow to form macrocracks. Crack propagation in thermally shocked ceramics may be arrested depending on the severity of thermal shock, thermal stress field characteristics and material properties. What is more, the thermal shock residual strength is one of the most important properties that evaluate the ceramic materials for further use after thermal shock. However, few researchers do it in theoretical way [17] , and they didn't consider the effects of temperature on the thermo-physical properties. But in its actual operating condition the temperature range of the UHTCs is very large and the material properties are always function of temperature, the effects of temperature on the UHTCs material properties must been taken into consideration [7].

In this paper, thermal shock residual strength of UHTCs is studied. As basic research, firstly we only consider the strength degradation due to propagation of a single crack, which has proven reasonable in evaluating thermal shock residual strength of monolithic ceramics [18,19]. Effects of multiple crack propagation and particle-reinforced on strength degradation will be considered in the future study. And the material properties are function of temperature to take the effects of temperature on the UHTCs material properties into account. The critical thermal shock temperature that causes the material strength drop and thermal shock residual strength is determined by calculation and the results demonstrate the differences from the one without temperature-dependent material properties.

2. Temperature and thermal stress fields

2.1. Temperature fields of UHTC strip under cold shock

Consider a long UHTC strip with an edge crack as shown Fig. 1, where $2a$ is the thickness of the strip and c_0 is the crack length. The strip is initially at a constant temperature T_0, and its surfaces $x = 0$ are suddenly cooled by cooling media of temperatures T_∞ with the heat transfer coefficients h.

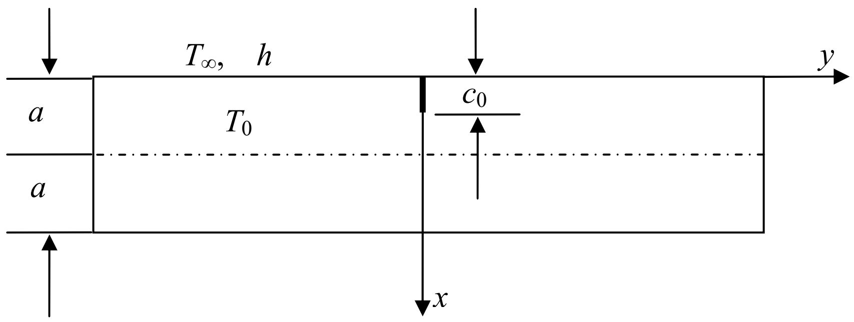

Figure 1. A UHTC strip with an edge cracks subjected to thermal shock

Assume that the crack whose plane is normal to the surface of the strip does not perturb the transient temperature distribution. Therefore, this is a one-dimensional heat conduction problem as the Fig. 1 shows. Taking the temperature-dependent material properties into account, the governing equation can be written in the form

$$\frac{\partial}{\partial x}\left(k(T)\frac{\partial T(x,t)}{\partial x}\right)=\rho(T)C_{\mathrm{p}}(T)\frac{\partial T(x,t)}{\partial t}, \qquad 0<x<2a,\ t>0 \tag{1}$$

The corresponding boundary and initial conditions are as follows

$$k(T)\frac{\partial T(x,t)}{\partial x}=h\left(T(x,t)-T_\infty\right), \qquad x=0,\ t>0 \tag{2}$$

$$\frac{\partial T(x,t)}{\partial x}=0\,,\qquad x=2a,\ t>0 \tag{3}$$

$$T(x,t)=T_0\,,\quad t=0, 0<x<2a \tag{4}$$

where $k(T)$, $\rho(T)$ and $C_p(T)$ are the temperature-dependent thermal conductivity, mass density and specific heat capacity, respectively. And t represents time.

Obviously this is a transient nonlinear heat conduction problem. In order to solve Eq. (1), we linearize this partial differential heat conduction equation using the Kirchhoff transformation [20], namely

$$\theta(T)=\frac{1}{k_0}\int_{T_0}^{T}k(T)dT \tag{5}$$

where k_0 is the thermal conductivity at reference temperature T_0. Under the transformation (5), equations (1), (2), (3) and (4) reformulate as

$$\frac{\partial^2\theta(x,t)}{\partial x^2}=\frac{1}{\kappa}\frac{\partial\theta(x,t)}{\partial t}\,,\qquad 0<x<2a,\ t>0 \tag{6}$$

$$k_0\frac{\partial\theta(x,t)}{\partial x}=h\left(\theta(x,t)-\theta_\infty\right),\quad x=0, t>0 \tag{7}$$

$$\frac{\partial\theta(x,t)}{\partial x}=0\,,\quad x=2a, t>0 \tag{8}$$

$$\theta(x,t)=\theta_{\mathrm{i}}\,,\quad 0<x<2a, t=0 \tag{9}$$

However, in Eq. (6)

$$\kappa=\frac{k(T)}{\rho(T)C_{\mathrm{p}}(T)} \tag{10}$$

is still temperature-dependent. For the convenience of derivation and calculation, we determine a κ_0 with the use of Eq. (11) to replace in Eq. (6).Therefore, Eq.(6) becomes a total linear equation.

$$\kappa_0=\frac{1}{T_0-T_\infty}\int_{T_\infty}^{T_0}\frac{k(T)}{\rho(T)C_{\mathrm{p}}(T)}dT \tag{11}$$

Applying the variable separation approach, the expression of $\theta(x,t)$ is obtained.

$$\theta(x,t)=\theta_\infty+2(\theta_{\mathrm{i}}-\theta_\infty)\sum_{m=1}^{\infty}\frac{\left(\beta_m^2+H^2\right)\sin\beta_m L}{\beta_m\left(H+\left(\beta_m^2+H^2\right)L\right)}\cos\left(\beta_m(L-x)\right)e^{-\kappa_0\beta_m^2 t} \tag{12}$$

in which $h/k_0=H$, L=2a, and β_m is determined by the following Eq. (13). Therefore, the temperature fields $T(x,t)$ can be acquired from $\theta(x,t)$ in Eq. (12) making the use of their relationship in Eq. (5).

$$\beta_m \tan \beta_m L = H \tag{13}$$

2.2. Thermal Stress in UHTC strip under cold shock

After the temperature is obtained, the transient thermal stress in a fully free strip can be obtained from the classical beam analysis [21]. For plane-stress $\sigma_{yy}(x,t)$ has the form

$$\sigma_{yy}(x,t) = E\left(T(x,t)\right)\left[Ax + B - \alpha\left(T(x,t)\right)\left(T(x,t) - T_0\right)\right] \tag{14}$$

where E and α are the temperature-dependent elastic modulus and thermal expansion coefficient, respectively. Values for constants A and B are determined from:

$$\int_0^{2a} \sigma_{yy}(x,t)dx = 0 \quad \text{and} \quad \int_0^{2a} \sigma_{yy}(x,t)\,xdx = 0 \tag{15}$$

3. Thermal stress intensity factor and thermal shock cracking

The transient thermal stress intensity factor (TSIF) for an edge crack of quasi-static fracture problem can be obtained by using a non-dimensional weight function and the thermal stress.

$$K_{\mathrm{I}}(t) = \frac{\int_0^c \sigma_{yy}(x,t)\,dx}{c}\sqrt{\pi c}F\left(\frac{c}{2a}\right) \tag{16}$$

where c is the crack length, and F is the weight function[22], $K_{\mathrm{I}}(t)$ represents the TSIF at t.

It is obvious that the TSIF is proportional to thermal shock temperature difference ΔT, crack propagation will not occur if the thermal shock has no reached a critical value ΔT_{c}, at which the peak value of transient TSIF reaches the fracture toughness K_{IC}. At ΔT=ΔT_{c}, the peak value $K_{\mathrm{I}}(t)$ reaches K_{IC} and crack propagation is initiated. Therefore, when $\Delta T \geqslant \Delta T_{\mathrm{c}}$, as the thermal shock proceeding, the crack propagation will occur when TSIF $K_{\mathrm{I}}(t) > K_{\mathrm{IC}}$ and results in severe damage in UHTC plate; And it will be arrested after extending when $K_{\mathrm{I}}(t) > K_{\mathrm{IC}}$ again, thus the crack will reach a final length c_{f} after thermal shock determined by Eq. (17).

$$K_{\mathrm{I}}(t) = \frac{\int_0^{c_{\mathrm{f}}} \sigma_{yy}(x,t)\,dx}{c_{\mathrm{f}}}\sqrt{\pi c_{\mathrm{f}}}F\left(\frac{c_{\mathrm{f}}}{2a}\right) = K_{\mathrm{IC}}, \quad \Delta T > \Delta T_{\mathrm{c}} \quad \text{and} \quad t > 0 \tag{17}$$

Therefore, the thermal shock residual strength can be determined by the final crack length as shown in Eq. (18).

$$\sigma_{\mathrm{R}} = \frac{K_{\mathrm{IC}}}{\sqrt{\pi c_{\mathrm{f}}}F\left(\frac{c_{\mathrm{f}}}{a}\right)} \tag{18}$$

4. Results and discussion

Refractory diborides of zirconium (ZrB_2) based ceramics are the most used UHTCs. Take it as an example, the temperature-dependent material properties of the diborides of zirconium based UHTCs are shown Table 1 [8, 16, 23]. And the thickness of UHTC strip $2a$ = 5mm.

Fig. 2 shows temperature has significant effect on crack resistance [5]. It shows that a higher temperature leads to a higher crack resistance. The highest crack resistances are about 5.5MPa·m$^{1/2}$ and 6MPa·m$^{1/2}$ for 20°C and 600°C respectively. Due to lack of temperature-dependent crack resistance data, while determining the thermal shock residual strength with temperature-dependent material properties, we consider that it is still the same as the crack resistance at 600°C when thermal shock initial temperature is higher than 600°C. For without temperature-dependent material properties, it is considered to be the same as the crack resistance at 20°C.

Table1. Temperature-dependent material properties of the diborides of zirconium based UHTC

Material parameters	Values and expressions
E(GPa)	$E = E_0 - BTe^{-\frac{T_m}{T}} + B_1\left(T - B_2T_m + \left\|T - B_2T_m\right\|\right)\ e^{-\frac{T_m}{T}}$
E_0(GPa), B_0, B_1, B_2	500, 2.54, 1.9, 0.363
α (°C^{-1})	$(2.01\ln(T)\text{-}6.7652)\times10^{-6}$
k (W·(m·°C)$^{-1}$)	$-16.79\times\ln(T)+178.2$
ν	0.16
$C_p(T)$ (cal/mol)	$15.34+2.25\times10^{-3}T\text{-}3.96\times10^{5}T^{-2}$
ρ(g.cm-3)	6.1

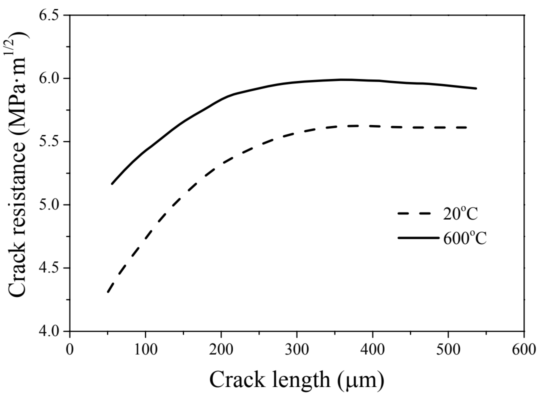

Figure 2. Crack resistance under different temperature

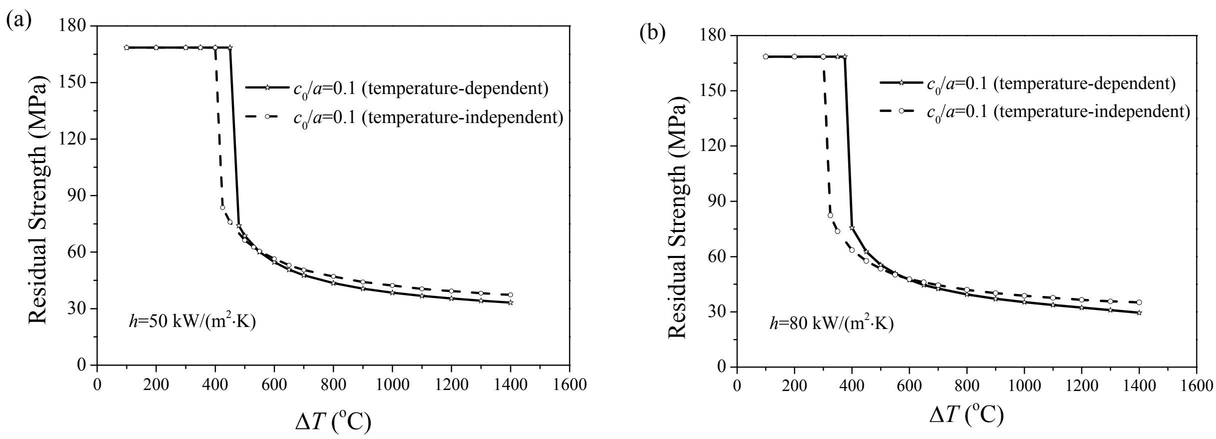

Figure 3. The relationship between thermal residual strength and thermal shock temperature difference ΔT ((a), h=50kW/(m^2·K), (b), h=80kW/(m^2·K))

As can be seen in Fig. 3, the curves of thermal shock residual strength have the same trends with the experiments results' trends which are common in literatures [5,9]. When the thermal shock temperature difference ΔT is less than the critical thermal shock temperature difference ΔT_c, crack propagation didn't occur and the strength remains unchanged. At $\Delta T = \Delta T_c$, the strength drops precipitously, then decreases gradually and tends to be a constant as the increase of thermal shock temperature difference ΔT. Also the Fig. 3 shows that the critical thermal shock temperature difference ΔT_c with temperature-dependent material properties is higher than the one which does not take the effect of temperature on material properties into account. And, if the ΔT is less than a certain value the thermal shock residual strength with temperature-dependent material properties is higher than the one without the consideration of temperature-dependent material properties. However, the results are reversed as the ΔT becomes larger than the certain value. Therefore, if the temperature dependence of material is ignored, the critical thermal shock temperature difference ΔT_c will be underestimated, and the thermal shock residual strength will be wrong determined. Thus, consideration of temperature-dependent material properties is essential for correct evaluation of thermal shock resistance and thermal shock residual strength of a material, especially for UHTCs suffered high temperature thermal shock.

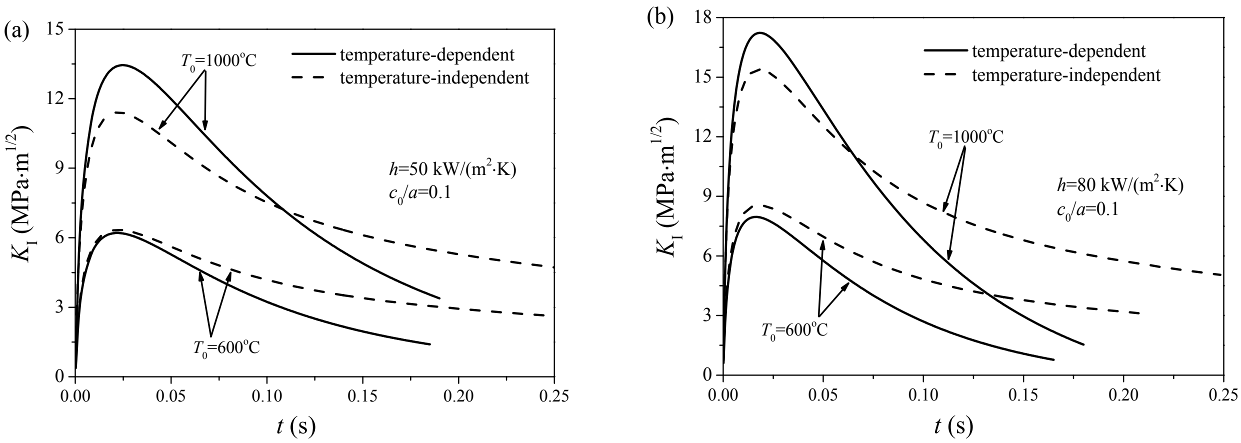

Figure 4. Thermal stress intensity factor as a function of time ((a), h=50kW/(m^2·K), (b), h=80kW/(m^2·K))

In Fig. 4, setting the crack to be the initial length during the thermal shock proceeding, the TSIF K_I is plotted as a function of thermal shock time for thermal shock initial temperature T0=600°C and 1000°C with surface heat transfer coefficient h=50kW/(m^2·K) in Fig. 4 (a) and h=80kW/(m^2·K) in Fig. 4 (b), respectively. The results show that the peak values TSIF K_I for 600°C with temperature-dependent material properties are lower than the one without temperature-dependent material properties, on the contrary, when thermal shock initial temperature is 1000°C, the peak values with temperature-dependent material properties is higher than the one which does not take the effect of temperature on material properties into account. Because the coefficient of thermal diffusion of high temperature without temperature-dependent material properties is larger than the one with temperature-dependent material properties, the serious temperature gradient will moderate sooner, which can result in relaxing of thermal stress induced by thermal shock. Therefore, the phenomenon, that if the ΔT is less than a certain value the thermal shock residual strength with temperature-dependent material properties is higher than the one without the consideration of temperature-dependent material properties but the results are reversed as the ΔT increase shown in Fig. 3, is explained. And it is obvious that the thermal shock residual strength is strongly affected by the dependence of temperature of material properties. Thus, when determining the thermal residual strength of UHTCs for high temperature used, the result of high temperature thermal shock, that thermal residual strength with the consideration of temperature-dependent material properties is higher than the one without temperature-dependent material properties, is not always right. It must fully consider the effect of temperature on the material properties.

5. Conclusions

In this paper, theoretical prediction thermal shock residual strength with the temperature-dependent material properties of UHTCs is presented. The theoretical model is capable of predicting qualitatively thermal shock residual strength behavior of UHTCs observed in experiments, i.e., when the thermal shock temperature difference ΔT is less than the critical thermal shock temperature difference ΔT_c, crack propagation didn't occur and the strength remains unchanged. At $\Delta T = \Delta T_c$, the strength drops precipitously, then decreases gradually and tends to be a constant as the increase of thermal shock temperature difference ΔT. The results of the theoretical model applying to the diborides of zirconium based UHTCs are compared to the results which haven't take the effect of temperature on material properties into consideration. It shows that the thermal shock residual strength and thermal shock resistance is very sensitive to their temperature-dependent material properties. If the temperature dependence of material is ignored, the critical thermal shock temperature difference ΔT_c will be underestimated. And the thermal shock residual strength with temperature-dependent material properties is higher than the one without the consideration of temperature-dependent material properties if the ΔT is less than a certain value, but the results are reversed as the ΔT is larger than the certain value. Therefore, when determined the thermal shock residual strength, it must take the temperature-dependent material properties into fully account.

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