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Brittle vs ductile fracture behavior in ceramic materials at elevated temperature

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ABSTRACT

An intergranular crack initiated at a pore located in a triple junction of grain boundaries in a ceramic material is considered in order to investigate the brittle versus ductile fracture in different temperature ranges. The critical fracture stress and critical dislocation slip stress are estimated in dependence on temperature for the case of Al_2O_3 ceramics. The temperature dependless local stresses in vicinity of blunt cracks and a triangular-shaped pore are calculated by the finite element method. The provided analysis reveals the favorability of the fracture scenarios upon the temperature conditions and bluntness of a crack tip as well.

KEYWORDS

ceramic materials • pore •crack • intergranular fracture •dislocation emission • finite element simulation

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Introduction

Due to relatively high melting point and ability to arouse plastic deformation at elevated temperatures, the ceramic materials are widely used in modern industry [1–3]. The mechanical properties as well as the fracture tolerance of these materials are strongly determined by the temperature range of the operational conditions [4,5]. Commonly, the brittle behavior of fracture is expected to experience at relatively low temperatures while the ductile one occurs at relatively high temperatures. The first scenario stems from the propagation of cracks whereas the second one is accompanied with activation of dislocation glide and grain boundary (GB) sliding. In particular, the dislocation emission from the crack tip can significantly inhibit the crack growth due to blunting of the crack tip.

The problem of brittle-to-ductile transition has been long studied in literature [6]. For instance, some studies [7–11] were focused on the influence of GBs on the dislocation emission, other works [12–14] concerned with the effect of crack blunting on the material toughening and research [15–17] examined the critical condition of the GB sliding. However, the aforementioned models did not consider the brittle vs ductile response to the increment of mechanical properties of the materials under temperature increase. The analysis of the occurrence of either brittle or ductile behaviors of ceramics with regard to the temperature conditions seem to be an essential issue that could be ascertained

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through thorough investigation of the critical conditions for both crack propagation and dislocation emission as well as stress concentration effects associated with cracks.

In our previous research, the stress concentration induced by triangular-shaped pores [18] and inhomogeneities [19] in ceramics was investigated by both the perturbation technique and finite element method. It was demonstrated that the first-order semi-analytical solution is in a good agreement with the results of finite element simulations. Besides, a finite element simulation was employed in [20] to reveal the favorability of various crack configurations in a ceramic composite containing a lamellar inhomogeneity viz. crack initiation in the matrix, in the inhomogeneity and at the interface. It was shown that, in the case of relatively rigid inhomogeneities, the crack initiation is more feasible in the matrix region near the interface, in contrast to the case of relatively soft inhomogeneities, when the cracks are expected to occur either in the inhomogeneity or at the interface.

This work is aimed at analyzing the favorability of failure scenarios considering the intergranular fracture initiated on a pore at a triple junction (TJ) of GBs in a monolithic ceramics. The GBs are assumed to be the preferred pathways for crack propagation. In doing so, we investigate the critical conditions for crack cleavage and dislocation slip with respect to the temperature, implement the finite element simulation to determine stress concentration effects due to both rounded triangular pore and elliptical crack, and exhibit the preferred fracture scenarios in dependence of the temperature and geometric parameters of the problem. It is worth noting that this study considers the plasticity through the dislocation mechanisms and does not concern other mechanisms such as the GB sliding.

Model

Consider a pore located in an equilibrium TJ of GBs in a ceramic material exerted by axial loading S_0 (see Fig. 1(a)). The following failure scenarios can be expected: (i) intergranular fracture due to crack initiation at the pore and subsequent growth along the GB, (ii) ductile fracture due to dislocation nucleation on either the crack or the pore. The preference of these scenarios is mainly determined by both local stresses prescribed by the pore or crack geometry and temperature conditions defining the critical cleavage stress for crack propagation and the critical stress for dislocation nucleation.

According to [21], the critical cleavage stress (theoretical strength) for crack advance can be estimated as follows:

$$S_c = \sqrt{\frac{E\gamma}{x_0}}, \qquad (1)$$

where E is the Young modulus, γ is the specific surface energy, and x_0 is the interatomic distance of the material. Generally speaking, the values of material parameters E and γ are strongly defined by the temperature of a sample. For instance, Nie et al [22] investigated the Young modulus of α-Al_2O_3 ceramics at high temperatures by applying the impulse excitation technique and the static three- and four-point bending tests. They demonstrated that the elastic modulus of alumina at first slowly decreased from 20 to 1000 °C and then rapidly dropped with the increase in temperature from 1000 to 1300 °C. The results of these measurements are given in Table 1.

Table 1. Temperature dependence of the Young modulus of α-Al_2O_3 ceramics [22]

Temperature, °C	20	400	600	800	1000	1100	1200	1300
Young modulus, GPa	282	269	250	235	195	132	88	27

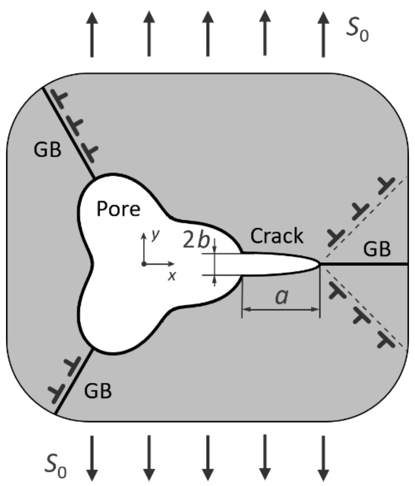

Fig. 1. Various scenarios of microfracture: the intergranular fracture due to the crack initiation at the TJ pore and the ductile fracture due to dislocation emission from the pore and the crack tip

As for the specific surface energy γ, the experiments [23] and theoretical modelling [24] clearly indicate its linear decrease in ceramics when the temperature increases from 0 K to the melting point. For α-Al_2O_3 ceramics, the following approximation is valid:

$$\gamma = \gamma_0 - \beta T, \quad (2)$$

where the temperature T is given in K, $\beta \approx 0.83$ mJ / (m^2 K) and $\gamma_0 \approx 2138$ mJ / m^2.

In addition, the interatomic distance x_0 in the α-Al_2O_3 ceramics can be estimated as ~ 0.25 nm over the wide range of temperatures.

To evaluate the critical stress for dislocation slip in dependence on temperature in the α-Al_2O_3 ceramics, the following empirical formulas can be employed [25]:

$$\ln \tau_{cb} = \ln \tau_{0b} - 0.0052T, \quad (3)$$

where τ_{cb} is a critical shear stress for basal dislocation slip, τ_{0b} = 109 GPa, and T is given in K.

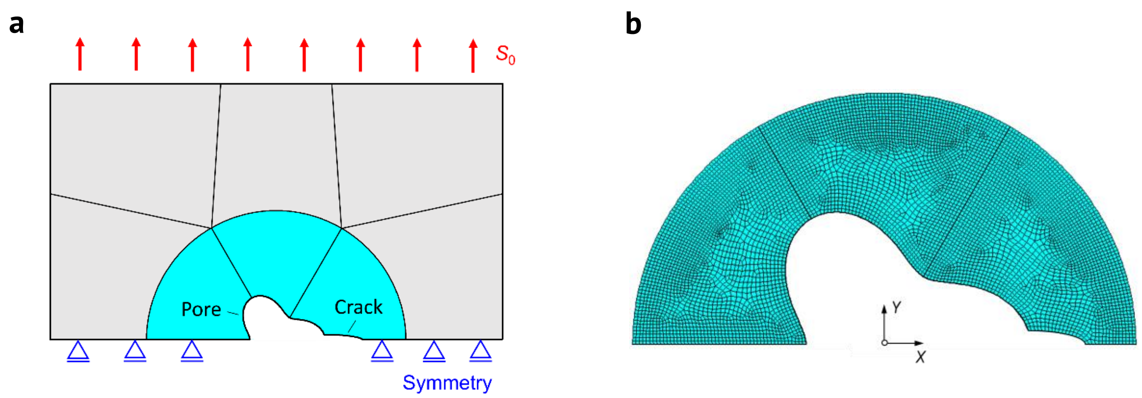

Fig. 2. (a) The finite element model of a ceramic material containing a triangular-shaped pore and an elliptical crack. The prescribed boundary conditions are shown. (b) The magnified inset highlights the irregular finite element mesh in vicinity of the pore and the crack for ε = 0.3

The local stress associated with the geometrical aspects of the crack and the pore can be calculated within finite element simulations. A 2D finite element model of a ceramic material containing a triangular-shaped pore and an elliptical crack has been prepared in a commercial software as shown in Fig. 2. The rounded triangular shape of three-fold symmetry of the pore is prescribed by the following analytical equations [18,19]:

$$x = (R_0 + \varepsilon \cos 3\theta) \cos\theta, \quad (4)$$

$$y = (R_0 + \varepsilon \cos 3\theta) \sin\theta, \quad (5)$$

where (x,y) are the coordinates of the pore boundary, θ is the polar angle, and the parameter ε describes the maximum deviation of pore boundary from the circle of radius R_0.

The crack shape is treated as an elliptical one with semi-axes a and b. The radius of the crack tip can be determined as follows $\rho = b^2 / a$. The model is built up from 2D plane elements containing 8 nodes to better approximate the pore and crack geometry. The top of the model is loaded by an external pressure S_0, while the bottom is fixed in the y-direction due to the symmetry of the problem under consideration. The size of the model is considered to be big enough to neglect the shielding effects of the external boundaries. The material is supposed to be linearly elastic and isotropic, determined by the Young modulus E according to Table 1 and the Poisson ratio $\nu = 0.25$.

Results

The derived temperature dependences of the critical stress for crack propagation (Eq. 1) and the critical stress of dislocation nucleation (Eq. 3) for the case of α-Al_2O_3 ceramics are shown in Fig. 3. The latter stress is expressed through the equivalent tensile stress as follows: $S_{db} = 2\tau_{cb}$. As is seen from Fig. 3, the critical stresses decrease when the temperature increases. Moreover, at relatively low temperatures, the critical cleavage stress S_c is much lower than the critical stress for dislocation generation S_{db}, i.e. the material tends to the brittle fracture. On the contrary, at relatively high temperatures, the critical cleavage stress exceeds the critical stress of dislocation slip, i.e. the ductile fracture is expected. It is worth noting that, in the case of α-Al_2O_3 ceramics, the threshold temperature T_1 takes a value close to 300 K ($T_1 \sim 20$ °C). Besides, the cleavage stress S_c estimated at 0 K takes a value close to 48.9 GPa shown by density functional calculations [26].

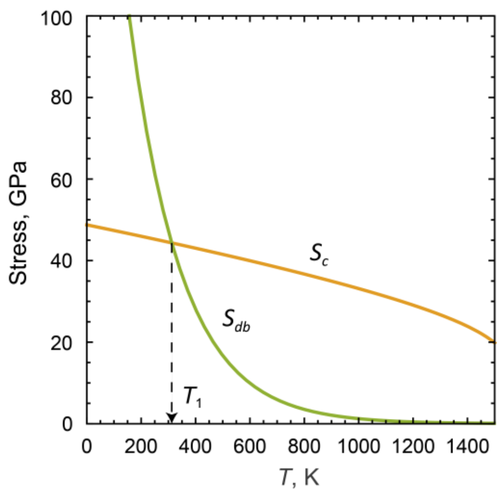

Fig. 3. Dependence of the critical cleavage stress S_c and the critical stress of dislocation slip S_{db} on the temperature for α-Al_2O_3 ceramics

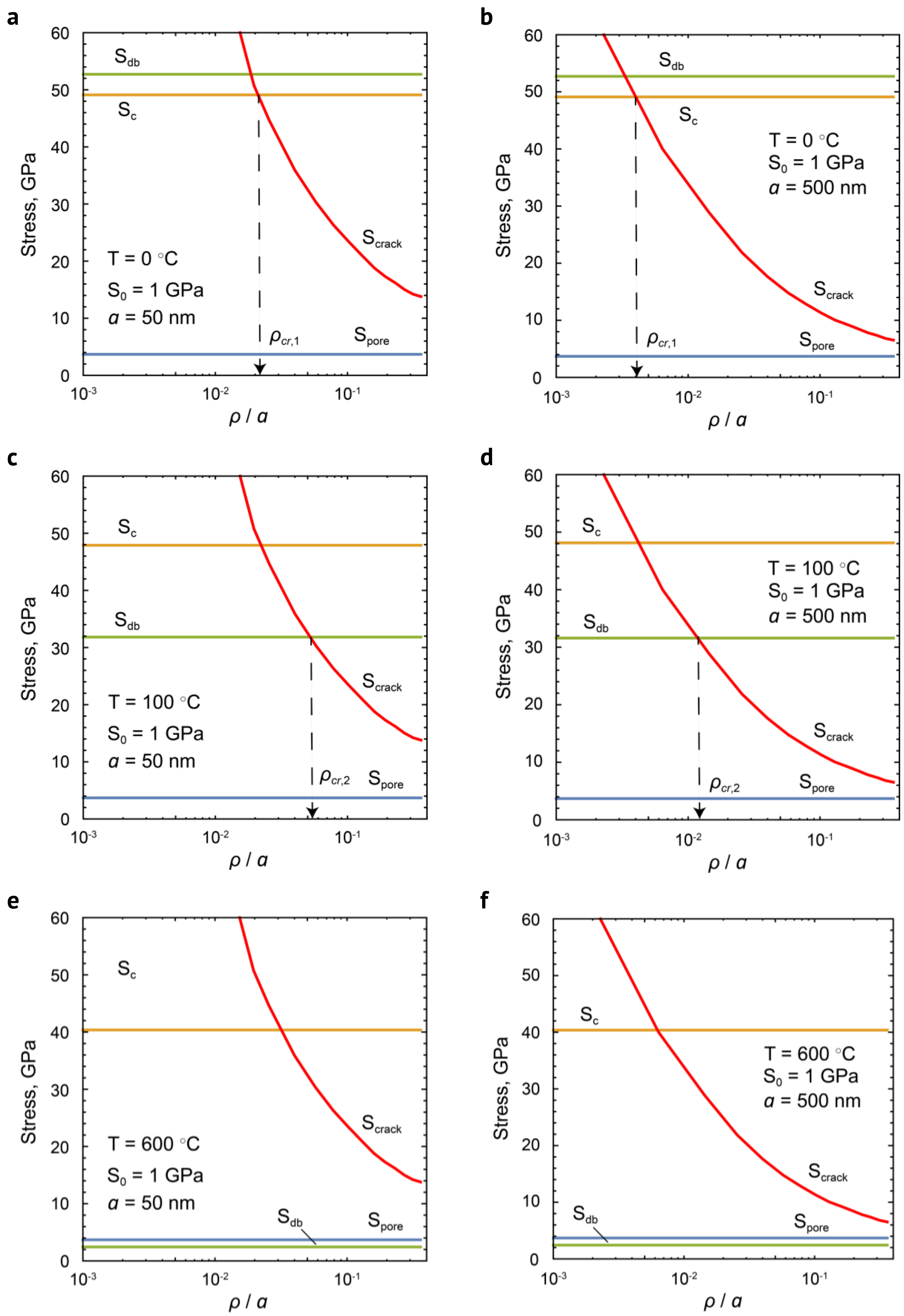

Fig. 4. Maximum local stress in vicinities of the crack tip, S_{crack}, and the rounded triangular pore, S_{pore}, under the uniaxial tensile stress S_0 = 1 GPa vs the crack tip radius to crack length ratio ρ / a at a / R_0 = 1/2 and crack lengths 50 (a,c,e) and 500 nm (b,d,f) for the three different temperatures: (a,b) 0, (c,d) 100, and (e,f) 600 °C

Thus, the cracks tend to propagate if the temperature is less than the threshold one that is T_1. Otherwise, one can expect the emission of dislocations from the crack with subsequent blunting of its tip at elevated temperatures, when $T > T_1$. This phenomenon can lead to significant decrease of local stress in the crack tip, thus suppressing the brittle behavior of cracks.

Taking into account the above theoretical analysis, some numerical calculations have been carried out to demonstrate the impact of the crack and pore geometry on the local stress concentration. Figure 4 depicts the local stress calculated by the finite element simulation at the elliptic crack and the rounded triangle pore in dependence on the normalized crack tip radius ρ / a. The following failure scenarios are elucidated below.

(i) *Brittle fracture*. This scenario is attributed to relatively low temperatures when the critical stress of dislocation slip S_{db} is higher than the critical cleavage stress S_c. As is seen from Fig. 4(a,b), for $T < T_1$, the local stress at the crack tip, S_{crack}, exceeds the critical cleavage stress S_c for relatively sharp cracks with $\rho < \rho_{cr,1}$. It means that these cracks have a tendency to advance provoking the brittle fracture. On the contrary, the local stress influenced by the blunting is not high enough to exert the crack propagation if the crack tip radius ρ exceeds the critical one $\rho_{cr,1}$, $\rho > \rho_{cr,1}$. On the other hand, the local stress at the pore is considerably lower than that at the crack tip and does not depend on the crack length.

(ii) *Quasi-brittle fracture*. In contrast to the previous scenario, the critical stress for the dislocation slip activation is lower than the critical cleavage stress ($T > T_1$), i.e. the dislocation emission becomes the most favorable mechanism. Fig. 4(c,d) shows that the local stress at the crack tip S_{crack} can be high enough to provide the dislocation emission that is accompanied by the crack tip blunting when $\rho < \rho_{cr,2}$. One can expect that S_{crack} decreases due to the blunting process as long as the radius of the crack tip reaches its critical value $\rho_{cr,2}$. The cracks with tip radius $\rho > \rho_{cr,2}$ are unable to either propagate or emit dislocations until the external tensile stress S_0 gets a necessary level. The local stress at the pore S_{pore} remains so low that the pore can not emit dislocations.

(iii) *Ductile fracture*. In the case of relatively high temperatures ($T > 500$ °C), the critical stress of dislocation slip becomes so low that the pore is enabled to emit dislocations as is seen from Fig. 4(e,f). It means that the fracture fashion in monolithic ceramic materials at elevated temperatures can be largely determined by the dislocation emission from pre-existing pores.

It is worth noting that the local stress in vicinity of relatively small cracks (of length $a = 50$ nm) is essentially influenced by the concentration effect of the triangular-shaped pore while the relatively large cracks (of length $a = 500$ nm) are not responsive to the pore effect. As a result, small cracks have a tendency to accelerate the evolution process through either growing or blunting.

Conclusions

In this study, different failure scenarios in monolithic ceramics at evaluated temperatures have been elucidated. In doing so, a Mode I crack initiated at a triple-junction pore under uniaxial tensile stress has been considered. The critical stresses for crack cleavage and dislocation emission have been derived for the case of α-Al_2O_3 ceramics with regard to the temperature. The finite element analysis incorporating both the elliptical shape of the crack and rounded triangle shape of the pore has been employed to determine the local stress concentration effects. It has been assumed that the cracks tend to propagate when the maximum local stress exceeds the critical cleavage stress whereas the dislocation emission occurs when the maximum local stress attains the critical stress of dislocation slip. As a result, the following failure scenarios with respect to the temperature and defect geometry are suggested. It is shown that, at relatively low temperatures ($T < T_1$), the critical fracture stress is less than that for dislocation slip. In this case, the local stress at the crack tip is sufficient to provoke the cleavage if the crack tip is sharp enough, $\rho < \rho_{cr,1}$. This fracture fashion is considered as a brittle failure. In the range of medium temperatures ($T > T_1$), the dislocation emission precedes cleavage as the critical stress of dislocation slip becomes lower than the critical fracture stress. As a result, the multiple emission of dislocations from the tip converts a sharp crack into the blunt one until the crack tip radius ρ takes its critical value $\rho_{cr,2}$. The cracks with tip radii $\rho > \rho_{cr,2}$ are able to advance only when the temperature and the loading conditions are changed. This fracture fashion is treated as quasi-brittle failure. At elevated temperatures ($T > 500$ °C), the critical stress for dislocation emission becomes lower than the maximal local stress at the triangular-shaped pore. It means that the dislocation emission from the pore is the most favorable response to external loading. In this case, the significant plastic deformation preceding the failure is expected.

Thus, it has been shown that the preference of the considered fracture scenarios in a ceramic material is determined by temperature range and geometrical parameters of pre-existing pores and cracks. Another important finding is that the significant plasticity of ceramics at elevated temperatures can be explained in terms of dislocation emission from the pre-existing pores.

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