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Feature article

Critical inclusion size prediction in refractory ceramics via finite element simulations

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ABSTRACT

Thermal expansion mismatch between matrix and aggregates can generate microcracks or decohesions when refractory ceramics are submitted to temperature variation. Earlier analytical studies have shown that these phenomena occur for inclusions with dimensions higher than a critical radius. These models are not reliable for inclusion amounts higher than 30 vol.%. In this paper, the critical inclusion size prediction by numerical simulation is presented resulting in more realistic models. The values obtained were compared to experimental ones from the literature with inclusion fractions of up to 45 vol.%. Finite element method results pointed out a change in the maximum thermomechanical stress location for volume fractions close to 43 vol.%. Up to this content, the maximum stress is at the matrix/inclusion interface, whereas for higher volume fractions, it is located in the midpoint between the inclusions. The advances attained by the present paper provide a suitable scientific foundation for designing flexible refractory compositions.

1. Introduction

Thermal expansion mismatch between matrix and inclusion can induce mechanical damage when the ceramic is subjected to temperature variation [1–3]. If the matrix thermal expansion coefficient is lower than that of the inclusions, decohesions can occur at the matrix/inclusion interface during cooling. Conversely, when the thermal expansion coefficient of the matrix is higher, radial microcracks can be nucleated in the matrix due to the tensile stresses at the circumferential directions [1–9]. In both cases, microcracks or decohesion will occur when the total elastic deformation energy overcomes its surface formation one [1]. Analytical and numerical models are important tools to predict these critical conditions that help to design refractory ceramics.

Prediction models related to thermal stresses have been studied since the sixties [1,10]. Selsing [10] calculated internal stresses in biphasic ceramics considering spherical inclusions. Davidge and Green [1] proposed an analytical model which takes into account the mechanical and thermomechanical properties of the phases and the cooling condition to determine the inclusion critical radius, above which spontaneous microcracks originate. Critical size prediction models are always important, as they guide the selection of inclusion dimensions for components where microcracks may be desirable or not.

Analytical models consider a constant pressure along the matrix/inclusion interface [1,10]. This assumption is not valid for higher volume fractions as the proximity of the inclusions may affect their stress field vicinity [11]. FEM has already been applied for thermal stress studies on metal/ceramic composite [12,13] and for ceramic/ceramic ones [14–17]. Other authors used this technique to identify crack patterns induced by thermal stresses [18,19]. Joliff et al. [20] considered an axisymmetric model based on FEM to investigate stress distribution between two inclusions for volume fractions of up to 40 vol.%, focusing on the matrix/inclusion interaction, however they were not concerned with the critical radius prediction. This sort of simulation is based on a revolution symmetry as a simplifying assumption, which reduces the computational cost when compared with three-dimensional models [20].

In this context, the objective of this study is to estimate the critical inclusion radii on biphasic refractory materials with the help of FEM numerical simulation. This allows non-uniform stress states attained in samples with high volume fractions of inclusions (>30 vol.%) to be considered. In this paper, investigations of stress field distributions have been carried out up to 60 vol.%. Nevertheless the method developed can also be applied to higher inclusion fractions (<74 vol.%).

Firstly, a synthesis of the analytical model based on the literature is shown in Section 2 and their assumptions are pointed out.

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In Section 3, the materials and their respective properties, which integrate the numerical models, are presented. Different finite element models for predicting critical parameters are highlighted and a strategy for solving them is explored in Section 4. Finally, a comparison between the numerical simulation results and literature experimental observations, as well as a discussion about the interaction among inclusions for volume fractions higher than 30 vol.% are shown in Section 5.

2. Analytical models for the critical radius prediction

Davidge and Green [1] proposed one of the first models which considers a single inclusion embedded in an infinite matrix volume. The critical inclusion radius is calculated by comparing the total energy stored during elastic deformation, U_t[J], and the surface formation energy, U_s. According to Davidge and Green [1], U_t, for their microstructure configuration, it is written as:

$$U_t = P^2 \pi a^3 \left[\frac{1+\nu_m}{E_m} + \frac{2(1-2\nu_i)}{E_i} \right] \tag{1}$$

where P [Pa] is the pressure at the matrix/inclusion interface; E_m, E_i [Pa] is the Young's moduli; ν_m, ν_i is the Poisson's ratios; a [m] is the inclusion radius; the subscript m and i refer to the matrix and inclusion, respectively.

According to Selsing [10], the P value is related with the matrix and inclusion properties using the following equation:

$$P = \frac{(\alpha_m - \alpha_i)\,|\Delta T|}{(1+\nu_m)/2E_m + (1-2\nu_i)/E_i} \tag{2}$$

where α_m and α_i [°C^{-1}] are the linear thermal expansion coefficients and ΔT [°C] the temperature variation. In this paper only the cooling process was considered.

The critical inclusion radius, a_c, can be determined by comparing U_t (Eq. (1)) and U_s, based on an energy balance. Considering $\alpha_i > \alpha_m$ (debonding), U_s can be expressed as $2(4\gamma_s\pi a^2)$, where γ_s is the effective surface energy of the matrix [1] [J m^{-2}]. It must be emphasized that γ_s is a property of the matrix, assuming that the cracks or de-cohesions will originate in the matrix, making γ_s independent of the inclusions volume fraction ϕ. The fact that the total deformation energy is proportional to a^3, whereas the surface formation energy is proportional to a^2, enables the determination of a critical radius (a_c) when both energies are equalized [$U_t(a_c) = U_s(a_c)$]:

$$a_c = \frac{8\gamma_s}{P^2[1+\nu_m/E_m + 2(1-2\nu_i)/E_i]} \tag{3}$$

For ceramics with low inclusion volume fraction, the mean distance between their inclusions is large enough to assume that their stress and strain fields are similar to a single inclusion embedded in an infinite matrix volume [1]. Increasing the volume fraction, for a given value of a, inclusions become closer and their stress and strain fields mutually interact. For this latter case, the assumption of constant pressure along the matrix/inclusion interface is not valid [11]. The interaction among inclusions and the influence of the volume fraction has been evaluated by Liu and Winn [11]. They proposed an analytical model with two inclusions and assumed that the effects among them are calculated as a linear combination of effects in the axis crossing the inclusions' centers. The volume fraction of inclusion (ϕ) is a function of the inclusion's distance ($\phi = a^3/b^3$) and the stress state in a generic point P is a linear combination of effects of the inclusion which distance is r and that distant $2b - r$ regarding to this point. Liu and Winn [11] investigated the radial and circumferential stresses between two inclusions and concluded that, for a volume fraction higher than 12.5 vol.% ($b < 2a$), significant changes are attained for the radial stress field. Therefore, the assumption of isolated inclusion embedded in a infinite matrix is not reasonable when increasing the volume fraction.

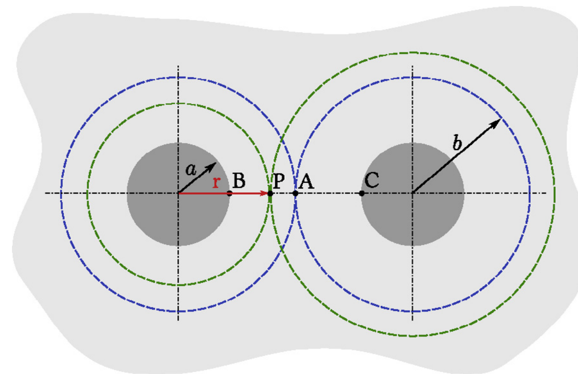

Fig. 1. Two inclusions embedded in a finite matrix (blue circles' radius are function of the volume fraction of inclusions and green circles represents the distance of the two nearest inclusions of a generic point), based on Liu and Winn [11] model. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article.)

In order to evaluate the radial and circumferential stress distributions between two inclusions, Liu and Winn [11] used the stress coefficients ($\overline{\sigma_\rho}$ and $\overline{\sigma_\theta}$) as dimensionless parameters to analyze the matrix stress distributions. These coefficients are determined by the ratio of the radial or circumferential stress at point $P \in \overline{BC}$ (Fig. 1), $\sigma(r)$, over the stress (radial or circumferential) at the matrix/inclusion interface, $\sigma(a)$. The radial stress coefficient, $\overline{\sigma_\rho}$, and the circumferential stress one, $\overline{\sigma_\theta}$, are expressed as:

$$\overline{\sigma_\rho} = \frac{\sigma_\rho(r)}{\sigma_\rho(a)} = \left[\left(\frac{a}{r}\right)^3 - \left(\frac{a}{2b-r}\right)^3 \right] \frac{1}{1-\phi} \tag{4}$$

$$\overline{\sigma_\theta} = \frac{\sigma_\theta(r)}{\sigma_\theta(a)} = \left[\frac{1}{\phi}\left(\frac{a}{r}\right)^3 + \left(\frac{a}{2b-r}\right)^3 + 4 \right] \frac{1}{2+1/\phi} \tag{5}$$

where ϕ is the inclusion volume fraction, ρ and θ refer to the radial and circumferential directions, respectively, and r is a point position over the $\overline{BC}$ straight line, i.e. $r \in [a, 2(b-a)]$.

Liu and Winn [11] also developed a critical radius equation, which is presented as:

$$\overline{a_c} = \frac{3\gamma_s}{\left[({F_\rho}^2 + {F_\theta}^2) - 2\nu_m F_\theta(2F_\rho + F_\theta)\right](2{\sigma_\alpha}^2/E_m) + ({\sigma_\alpha}^2(1-2\nu_i)^2/E_i)} \tag{6}$$

where

$$F_\rho = \frac{1-(2\phi^{-1/3}-1)^{-2}}{(1-\phi)(\phi^{-1/3}-1)}$$

$$F_\theta = \frac{1+(2\phi^{-1/3}-1)^{-2}}{4(1-\phi)(\phi^{-1/3}-1)}$$

$$\sigma_\alpha = \frac{(\alpha_m - \alpha_i)\,|\Delta T|}{(2\phi(1-2\nu_m) + (1+\nu_m)/2E_m(1-\phi)) + (1-2\nu_i/E_i)}$$

3. Materials

Three examples in which ceramic composite materials resulted in cracks during the cooling process due to the thermal expansion mismatch, have been selected from the literature to apply the finite element simulations and the extension of the Davidge and Green [1] critical radius model.