Calculation of fracture toughness for a biphase ceramic material

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A model for biphase ceramic material fracture toughness prognosis is proposed based on the estimation of influence of second phase mechanical properties and grain size and taking into account the possibility of rounding of the second phase grains by the crack front. The dependence of grain composite fracture toughness on high modulus grain volume fraction is shown to have an extreme. The maximum magnitude as well as its position is shown to be depended on matrix-inclusion grain size ratio.

Представлена модель для прогнозирования коэффициента трещиностойкости двухфазного керамического материала, основанная на оценке вклада в трещинностойкость зерен второй фазы, исходя из их размеров, физико-механических свойств и учитывая возможность огибания их фронтом трещины. Показано, что зависимость трещиностойкости зернистого композита от объемного содержания высокомодульных включений имеет экстремальный характер, причем как высота, так и положение максимума зависит от соотношения размеров зерен матрицы и включений.

There are several approaches to forecast multiphase ceramic fracture toughness (the strength characteristic of a material containing a crack defect, $K_{1C} = (\pi c)^{1/2}\sigma_c$ where σ_c is the material tensile strength; c, the crack length). In most cases, the influence of second phase introduction on the composite mechanical properties is considered. Within the frame of an approach proposed in [1], the crack passes consecutively and rectilinearly through grains and grain boundaries. The problem statement implies that the model, although having an advantage consisting in the possibility to estimate the K_{1C} for a multiphase composite, does not take into account that the crack is able of rounding obstacles as well as the failure may occur along the grain boundaries at all.

It is just F.F.Lange [2] who has considered the fracture surface of an epoxy resin sample containing glass beads and connected the destruction energy increasing with the crack front bending in the propagation plane due to its delay on "stoppers" that are the second phase grains. However, this model does not take into account different ability of stoppers to delay the crack front before failure. This work is an attempt to estimate the contribution of a second phase grains to fracture toughness, taking into account their sizes, mechanical characteristics and the possible rounding them by the crack.

Let a crack in biphase material be considered. We shall keep the concept of quasibrittle failure [3] and consider that the crack size is much greater than the composite structure parameter. Let us consider the critical stress intensity factor:

$$K_{1C} = \eta_{11}K_{1C_{11}} + \eta_{22}K_{1C_{22}} + \\ + \eta_{12}K_{1C_{12}} + \eta_{21}K_{1C_{21}}, \tag{1}$$

where $\eta_{i,j}$, K_{1Cij} are the fracture toughness characteristics and the volume fractions, respectively, of the i-th phase grains limited by the contact surface with those of the j-th one. The volume fractions can be expressed via the specific contact areas of corresponding phases, S_{11}, S_{12}, S_{22}. Then,

$$\eta_{11} = 2\frac{R_1}{3}S_{11},\ \eta_{22} = 2\frac{R_2}{3}S_{22},$$
$$\eta_{12} = 2\frac{R_1}{3}S_{12},\ \eta_{21} = 2\frac{R_2}{3}S_{21}.$$

It is known [4] that if $R_1/R_2 = \rho$ (where R_1 and R_2 are grain radii and $R_2 > R_1$), then

$$S_{12} = \frac{S_2\eta_2(1-\eta_2)}{1-\eta_2(1-\beta)}$$

(here S_2 is the specific area of phase 2; $S_2 = 3/R_2$), or

$$S_{12} = \frac{3\eta_2\eta_1}{R_2\left(1-\eta_2(1-\beta)\right)},$$
$$S_{11} = \frac{3\eta_1^2}{2R_1\left(1-\eta_2(1-\beta)\right)},$$
$$S_{22} = \frac{3\beta\eta_2^2}{2R_2\left(1-\eta_2(1-\beta)\right)},$$

and the formula (1) can be written as

$$K_{1C} = \frac{\eta_1^2}{1-\eta_2(1-\beta)}K_{1C_{11}} + \quad (2)$$
$$+\frac{\beta\eta_2^2}{1-\eta_2(1-\beta)}K_{1C_{22}} + \frac{\eta_1\eta_2\left(K_{1C_{21}} + \beta K_{1C_{12}}\right)}{1-\eta_2(1-\beta)}.$$

Here K_{C11} and K_{C22} are fracture toughness factors for materials of phases 1 and 2 that can be determined in experiment on pure materials manufactured in conditions selected to synthesize the corresponding composite. To estimate K_{C21}, it is to consider the behavior of a crack propagating from the matrix (phase 1) into an inclusion (phase 2). Let $E_2 > E_1$ (E is the Young modulus). In this case, there are two possible ways of the crack further propagation: within the grain and along the grain boundary.

Let the rectilinear crack front that had place in isotropic medium be referred to as the "efficient" one. The efficient front is assumed to coincide with the real one in areas where the crack passes within the grain and to differ from the real one where the crack rounds a stronger phase grain. Proceeding from known dependences of stresses at the crack top on the angle between chosen direction and the crack plane [3], we can write:

$$\sigma_{ef}(\theta) = \frac{K_I}{\sqrt{2\pi r}}\cos\frac{\theta}{2}\sqrt{1 + 2\sin\frac{\theta}{2}\sin\frac{7\theta}{2} + \sin^2\frac{\theta}{2}},$$

where $\sigma_n(\theta)$ is the efficient stress which may provoke the crack propagation at an angle θ. This case is conditioned by equality between $\sigma_{ef}(\theta)$ and σ_{1cr}, the critical stress of phase 1 (so-called "theoretical toughness" is meant). On the other hand, the condition of the crack propagation within the inclusion is the equality between $\sigma_{ef}(\theta)$ and σ_{2cr}.

$$\sigma_{2cr} = \frac{K_I}{\sqrt{2\pi r}}.$$

Then the expression for critical angle (θ_0) is:

$$\frac{\sigma_{1cr}}{\sigma_{2cr}} = \quad (3)$$
$$\cos\frac{\theta_0}{2}\sqrt{1 + 2\sin\frac{\theta_0}{2}\sin\frac{7\theta_0}{2} + \sin^2\frac{\theta_0}{2}}.$$

It is obviously that when $\theta < \theta_0$, the crack will move along the grain boundary, and when $\theta > \theta_0$, within the grain bulk.

Let $V(\theta_0)$ be the volume of a segment cut from the grain by the plane α (Fig. 1); $V_{1/2}$, the grain hemisphere volume; K_{1C}', the stress intensity coefficient required for moving the crack front sections around the second phase grain; and K_{1C}'', the same but within the grain. Then, similarly to (1)

$$K_{1C_{21}} = \frac{V(\theta_0)}{V_{1/2}}K_{1C}' + \frac{V_{1/2} - V(\theta_0)}{V_{1/2}}K_{1C}''. \quad (4)$$

Let us consider now area dS_0 before the real front which bends the phase 2 grain (Fig. 1), corresponding to area dS before the efficient front. Then the stress intensity factor in dS_0: are

$$K_{II}^* = \sqrt{\pi c}\,\sigma\sin\theta\cos\theta\sin\varphi$$
$$K_{III}^* = \sqrt{\pi c}\,\sigma\sin\theta\cos\theta\cos n\varphi,$$

where c is the crack size. Accordingly to the general energy criterion of Griffits [3], a crack front advancement starts if

$$K_I^{*2} + K_{II}^{*2} + \frac{4}{1+k}K_{III}^{*2} = K_{1C}^{*2},$$

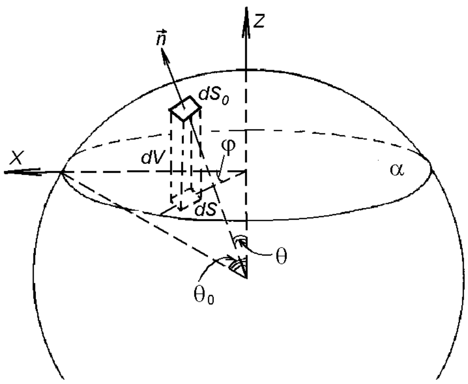

Fig. 1. Areas before real and efficient front elements.

where $k = 3 - \nu/(1 + \nu)$ (for planar stressed state). For brittle materials, $\nu \approx 0.2$, so for generalization, it is assumed that $4/(1 + k) \approx 1$ and thus $K^*_{1C} \approx \sqrt{K^{*2}_I + K^{*2}_{II} + K^{*2}_{III}}$.

Let us assume that the front segments which bend around the second phase grains start to move if and when the average value K^*_{1C} reaches K_{IC_1} (fracture toughness of phase 1) that is possible when the phase interface strength is equal to or higher than that of the phase 1. The average value $<K^*_{1C}>$ of K^*_{1C} along all the crack front segments rounding the second phase grains is:

$$<K^*_{1C}> = \frac{1}{V(\theta_0)} \int_{V(\theta_0)} \sqrt{K^{*2}_I + K^{*2}_{II} + K^{*2}_{III}} dV,$$

or

$$<K_{1C}> =$$

$$= \frac{2R^3\pi}{V(\theta_0)} K_{1C}' \int_0^{\theta_0} \cos\theta_0 \cos^2\theta - \cos^3\theta) d\cos\theta,$$

($\sqrt{\pi c}\sigma$ *equiv* K_{1C}'). After integration, taking into account that $\frac{8}{3}\pi R^3 \sin^4\frac{\theta_0}{2}(1 + 2\cos^2\theta_0)$ we get

$$<K^*_{1C}> = \frac{1}{\alpha} f(\theta_0) K_{1C}', \quad (5)$$

where

$$f(\theta_0) = \begin{cases} \dfrac{3}{4\sin^4\frac{\theta_0}{2}(1 + 2\cos^2\theta_0)}\left(\dfrac{1}{4} - \dfrac{\cos\theta_0}{3} + \dfrac{\cos^4\theta_0}{12}\right), & \text{when } \theta_0 < \dfrac{\pi}{2} \\ \dfrac{3}{4}, & \text{when } \theta_0 \geq \dfrac{\pi}{2} \end{cases}.$$

The factor $1/\alpha$ in (5) is introduced to take into account the non-sphericity of a real grain and is a ratio of sphere specific area of to that of corresponding figure. Thus, $\alpha \geq 1$. Therefore, $K_{1C}' = \alpha K_{1C_1}/f(\theta_0)$. K_{1C}'' in (4) is in fact K_{1C_2}, i.e., fracture toughness of nonporous sample of the phase 2. Then,

$$K_{1C_{21}} = \frac{V(\theta_0)\alpha}{V_{1/2} f(\theta_0)} K_{1C_1} + \left(1 - \frac{V(\theta_0)}{V_{1/2}}\right) K_{1C_2}, \quad (6)$$

where

$$\frac{V(\theta_0)}{V_{1/2}} = 4\sin^4\frac{\theta_0}{2}(1 + 2\cos^2\theta_0).$$

When the joint between phases 1 and 2 is strong (e.g. due to sintering), then $K_{IC_{12}} = K_{IC_{11}}$ and it is just the fracture toughness of nonporous material of the phase 1.

For a metal-ceramic composite, $\beta = 0$ (the ceramic phase grain are not in contact with each other), $K_{IC_{11}} = K_{IC_1}$, and the formula (2) takes the view:

$$K_{1C} = \eta_1 K_{1C_1} + \eta_2 K_{1C_{21}}. \quad (7)$$

To conclude, let us consider some interesting cases of component selection for a composite at various ratios of mechanical characteristics.

1). Let we have two nonporous phases having $K_{IC_{11}} = K_{IC_{22}}$ and $\sigma_{cr1} = \sigma_{cr2}$. Let at the selected synthesis conditions $K_{IC_{11}} = K_{IC_{22}} = 0.75K_{IC_1} = 0.75K_{IC_2}$. Let at the same synthesis conditions we have ideal mutual contact between grains of different phases due to chemical interaction. In this case, the enhancement in mechanical characteristics due to the second introduction can be referred to as a "purely chemical" one. Proceeding from (2), it is seen that $K_{IC_{21}} = K_{IC_{12}} = 4/3K_{IC_{11}}$. The results for $R_1/R_2 = 10$; 1; and 0.1 are presented in Fig. 2.

2). Let $K_{IC_{11}} = K_{IC_{22}}$ as in the previous case, but $E_2 = 3E_1$. In this case, $K_{IC_{12}} = 4/3K_{IC_{11}}$. The $K_{IC_{21}}$ value can be obtained from formula (6) where $\theta_0 \geq \pi/2$ and $\alpha \approx 1.2$ (cube-to-sphere specific surface ratio). Then $K_{IC_{21}} \approx 1.63K_{IC_{11}}$. Thereby,

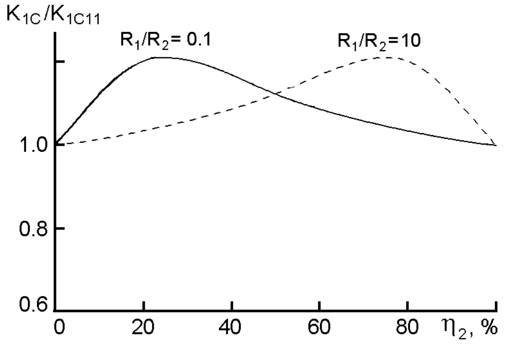

Fig. 2. Fracture toughness as a function of the second phase volume fraction (η_2) ($K_{IC_{11}} = K_{IC_{22}}$ and $E_1 = E_2$).

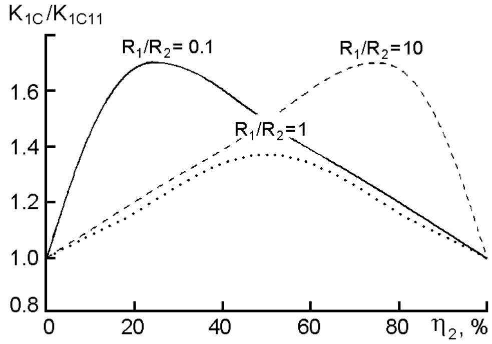

Fig. 3. Fracture toughness as a function of the second phase volume fraction (η_2) ($K_{IC_{11}} = K_{IC_{22}}$ and $3E_1 = E_2$).

$$K_{1C} = \left(\frac{\eta_1^2}{1 - \eta_2(1 - \beta)} + \frac{\beta \eta_2^2}{1 - \eta_2(1 - \beta)} + \frac{\frac{4}{3}\eta_1\eta_2(1.63 + \beta)}{1 - \eta_2(1 - \beta)} \right) K_{1C_{11}}.$$

The results for $R_1/R_2 = 10$; 1; 0,1 are presented in Fig. 3.

Thus, the dependence of composite fracture toughness on its composition at a good chemical compatibility of different phases includes an extreme. The optimum second phase concentration, as well as the maximum fracture toughness, depends on correlation between grain sizes of different components. Thereby, the presented model allows to forecast two-phase ceramic system fracture toughness, proceeding from mechanical features of its components and their boundaries, taking into account the case when a crack rounds high-strength phase inclusions.

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Розрахунок коефіцієнта тріщиностійкості двофазного керамічного матеріалу

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Представлено модель для прогнозування коефіцієнта тріщиностійкості двофазного керамічного матеріалу, що базується на оцінці вкладу у тріщиностійкість зерен другої фази, виходячи з їхніх розмірів, фізико-механічних властивостей та враховуючи можливість огинання їх фронтом тріщини. Показано, що залежність тріщиностійкості зернистого композиту від об'ємного вмісту високомодульних включень має екстремальний характер, причому як величина, так і положення максимуму залежить від співвідношення між розмірами зерен матриці та включень.