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The stiffness and strength of transformation toughening ceramics with misoriented microcracks

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Theoretical studies on misoriented transformation particles and microcracks in transformation toughening ceramics are presented using the Eshelby equivalent inclusion method. The stress field, stiffness and strength were calculated. Experiments were done by the three-point bend method using Al_2O_3/ZrO_2 ceramics and the stiffness and strength were also measured. Comparison between theoretical and test results confirmed the important role of microcracks.

1. Introduction

In ceramics in which the main component is ZrO_2, some tetragonal ZrO_2 particles transform into a monoclinic phase, accompanied by a strain increment in the particles, consisting of a mean strain of 5% and a shear strain of 14%, upon cooling and loading. During the process, local high energy is absorbed and the crack opening is restrained. Meanwhile, microcracks occur in particles and in the matrix due to the external load and the thermo-strain mismatch of components. A large number of microcracks are of benefit for the toughening of ceramics, although the material strength is reduced; therefore, the influence of microcracks is a factor which has to be accounted for. In the process zone, i.e. at a crack tip, in transformation ceramics, the transformation and microcracks occur at the same time and contribute to the toughness in a similar way, namely crack shielding. Therefore, the properties of the zone are very important to the understanding of the mechanical properties of transformation ceramics, including stiffness, strength and critical load during transformation. Generally, microcracks are misoriented, and are distributed randomly. The transformation particles are not spherical. Some of them are irregular in shape, such as ellipsoidal and lense shaped particles dispersed randomly in the matrix. Rühle [1] observed *in situ* microcracking in Partially Stabilized Zirconia (PSZ) ceramics and found that the aspect ratio of microcracks was about 1:100 and that displacement of the crack opening could be neglected. The length of microcracks is greater than the size of the particles. Research on transformation and microcracking was done independently, and interaction between the two was introduced. Some models on transformation ceramics have been proffered without microcracking being considered [2–4]. Also, the stiffness and strength of microcrack-toughening ceramics have been researched without transformation strain being considered [5]. In the present paper, interaction between microcracking and transformation is accounted for using the equivalent inclusion method of Eshelby [6]. The influence of microcracking on the properties of ceramics can be studied, involving the stress, strength and effective modulus, by a theoretical model in which the misorientation of microcracks and transformation particles are considered i.e. by the three-point bend experiment in Al_2O_3/ZrO_2 ceramics. Comparison between experimental and theoretical results confirmed the rationality of the theory in this paper.

2. Stress field

Fig. 1 shows the random distribution of microcracks and particles in the material element. The particles are viewed as prolate spheroids and the microcracks as penny shaped voids (Fig. 2). Suppose that all the particles are of the same shape and transform at the same time; and also, that the transformation does not develop progressively. Meanwhile, the microcracks are of the same length and the crack opening displacement is much less than the length.

Under external load, σ^o, the tetragonal ZrO_2 particles, of volume fraction f_1, transform by a strain increment, ε^T, and microcracks of volume fraction, f_2, exist. The interaction strain between the particles and microcracks is represented by a mean strain $\bar{\varepsilon}$. The mean stress in the matrix is

$$\sigma_m = \sigma^o + C\bar{\varepsilon} \quad (1)$$

and the stress of a particle under the global co-ordinate system is as follows

$$\begin{aligned}\sigma^1 &= C_1(\varepsilon^o + \bar{\varepsilon} + T'_1 S_1 T_1 \varepsilon^{**} - \varepsilon^T) \\ &= C[\varepsilon^o + \bar{\varepsilon} + (T'_1 S_1 T_1 - I)\varepsilon^{**}] \quad (2)\end{aligned}$$

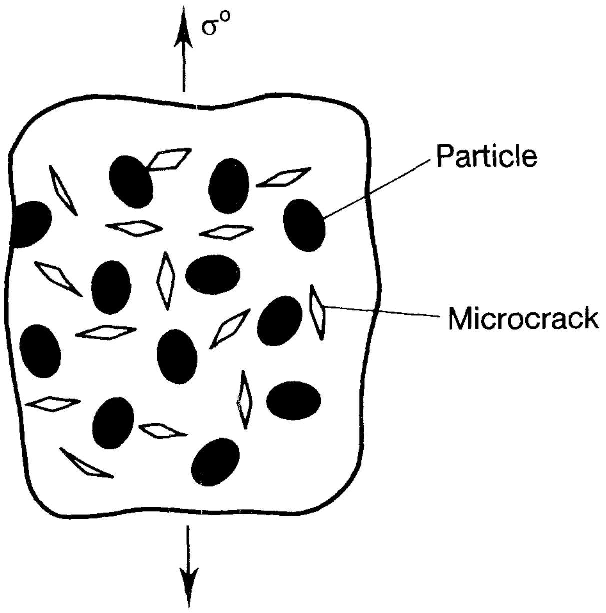

Figure 1 The element of material.

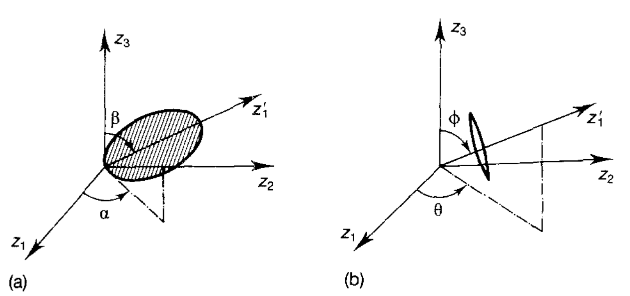

Figure 2 The orientation of: (a) particle and (b) microcrack.

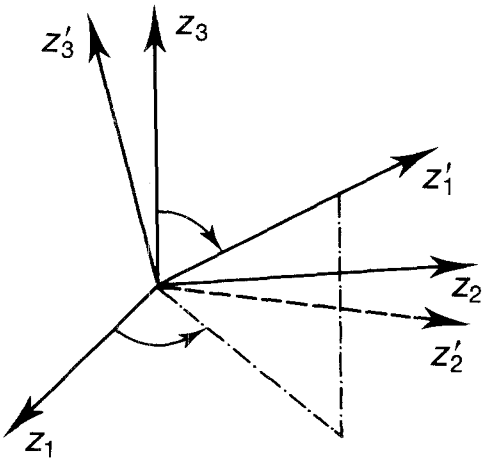

Figure 3 Transformation of co-ordinate system.

where C and C_1 are the moduli of the matrix and particles, respectively; ε° satisfies that $\sigma^{\circ} = C\varepsilon^{\circ}$; ε^{**} is the equivalent strain; S_1 is the Eshelby tensor; and T_1 the transformation matrix of a particle. The equivalent relation of a microcrack under the global system is

$$\sigma^2 = C[\varepsilon^{\circ} + \bar{\varepsilon} + (T'_2 S_2 T_2 - I)\varepsilon^{2*}] = 0 \quad (3)$$

where T_2 is transformation matrix, S_2 is the Eshelby tensor of a microcrack and ε^{2*} is the equivalent strain. From Equations 3 and 4, ε^{**} and ε^{2*} are given as

$$\varepsilon^{**} = (\Delta C T'_1 S_1 T_1 + C)^{-1}[-\Delta C(\varepsilon^{\circ} + \bar{\varepsilon}] \quad (4)$$

$$\varepsilon^{2*} = -(T'_2 S_2 T_2 - I)^{-1}(\varepsilon^{\circ} + \bar{\varepsilon}) \quad (5)$$

where $\Delta C = C_1 - C$ and I is the identity tensor. Because the interaction stress satisfies equibalance by itself, namely, $\int_v \sigma \, dv = 0$

$$\int_{v - v_1 - v_2} C\bar{\varepsilon} \, dv + \int_{v_1} C[\bar{\varepsilon} + (T'_1 S_1 T_1 - I)\varepsilon^{**} \, dv + \int_{v_2} C[\bar{\varepsilon} + T'_2 S_2 T_2 - I)\varepsilon^{2*}] \, dv = 0 \quad (6)$$

where v, v_1 and v_2 are the volumes of material element, particles and microcracks, respectively. The orientation distributing functions of the particles and microcracks are $g_1(\alpha, \beta)$ and $g_2(\theta, \phi)$. $\alpha \in [\alpha_1, \alpha_2]$, $\beta \in [\beta_1, \beta_2]$, $\theta \in [\theta_1, \theta_2]$, $\phi \in [\phi_1, \phi_2]$, α_i, β_i and θ_i, ϕ_i are the orientation scopes. f_1 and f_2 are given as follows

$$f_1 = \frac{1}{v}\int_{v_1} \Omega_1 g_1(\alpha, \beta) \sin\beta \, d\alpha \, d\beta \quad (7)$$

$$f_2 = \frac{1}{v}\int_{v_2} \Omega_2 g_2(\theta, \phi) \sin\theta \, d\theta \, d\phi \quad (8)$$

where Ω_1, Ω_2 are the volumes of a single particle and a microcrack, respectively.

$$a_1 = \int_{\beta_1}^{\beta_2}\int_{\alpha_1}^{\alpha_2} g_1(\alpha, \beta) \sin\beta \, d\alpha \, d\beta \quad (9)$$

$$a_2 = \int_{\phi_1}^{\phi_2}\int_{\theta_1}^{\theta_2} g_2(\theta, \phi) \sin\phi \, d\theta \, d\phi \quad (10)$$

Combining Equations 4–6, $\bar{\varepsilon}$ is given as

$$\bar{\varepsilon} = \left[(1 - f_2)I - \frac{f_1}{a_1} R\Delta C\right]^{-1} \times \left[\left(\frac{f_1}{a_1} R\Delta C - f_2 I\right) C^{-1}\sigma^{\circ} - \frac{f_1}{a_1} R C_1 \varepsilon^{\mathrm{T}}\right] \quad (11)$$

$$R = \int_{\beta_2}^{\beta_2}\int_{\alpha_1}^{\alpha_2} (T'_1 S_1 T_1 - I)(\Delta C T'_1 S_1 T_1 + C)^{-1} \times g_1(\alpha, \beta) \sin\beta \, d\alpha \, d\beta \quad (12)$$

The stress in a particle of orientation (α, β) is

$$\begin{aligned} \sigma^1 &= \sigma^{\circ} + C\bar{\varepsilon} + C(T'_1 S_1 T_1 - I)\varepsilon^{**} \\ &= \sigma^{\circ} + C\bar{\varepsilon} + C(T'_1 S_1 T_1 - I) \\ &\quad \times (\Delta C T'_1 S_1 T_1 + C)^{-1} \\ &\quad \times [C\bar{\varepsilon} - \Delta C(C^{-1}\sigma^{\circ} + \bar{\varepsilon})] \end{aligned} \quad (13)$$

Equation 13 suggests that the stress in the particles does not depend on the distribution of microcracks. When $f_2 \ll 1$, the influence of microcracks vanishes.

3. Material strength

The change in free energy with microcracking is

$$E_{\text{int}} = -\frac{2\pi a^2 t}{3a_2}\int_{\phi_1}^{\phi_2}\int_{\theta_1}^{\theta_2} \varepsilon^{2*} g_2(\theta, \phi) \sin\phi \, d\theta \, d\phi \quad (14)$$

where a and t are the radius and crack opening displacement of a microcrack. The strength, σ_u, satisfies the following equation

$$G = \left| \frac{\partial E_{\text{int}}}{\partial (\pi a)^2} \right| = G_c \tag{15}$$

where G_c is the toughness of the matrix. Combining Equations 5 and 14, Equation 15 is changed into the following

$$a\sigma_u Q(C^{-1}\sigma_u + \bar{\varepsilon}) = \frac{\pi(2-\mu)(1-2\mu)}{8(1-\mu)^2} G_c \tag{16}$$

and

$$Q = \int_{\phi_1}^{\phi_2} \int_{\theta_1}^{\theta_2} T g_2(\theta, \phi) \sin\phi \, d\theta \, d\phi \tag{17}$$

where T is given as

$$T = \frac{4a(1-\mu)^2}{\pi(1-2\mu)(2-\mu)} T_2' \boldsymbol{T}_o T_2 \tag{18}$$

and $\boldsymbol{T}_o$ is

$$\boldsymbol{T}_o = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ \frac{\mu}{1-\mu} & 0 & 0 & 0 & 0 \\ \frac{\mu}{1-\mu} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1-2\mu}{1-\mu} \\ 0 & 0 & 0 & 0 & \frac{1-2\mu}{1-\mu} \end{bmatrix} \tag{19}$$

when the external load $\sigma_i^o \neq 0$ and $\sigma_j^o = 0 (i \neq j)$, the strength, σ_{ui}, is solved from the following equation

$$\left(Q_{ij}C_{ij}^{-1} + \frac{f_1}{a_1} Q_{ij} RI_{jk} R_{kl} \Delta C_{lm} C_{mi}^{-1}\right)(\sigma_{ui})^2 - \frac{f_1}{a_1} RI_{ij} R_{jk} C_{kl}^{-1} \varepsilon_l^T \sigma_{ui} - \frac{\pi(2-\mu)(1-2\mu)}{8(1-\mu)^2} G_c = 0 \tag{20}$$

where i is not the dummy subscript, $RI = [(1-f_2)I - f_1/a_1 \, R\Delta C]^{-1}$.

4. Constitutive relation

Through volume averaging of the material element, the macro-strain is derived as

$$\langle \varepsilon \rangle = C^{-1}\sigma^o + \frac{f_1}{a_1} P[-\Delta C(C^{-1}\sigma^o + \bar{\varepsilon}) + C_1 \varepsilon^T] + \frac{32(1-\mu)^2 na^2}{3(1-2\mu)(2-\mu)a_2} Q(C^{-1}\sigma^o + \bar{\varepsilon}) \tag{21}$$

and

$$P = \int_{\beta_1}^{\beta_2} \int_{\alpha_1}^{\alpha_2} (\Delta C T_1' S_1 T_1 + C)^{-1} \times g_1(\alpha, \beta) \sin\beta \, d\alpha \, d\beta \tag{22}$$

Equation (22) is the constitutive relation for transformation ceramics. In effect, transformation develops progressively, and the transformation strain rate is related to stress in the particles. Meanwhile, the particles do not transform at the same time. Therefore, the non-linearity of materials would exist during the process. The factors above are not accounted for here, and the strain increment in particles under an external load is assumed. The increment of macro-strain is given by the difference in $\langle \varepsilon \rangle$ before and after transformation. The stiffness of the ceramics can be calculated by Equation 21.

5. Discussion

Calculation was performed assuming that the distribution of particles and microcracks was random and that the range of distribution angles was [−90°, 90°]. The calculation was based on Al_2O_3/ZrO_2 ceramics, and the results are shown in Figs 4–7. Figs 4 and 5 give the trends in strength with the length and the volume fraction of the microcracks. It is suggested that the main factor which causes the reduction of strength is the length of the microcracks rather than the volume fraction. Transformation reduces the

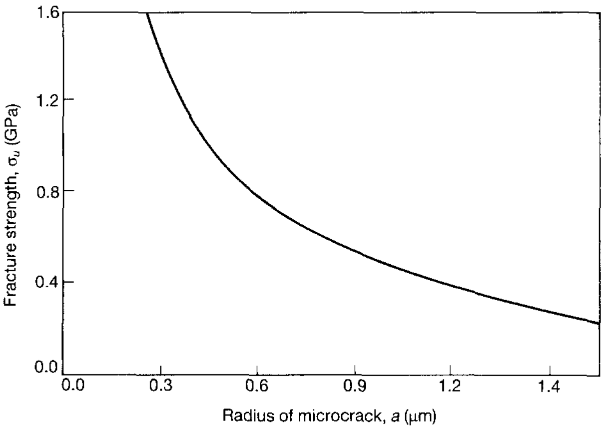

Figure 4 Trends in strength with crack radius.

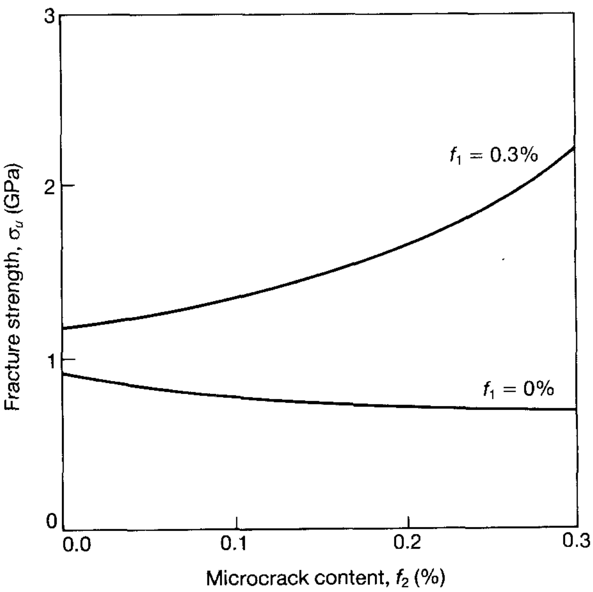

Figure 5 Relation between strength and microcrack content where f_1 is the volume fraction of ZrO_2 particles, and a, microcrack radius = 0.7 μm.

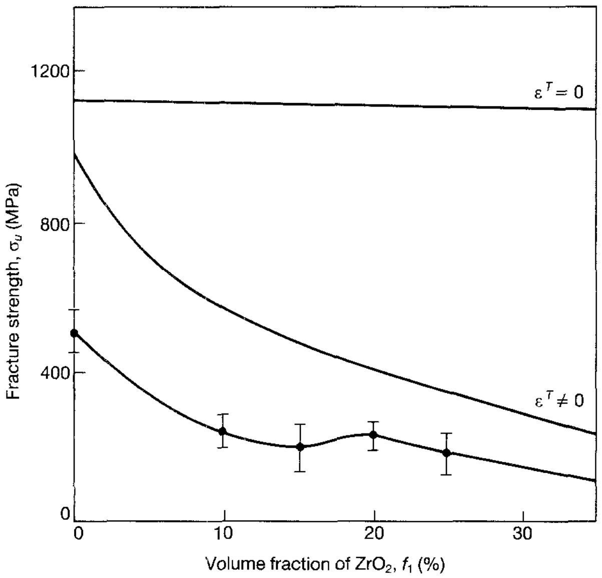

Figure 6 Trends in strength with the content of ZrO_2 in Al_2O_3/ZrO_2 (ε^T is the strain increment associated with the transformation of the ZrO_2 particles and a the microcrack radius = 0.7 μm).

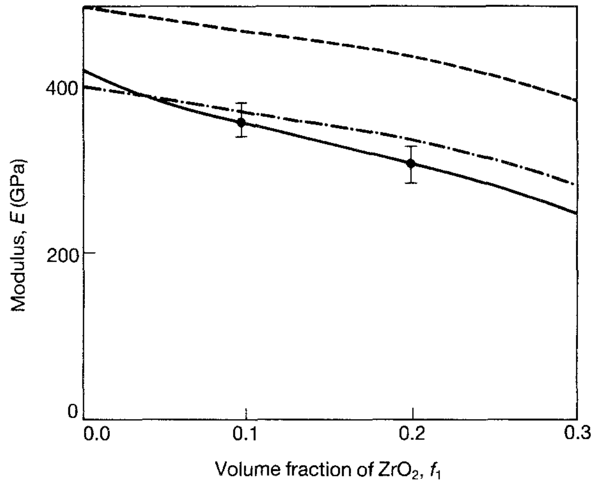

Figure 7 Comparison between theoretical and experimental value of the effective modulus (f_2 is the content of the microcracks). (-··-) theoretical $f_2 = 1\%$, (——) tested, (– – –) theoretical $f_2 = 0\%$.

strength because it induces tension stress in the matrix, and the stress concentration increases near the cracks. The suggestion can be seen from Fig. 6 in which strength reduces quickly with the increment of the volume fraction, f_1, of the particles when $\varepsilon^T \neq 0$. Fig. 7 shows the effective modulus of Al_2O_3/ZrO_2 ceramics as a function of ZrO_2 content for two kinds of microcracks: (a) $f_2 = 0$ (no microcrack exists) and (b) $f_2 = 1\%$ (dashed line). It is found that the modulus decreases with increasing ZrO_2 content, and that microcracks also cause the reduction of the modulus.

A three-point bend test of a rectangle beam of Al_2O_3/ZrO_2 is performed. The modulus and strength were measured and are shown in Figs 6 and 7. Agreement between the theoretical and experimental results is confirmed, and is better when $f_2 = 1\%$ for the effective modulus. The theoretical value of strength is higher than the tested value because of the assumption that all the microcracks extend at the same time when a critical load is attained. However, the trend is similar to the experimental strength value, except for $f_1 \approx 20\%$. In general, the present results and discussion suggest that stress in particles is not influenced by the distribution of microcracks, and that the microcracks have a large influence on the effective modulus. The strength, σ_u, is controlled by the following factors: length and content of the microcracks, the properties of the components and the transformation strain. In addition, transformation causes the reduction of the ceramic modulus. Comparison between theoretical and experimental results shows the rationality of the present theory.

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