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Transformation criterion of phase transformation toughening ceramics with misoriented microcracks

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Phase transformation criterion is the key to investigating the toughness of phase transformation ceramics. In this paper, the modified equivalent inclusion theory by the authors is employed to study the interaction between microcracking and transformation in ceramics. The transformation criterion is derived. The influence of microcracks and transformation particles on the critical transformation load is discussed.

1. Introduction

Microcracking in phase transformation ceramics is an important factor affecting the mechanical behaviour [1, 2]. Stiffness and strength are reduced and toughness is increased with microcracking [3]. The reason for microcracking is as follows: first, the volume expansion of the transformation particles induces microcracking in the matrix; second, residual thermal strain from the mismatch of thermal expansion causes microcracks; third, microcracks exist due to external load and environment. The microcracking and phase transforming at a crack tip can impede the expansion of the crack by crack shielding.

Rühle [1, 2] observed the microcracking in Partially stabilized zirconia (PSZ) ceramics by scanning electron microscopy (SEM) and found that the length of microcracks is almost the same as the size of the transformation particles. The opening displacement is only 1% of the length. In other works [3–5], the equivalent inclusion theory was applied to estimate the stiffness and strength of phase transformation ceramics with misoriented microcracks. Other authors [6, 7] suggested that the toughness can be estimated only if the critical transformation load is determined and the size of transformation zone is given. They derived the transformation criterion and constitutive relation without microcracking being considered. In this paper, suppose that the microcracks and transformation particles are distributed randomly. Based on the other works [3–5], the modified equivalent inclusion theory is employed to investigate the interaction between the microcracks and transformation particles. The transformation criterion and constitutive relation are derived. The influence of the microcracks and the particles is discussed quantitatively.

2. Phase transformation criterion

The orientation distribution functions of the transformation particles and the microcracks are $g_1(\alpha, \beta)$ and $g_2(\theta, \varphi)$ (Fig. 1), $\alpha \in [\alpha_1, \alpha_2]$, $\beta \in [\beta_1, \beta_2]$, $\theta \in [\theta_1, \theta_2]$, $\varphi \in [\varphi_1, \varphi_2]$. α_i, β_i and θ_i, φ_i are the orientation scopes. Suppose that all the particles are of the same shape and transform at the same time, and also, the transformation does not develop progressively. Meanwhile, the microcracks are of the same length and crack opening displacement much less than the length. Under external load σ^0, 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 stress in a particle under the global coordinate system is written [3–5] as

$$\sigma^1 = \sigma^0 + C\varepsilon + C(T'_1 S_1 T_1 - I) \times (\Delta C T'_1 S_1 T_1 + C)^{-1}[-\Delta C(C^{-1}\sigma + \bar{\varepsilon}) + C_1 \varepsilon_T] \quad (1)$$

where C and C_1 are the moduli of the matrix and particles, respectively; S_1 is the Eshelby tensor; T_1 is the transformation matrix of a particle; and I the identity tensor. $\Delta C = C_1 - C$; $\bar{\varepsilon}$ is the interaction strain between the particles and microcracks

$$\bar{\varepsilon} = \left[(1 - f_2)I - \frac{f_1}{a_1} R\Delta C\right]^{-1} \times \left[\left(\frac{f_1}{a_1} R\Delta C - f_2 I\right)C^{-1}\sigma^0 - \frac{f_1}{a_1} R C_1 \varepsilon^T\right] \quad (2)$$

and

$$a_1 = \int_{\beta_1}^{\beta_2}\int_{\alpha_1}^{\alpha_2} g_1(\alpha, \beta)\sin\beta \, d\alpha \, d\beta \quad (3)$$

$$R = \int_{\beta_1}^{\beta_2}\int_{\alpha_1}^{\alpha_2} (T'_1 S_1 T_1 - I)(\Delta C T'_1 S_1 T_1 + C)^{-1} \times g_1(\alpha, \beta)\sin\beta \, d\alpha \, d\beta \quad (4)$$

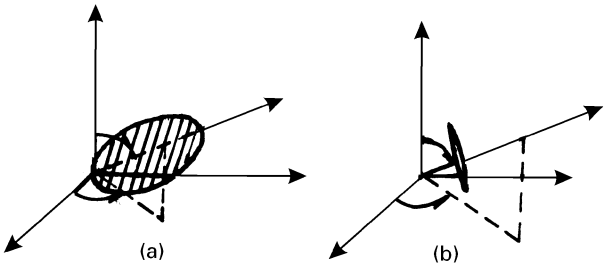

Figure 1 The orientation of (a) particles and (b) microcracks.

The energy change induced by the phase transformation strain of all the particles is derived as [5]

$$W = -\frac{1}{2}\int_V (\sigma^0 \varepsilon^{**} + \sigma^1 \varepsilon^T) dV \quad (5)$$

and

$$\varepsilon^{**} = (\Delta C T'_1 S_1 T_1 + C)[-C(\varepsilon^0 + \bar{\varepsilon}) + C_1 \varepsilon^T] \quad (6)$$

Through derivation, the interaction energy E_{int} with a particle is given as

$$E_{int} = -\frac{\Omega_1}{2a_1}\int_{\beta_1}^{\beta_2}\int_{\alpha_1}^{\alpha_2} (\sigma^0 \varepsilon^{**} + \sigma^1 \varepsilon^T) \times g_1(\alpha, \beta) \sin\beta \, d\alpha \, d\beta \quad (7)$$

where Ω_1 is the volume of a particle.

During phase transformation process, several kinds of energy change will take place, such as mechanical potential E_{int} and chemical free energy F_c, determining the possibility and direction of transformation. In addition, if twinning exists, the twinning energy G_T and crystal boundary energy G_c have to be considered. They can be given as follows

$$F_c = -\Omega_1 \Gamma_0 \quad (8)$$

$$G_T = \Omega_1 E_1 \gamma_t^2 [0.13/(1.2 + a_p/d)] \quad (9)$$

$$G_c = \Omega_1 \Gamma_t / d + \pi k a_p^2 \Gamma_i \quad (10)$$

where a_p is the size of a particle along its longitudinal axis; d and γ_t are the twinning space and shear strain. E_1 is the modulus of the particles; Γ_0, Γ_t and Γ_i are the chemical energy density, twinning boundary energy and grain boundary energy; k is the aspect ratio of the particles, i.e. $k = b/a_p$. When the energy balance is achieved, phase transformation will take place, namely

$$E_{int} + F_c + G_t + G_c = 0 \quad (11)$$

If the material element is loaded along axis z_i, the critical transformation load σ_c can be calculated from the following equation

$$l\sigma_c^2 + m\sigma_c + n = 0 \quad (12)$$

and

$$l = \frac{f_1}{a_1} A_{ii} + B_{ii} \quad (13)$$

$$m = 2\varepsilon_i^T + D_i + \frac{f_1}{a_1} G_i + H_i \quad (14)$$

$$n = -2E_c + 2L \quad (15)$$

where A_{ii}, B_{ii} are the elements of the second order tensor A and B when their two subscripts are both equal to i. $\varepsilon_i^T, D_i, G_i, H_i$ are the elements with subscript i of the vectors ε^T, D, G, H.

$$A = \frac{f_1}{a_1}\sigma^0 P \Delta C \left[(1 - f_2) I - \frac{f_1}{a_1} R \Delta C\right]^{-1} \times R \Delta C C^{-1} \quad (16)$$

$$B = P \Delta C C^{-1} \quad (17)$$

$$D = P C_1 \varepsilon^T \quad (18)$$

$$G = P \Delta C \left[(1 - f_2) I - \frac{f_1}{a_1} R \Delta C\right]^{-1} R C_1 \varepsilon^T \quad (19)$$

$$H = \varepsilon^T C \left\{\frac{f_1}{a_1}\left[(1 - f_2) I - \frac{f_1}{a_1} R \Delta C\right] \times \left[(1 - f_2) I - \frac{f_1}{a_1} R \Delta C\right]^{-1} - I\right\} R \Delta C C^{-1} \quad (20)$$

$$L = \varepsilon^T C \left\{\frac{f_1}{a_1}\left[(1 - f_2) I - \frac{f_1}{a_1} R \Delta C\right] \times \left[(1 - f_2) I - \frac{f_1}{a_1} R \Delta C\right]^{-1} - I\right\} R C_1 \varepsilon^T \quad (21)$$

$$P = \int_{\beta_1}^{\beta_2}\int_{\alpha_1}^{\alpha_2} (\Delta C T'_1 S_1 T_1 + C)^{-1} g_1(\alpha, \beta) \sin\beta \, d\alpha \, d\beta \quad (22)$$

$$E_c = F_0 - E_1 \gamma_T^2 [0.13/(1.2 + a_p/d)] - \Gamma_t/d - 3\Gamma_i/a_p \quad (23)$$

It is shown that the critical transformation load σ_c is not related to the distribution of microcracks, and is affected by the content f_2 of the microcracks. When $f_2 \ll 1$, the influence of the microcracks vanishes.

3. Constitutive relation

Through volume averaging of materials element, the macrostrain is derived as

$$\langle\varepsilon\rangle = C^{-1}\sigma^0 + \frac{f_1}{a_1} P[-\Delta C(C^{-1}\sigma^0 + \bar{\varepsilon}) + C_1 \varepsilon^T] + \frac{32(1 - \nu_0)^2 n a^2}{3(1 - \nu_0)(2 - \nu_0) a_2} Q(C^{-1}\sigma^0 + \bar{\varepsilon}) \quad (24)$$

Equation 24 is the constitutive relation for transformation ceramics. If transformation strain occurs in the particles, a macrostrain jump exists as the difference in $\langle\varepsilon\rangle$ before and after transformation. In fact, however, transformation develops progressively, and the fact that transformation strain rate is related to stress in the particles ought to be considered. Meanwhile, the particles do not transform at the same time. Therefore, the non-linearity of materials must exist during the process. Although the factors above are not taken into account here, the theoretical model is still rational because the non-linear period is much shorter than the whole failure process.

4. Discussion

Calculation was performed assuming that the distribution of the particles and microcracks is random and that the range of distribution angles is $[-90°, 90°]$. Twinning exists along the transverse axis of the particles and the number of the twinning crystals is a_p/d. The calculation was based on Al_2O_3/ZrO_2 ceramics and the values of the parameters in the formulas above are listed in Table I, in which E and ν are the modulus and Poisson ratio of the components. γ_t and v_t are the shear and bulk strain of phase transformation. Fig. 2 shows the influence of the volume fraction f_2 of microcracks on critical transformation load σ_c and strength σ_u. σ_c decreases almost linearly with the increment of f_2. It is possible that the stress intensity in matrix is increased with the increment of the microcracks' content and transformation is induced earlier. Fig. 3 gives the trends in σ_c with the content f_1 and size a_p of the particles, in which $\sigma_c \sim f_1$ curve is calculated when $a_p = 0.7$ μm and $\sigma_c \sim a_p$ curve when $f_1 = 0.3$. It is found that the critical transformation load decreases quickly with the increment of the size and content of microcracks. The reduction of σ_c induced with the size of the particles is greater than the microcracks' length. The influence of the particles' content originates from the stress transference from the particles to matrix because the particles are softer than the matrix. The density and boundary energy of twinning crystal depends on the size of the particles. The greater are the particles' size, the greater the twinning density and the less the boundary energy. The increment of the mechanical energy accelerates the phase transformation. In fact, the main factors affecting phase transformation are interphase chemical free energy and twinning. Twinning is the reason for the scale effect of the particles. Since the factors reducing the critical transformation load benefit toughening of ceramics, the increment of the size and content of transformation particles and the microcracks' content contribute to the toughening of ceramics. It is implied that microcracking contributes to the toughening of ceramics not only directly through crack shielding but also indirectly through the interaction with the transformed particles. From the calculation above, it is found that the material strength may be less than the critical transformation load when the length of microcracks is greater than some value, for example, $a = 1.5$ μm. Therefore, it is possible for the particles not to transform before material fails. Transformation, however, is still found on the fracture surface of Al_2O_3/ZrO_2, which suggests that transformation perhaps only concurs with fracture process before which none or few particles transform, because only the stress at a main crack tip is great enough to make the particles transform. This is also the reason that transformation toughening exists during fracture process.

Constitutive relation of Al_2O_3/ZrO_2 is calculated through Equation 16 and shown in Figs 4 and 5. When microcracks do not exist, the uniaxial modulus of the material element is almost the same before and after transformation, but the bulk modulus changes greatly due to the bulk strain of transformation. It is suggested that the reduction of the uniaxial modulus is only related to the microcracks and the one of the bulk

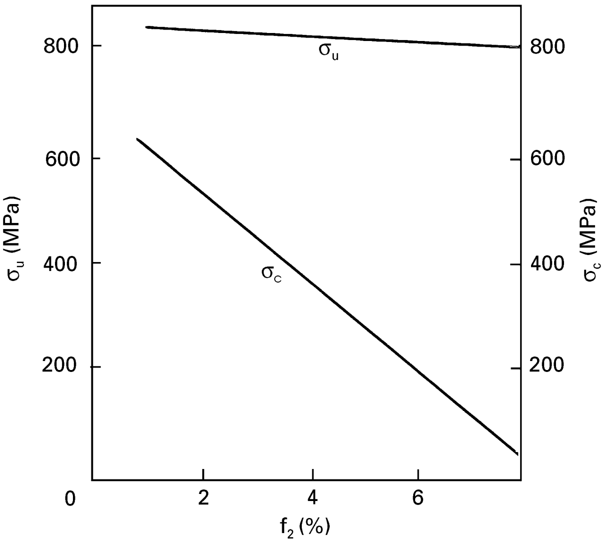

Figure 2 Influence of the microcracks' content f_2 on critical transformation load σ_c and fracture strength σ_u where f_1 (volume fraction of the particles) $= 0.3$; a (length of a microcrack) $= 0.7$ μm and a_p (size of a particle) $= 1$ μm.

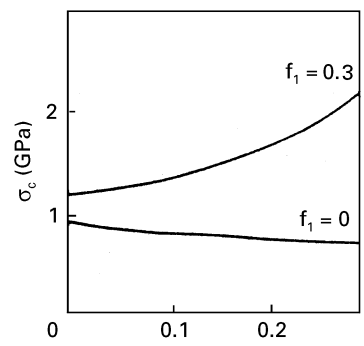

Figure 3 Trends in critical transformation load σ_c with the volume fraction f_1 and the size of the particles ($\sigma_c \approx f_1$ curve is calculated when $a_p = 0.7$ μm and $\sigma_c \approx a_p$ curve when $f_1 = 0.3$).

TABLE I The parameters of the components

Components	Parameters							
	E (GPa)	ν	γ_t	v_t	Γ_i (J/m^2)	Γ_t (J/m^2)	F_0 (MPa)	k
Al_2O_3	500	0.15	–	–	–	–	–	–
ZrO_2	170	0.20	0.14	0.05	1	1	280	0.8

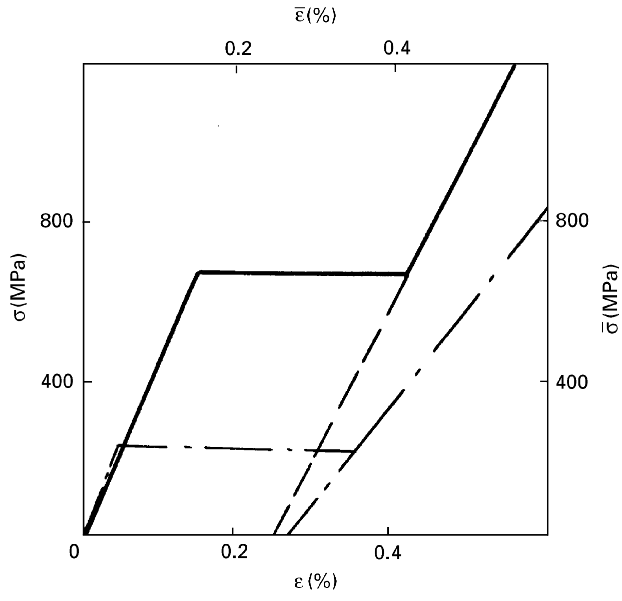

Figure 4 Stress–strain relation without microcracks. $f_2 = 0$; (——) $\sigma \approx \varepsilon$; (— · —) $\bar{\sigma} \approx \bar{\varepsilon}$.

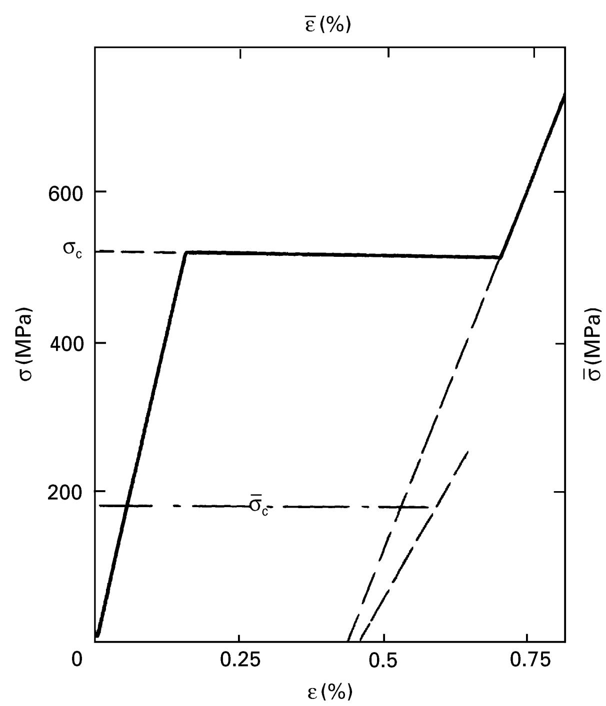

Figure 5 Stress–strain relation with microcracks of volume fraction $f_2 = 0.3$. (——) $\sigma \approx \varepsilon$; (— · —); $\bar{\sigma} \approx \bar{\varepsilon}$.

modulus, to the microcracks and transformation strain. Budiansky [7] proposed that the bulk modulus does not change before and after transformation and the stress decreases during the transformation process (Fig. 6). His proposal may be correct when the interaction between transformation and microcracks is not taken into account. Therefore, the conclusion of Budiansky may be not preferable in general cases. In the present paper, an assumption is given that transformation strain rate is not related to the stress in particles. The stress–strain relation during the transformation period is a straightline parallel to axis ε, not like the suggestion of Budiansky. When the bulk transformation strain of a particle is 5×10^4 με, the macrostrain increment of the material is 3×10^3 με without microcracks and 10^4 με with microcracks of volume fraction 2%. It is implied that microcracks are the main factor softening the ceramics.

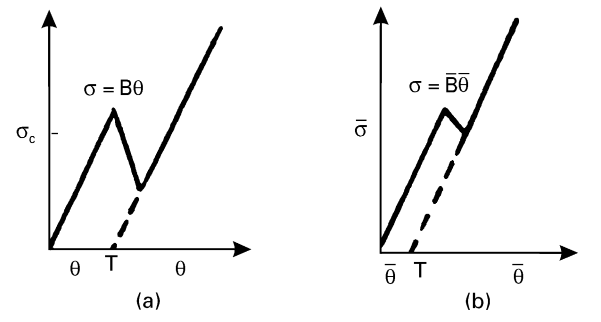

Figure 6 Stress–strain relation; (a) transformation particle; (b) composites with transformation particles of volume fraction *c*; B and $\bar{B}$ are constants.

5. Conclusion
The phase transformation criterion is not affected by the distribution of microcracks. The critical transformation load decreases slightly with the increment of microcrack length. The main factors affecting the criterion are the content, the size and the aspect ratio of the transformation particles, also, the microcracks' content and the chemical free energy difference of interphase. The greater are the size of the particles and the content of the microcracks, the lower the critical transformation load is. The scale effect results from the twinning. Microcracking contributes to the toughening of ceramics not only through crack shielding but also indirectly through the interaction with the transformed particles. For some cases, for example, when the length of the microcracks is greater than some value, the critical transformation load can exceed the material strength. It is implied that transformation exists during the failure period. For Al_2O_3/ZrO_2 ceramics, the length of microcracks is near to the grain size of ZrO_2. Therefore, the results from the theoretical model are rational.

Because of the consideration about the interaction between microcracking and transformation strain, the stress-strain relation is not same as the former results, (e.g. [6]). The modulus changes before and after transformation.

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