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Particle-size dependence of thermoelastic stress intensity factor in two-phase materials

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The stress intensity factor is estimated for an annular crack originating from the particle–matrix interface in residual stress fields associated with a spherical particle of lower thermal expansion than that of the matrix. It is shown that the stress intensity factor is a function of particle size and pre-existing crack length. Spontaneous matrix cracking will occur when the particle size exceeds a critical value, R_c. Close agreement between the calculated and experimental values for R_c is obtained. The analysis is applicable to all particulate composites where there is volume increase of a particle induced either by phase transformation or thermal expansion mismatch.

1. Introduction

It has been recognized by many investigators that the second-phase particle dispersed in a brittle matrix of different thermal expansion frequently serve as a potential source of fracture. Frey and Mackenzie [1] observed microcracking in a glass–Al_2O_3 composite of positive* differential thermal expansion and similar effects have been reported for BeO–SiC [2] and glass–ThO_2 [3] systems. Tummala and Friedberg [4] observed weakening of a glass–ZrO_2 system of positive thermal expansion difference between the matrix and second-phase but they did not indicate if the system was microcracked. Rossi [5] reported microcracking of a MgO–W composite for volume fractions of tungsten greater than 3 vol%.

Although the maximum thermoelastic stress concentration is independent of particle size [6], cracks have been observed adjacent to particles of certain size only, suggesting that some critical particle size, R_c, exists below which microfracture can be essentially suppressed. This was first pointed out by Binns [7] and later confirmed by Davidge and Green [3] for the glass–ThO_2 system. However, the analysis proposed by Davidge and Green [3] to explain the microcracking condition in two-phase materials does not take into account the effect of pre-existing crack length [8] and can only be taken as a crude approximation. Furthermore, their analysis does not consider the mechanism for crack extension, that is, that the stress intensity factor, K_I, must exceed the critical stress intensity factor, K_{Ic}, at pre-existing cracks located at the particle–matrix interface.

The object of the present paper is to present a simple analysis for crack extension in the stress fields associated with a spherical particle embedded within a homogeneous matrix material having a higher thermal expansion than the particle. The stress intensity factor, K_I, is estimated for an annular crack originating from the particle–matrix interface in the region of high thermoelastic stress field and then the solution is extended to establish the critical condition for crack extension.

2. Analysis

Due to differences in the thermal expansion coefficients of the matrix and the second-phase particle, localized stress fields develop around the particles as the body cools from high temperature. A spherical particle of radius R will be subjected to a uniform pressure P (hydrostatic in nature) and the matrix will be subjected to a radial, σ_r, and a

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*Positive thermal expansion is defined as when $\alpha_m > \alpha_p$, where α_m and α_p are the thermal expansion coefficients of the matrix and particle, respectively.

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tangential, σ_θ, stress given by the equation [6,9]

$$\begin{aligned} -\sigma_r &= 2\sigma_\theta \\ &= (\alpha_m - \alpha_p)\Delta T\left[\frac{1+\nu_m}{2E_m} + \frac{1-2\nu_p}{E_p}\right]^{-1}\left(\frac{R}{r}\right)^3 \\ &= P\left(\frac{R}{r}\right)^3, \end{aligned} \tag{1}$$

where α is the thermal expansion coefficient, ΔT is the temperature difference, ν is the Poisson's ratio, E is the Young's modulus, r is the distance from the centre of the particle, and the subscripts m and p refer to the matrix and particle, respectively.

Strictly speaking, Equation 1 holds for the case of a single particle in an isotropic linear elastic matrix. However, since thermoelastic stress in the matrix approaches a small value at short distance from the particle, i.e., at $r = 2R$, Equation 1 represents a satisfactory approximation at low volume-fractions of particles.

When $\alpha_m < \alpha_p$, the hydrostatic tensile stress developed within the spherical particle may initiate fracture in the particle, in the matrix or in the particle–matrix interface. This condition will be determined by the elastic and fracture properties of the phases involved. When $\alpha_m > \alpha_p$, the tangential stress outside the particle will cause the extension of annular cracks originating from the particle–matrix interface. For this case of crack extension, the thermoelastic stress field associated with the spherical particle cannot be completely relieved.

It is generally accepted that fracture in structural materials frequently originates from inclusions, particularly when there is a difference in the thermal expansions of the phases. The incidence of crack extension will be governed by the magnitude of stress intensity factor, K_I, at the cracks associated with the particles. If the stress intensity factor exceeds the critical value, K_{Ic}, for the matrix, then the cracks will extend, thereby developing into macrocracks. According to Evans [10], the stress intensity factor at small statistical flaws located at the interface or in the near vicinity of a particle–matrix interface, may be obtained by loading the crack faces with the tangential component of the thermoelastic stress (which is tensile in nature) and integrating over the crack length. Since the thermoelastic stress concentration imposed on the microflaws located outside the spherical boundary is independent of particle size, the solution for K_I [10] is not a strong function of R. However, in the following analysis it will be assumed that the crack (of length $R + c$) is kept open by a uniform thermoelastic stress, P, over a part of its surface, as shown in Fig. 1. According to Barenblatt [11, 12], the stress intensity factor, K_I, for an axisymmetrical stress distribution, $P(r)$, on both crack surfaces is

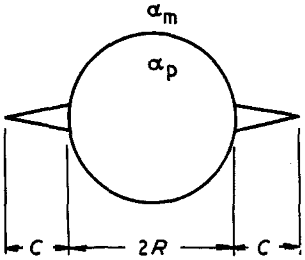

Figure 1 A spherical particle subjected to uniform hydrostatic compressive stress generated as a result of positive thermal expansion coefficient difference, $\alpha_m > \alpha_p$.

$$K_I = \frac{2}{(\pi a)^{1/2}}\int_0^a P(r) r\mathrm{d}r/(a^2 - r^2)^{1/2}, \tag{2}$$

where r is the distance from the centre of the particle and $a = R + c$ is the crack length (see Fig. 1).

Consider an annular crack originating from the particle–matrix interface in a region of high thermoelastic stress concentration, generated as a result of a thermal expansion coefficient difference, $\alpha_m > \alpha_p$. In case where $c > R$, and considering that the total crack length is $a = R + c$, the stress intensity factor, K'_I, due to a uniform thermoelastic stress P is obtained by substituting the value of P from Equation 1 into Equation 2 and integrating between limits of zero to $R + c$:

$$K'_I = 2P\left[\frac{R}{\pi}(s+1)\right]^{1/2}, \tag{3}$$

where $s = c/R$. Although Equation 3 gives correct expression for the stress intensity factor for $s > 1$, that is, when the interaction between the crack-tip stress field and the thermoelastic stress concentration is negligible, it is in error for $s < 1$. A corrected value for the stress intensity factor may be obtained by considering the tangential stress, $(P/2)(R/r)^3$, as acting across the crack surfaces in the direction to open the crack. This procedure neglects any perturbation caused by the presence of the crack and therefore can be used only as an approximation. Thus, for $s < 1$ the correction factor for the stress intensity factor is

$$K_I'' = P\left[\frac{c}{\pi}\frac{s+2}{(s+1)^5}\right]^{1/2} \qquad (4)$$

The same correction procedure has been applied by Green [13] to account for the influence of free surface caused by the annular crack located at the surface of a spherical void. The total stress intensity factor can now be obtained by the addition of Equation 3 and Equation 4:

$$K_I = P\left\{2\left[\frac{R}{\pi}(s+1)\right]^{1/2} + \left[\frac{c}{\pi}\frac{s+2}{(s+1)^5}\right]^{1/2}\right\}. \qquad (5)$$

It should be noted that numerical evaluation of Equation 5 shows that the correction term (second term in Equation 5) is small in comparison with the first term and, for many practical purposes, may be neglected.

To further illustrate the effect of s on the stress intensity factor, Fig. 2 shows the change of K_I for various particle sizes. Equation 5 shows explicitly that the stress intensity factor of a crack in a highly localized thermoelastic stress field associated with the spherical particle is a function of particle and defect size. Fig. 3 illustrates the variation of K_I as a function of particle radius.

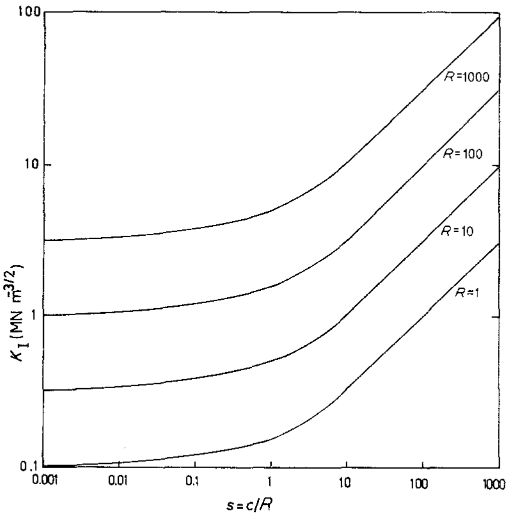

Figure 2 Variation of stress intensity factor, K_I, as a function of s and particle radius, R.

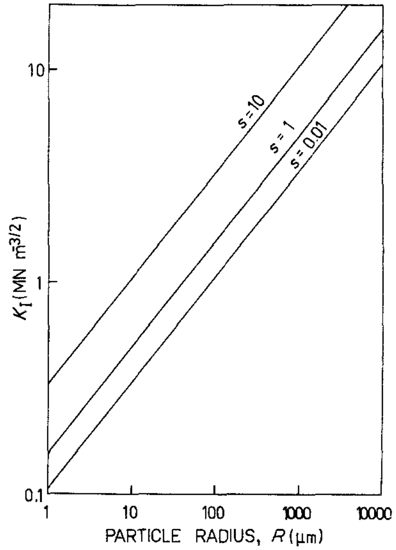

Figure 3 Variation of stress intensity factor, K_I, with particle radius and s.

The critical condition for crack extension in residual stress field can now be obtained by setting $K_I = K_{Ic} = [EG_{Ic}]^{1/2}$ and substituting for P from Equation 1 in Equation 5 yielding

$$\Delta\alpha\Delta T = [EG_{Ic}]^{1/2}\left[\frac{1+\nu_m}{2E_m} + \frac{1-2\nu_p}{E_p}\right] \times\left\{2\left[\frac{R}{\pi}(s+1)\right]^{1/2} + \left[\frac{c}{\pi}\frac{s+2}{(s+1)^5}\right]^{1/2}\right\}^{-1}, \qquad (6)$$

where E is the Young's modulus, G_{Ic} is the critical strain-energy release rate of the matrix and $\Delta\alpha$ is $\alpha_m - \alpha_p$. The results of Equation 6 are presented graphically in Fig. 4. Equation 6 shows that the minimum temperature difference or differential thermal contraction required to initiate pre-existing cracks is a function of particle radius, pre-existing crack length and the elastic and toughness properties of both the matrix and the second phase.

The same general approach may be applied to the case where $\alpha_m < \alpha_p$ if suitable crack geometry can be anticipated. However, due to the fact that, for this particular case ($\alpha_m < \alpha_p$), a spherical particle is subjected to a uniform hydrostatic tensile stress, an energy balance criteria may be more appropriate.

3. Discussion

The important result of the present analysis is that spontaneous matrix cracking in particulate brittle composites is governed by the particle size, the elastic and toughness properties of the matrix and the length of the pre-existing crack.

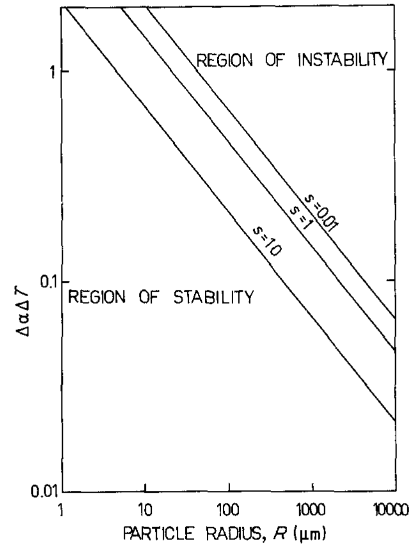

Figure 4 Minimum differential strain ($\Delta\alpha\Delta T$) required to initiate crack propagation as a function of particle radius and s.

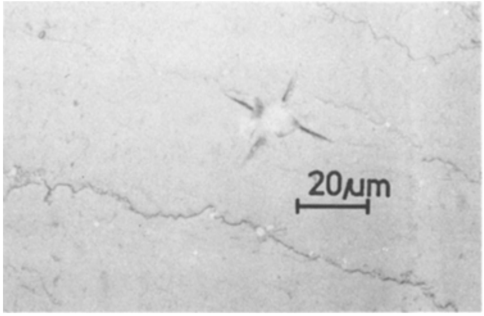

Figure 5 Extension of annular cracks around a MgF_2 particle dispersed in a LiF matrix.

On cooling from high temperature, thermoelastic stress will arise within each particle, regardless of its size (see Equation 1). Once the stress intensity factor, expressed by Equation 5, exceeds the critical value, K_{Ic}, cracks will be initiated adjacent to larger particles despite the fact that stress will also exist within and around small particles which did not satisfy the condition for crack extension. It can be inferred from Equation 6 that, for a given thermal strain ($\Delta\alpha\Delta T$), crack extension will occur when the inclusion size is larger than a critical value R_c. Consequently, very small particles ($R \ll R_c$) uniformly distributed in a brittle matrix are a prerequisite for the suppression of crack initiation. Thus, for a given $\Delta\alpha$ a brittle matrix containing spherical particles of lower expansion will tolerate a higher temperature drop if a lower particle-size dispersion is incorporated.

After the crack has been initiated, it will propagate some distance into the matrix until part of the stress associated with the particle is relieved. At this point crack-arrest will occur. A typical example of this is shown in Fig. 5 for a large inclusion of MgF_2 in a LiF matrix. As Fig. 5 shows, in some cases two annular cracks may originate from the particle–matrix interface. The critical temperature difference, ΔT, required to initiate annular cracks around a MgF_2 particle in a LiF matrix, may be obtained by substituting reported values into Equation 6 so that $E_m = 1.02 \times 10^5\,MN\,m^{-2}$, $\nu_m = 0.27$, $E_p = 1.419 \times 10^5\,MN\,m^{-2}$, $\nu_p = 0.271$ and $G_{Ic} = 1.3\,J\,m^{-2}$ [14]. For $s = 0.1$ and $R = 10\,\mu m$, Equation 6 predicts a critical value of $\Delta\alpha\Delta T = 0.6 \times 10^{-3}$. The actual differential strain* developed in the sample on cooling from 280° C was experimentally determined to be $\Delta\alpha\Delta T = 6.1 \times 10^{-3}$. Hence, matrix fracture was unavoidable.

To further test Equation 6, consider first the well-studied glass–ThO_2 system [3]. Substituting known values of $G_{Ic} = 8\,J\,m^{-2}$, $E_m = 7 \times 10^4\,MN\,m^{-2}$, $\nu_m = 0.2$, $E_p = 2.5 \times 10^5$, $\nu_p = 0.271$, $R = 75\,\mu m$ and $s = 0.1$ into Equation 6 gives a value of $\Delta\alpha\Delta T = 7.5 \times 10^{-4}$. Experimental observations have shown that glass containing ThO_2 spheres of 125 to 150 μm diameter broke on removal from the die. According to Davidge and Green [3] the differential strain which developed during cooling from the fabrication temperature was $\Delta\alpha\Delta T = 9.2 \times 10^{-4}$, substantially larger than the critical differential strain calculated from Equation 6. In order to suppress microcracking of a glass matrix, the maximum particle diameter of ThO_2 sphere must not exceed 100 μm. Similarily, for a glass–alumina composite, Equation 5 predicts that the critical radius, R_c, of Al_2O_3 sphere required to extend the cracks (for $c = 0.1R$) is of the order of $R_c = 50\,\mu m$. Experimental observations made by Frey and Mackenzie [1] revealed extensive cracking in this composite for alumina particles of 75 μm radius. If, how-

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*The LiF–MgF_2 sample was aged at 280° C for an extended time to produce large MgF_2 particles and then cooled to room temperature. For this system $\Delta\alpha = 2.4 \times 10^{-5}\,°C^{-1}$ and $\Delta T = 255°\,C$.

ever, the same size of alumina particles are incorporated in a glass matrix of $\Delta\alpha = 1.4 \times 10^{-6}$, Equation 6 predicts that the critical particle radius increases to $R_c \approx 80\,\mu$m. Thus, in this composite the particle size is sub-critical and spontaneous matrix cracking is not expected to occur. Experimental observations [1] showed no cracking in this composite, in agreement with Equation 6.

In the case of a MgO–W composite, where a large thermal expansion difference exists between the MgO matrix ($\alpha = 1.38 \times 10^{-5}\,°\mathrm{C}^{-1}$, $E = 2.1 \times 10^5\,\mathrm{MN\,m^{-2}}$ and $\nu = 0.19$) and the W particles ($\alpha = 4.8 \times 10^{-6}$, $E = 3.4 \times 10^5\,\mathrm{MN\,m^{-2}}$ and $\nu = 0.3$), Equation 6 predicts a minimum differential strain required to initiate annular cracks of $\Delta\alpha\Delta T = 3.5 \times 10^{-3}$. Assuming no stress relaxation during cooling from a hot-pressing temperature of 1400° C, the experimental value for the differential thermal strain was found to be $\Delta\alpha\Delta T = 1.26 \times 10^{-2}$, indicating that matrix cracking must have occurred. Electron microscopic examination revealed a microcrack network in composites containing 3 vol% of W [5]. The influence of stress field interaction may have played some role for volume fractions larger than 3 vol%. In addition to stress field interactions, it is worth noting that stress relaxation during cooling will always take place and the maximum thermoelastic stress calculated from Equation 1 will be overestimated. Therefore, the very close agreement between the experimental and calculated values for R_c justifies the use of Equations 5 and 6 for estimating the critical condition for crack extension in residual stress fields.

4. Summary

The effect of particle size on the stress intensity factor at small annular cracks in a region of high thermoelastic stress field is estimated. It is shown that the stress intensity factor for $\alpha_m > \alpha_p$, is a function of pre-existing crack length and particle radius in the sense that there will always be a critical particle radius below which spontaneous matrix cracking can be suppressed. However, an inclusion will be the most likely source of fracture as long as any tensile stress exists in the matrix outside an spherical inclusion. A strong particulate composite is expected to be the one with no positive differential strain ($\Delta\alpha\Delta T$) present.

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