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Transformation toughening

Part 2 *Contribution to fracture toughness*

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Two approaches are taken to determine the contribution of a stress-induced phase transformation to the fracture toughness of a brittle material. Both approaches result in an expression for the critical stress intensity factor, K_c, of

$$K_c = \left[K_0^2 + \frac{2RE_cV_i(|\Delta G^c| - \Delta U_{se}f)}{(1-\nu_c^2)}\right]^{1/2},$$

where K_0 is the critical stress intensity for the material without the transformation phenomenon, $(|\Delta G^c| - U_{se}f)$ is the work done per unit volume by the stress field to induce the transformation, E_c and ν_c are the elastic properties, V_i is the volume-fraction of retained, high-temperature phase and R is the size of the transformation zone associated with the crack. It is assumed that only those inclusions (or grains) close to the free surface of the crack will contribute to the fracture toughness; thus, $R \simeq$ the inclusion size. The chemical free-energy change associated with the transformation, $|\Delta G^c|$, will govern the temperature and alloying dependence of the fracture toughness.

1. Introduction

Part 1 [1] of this series of papers described the thermodynamics of the constrained phase transformation with particular emphasis on the effect of the inclusion size. In Part 2, two different approaches, those of Griffith and Irwin, will be used to determine the contribution of a stress-induced phase transformation to the fracture toughness of a brittle material. As in Part 1, special reference will be made to the ZrO_2 (tetragonal) → ZrO_2 (monoclinic) transformation.

2. The approach of Griffith

In this approach [2], the total energy of a system, defined as a cracked body and the applied load, is determined as a function of the crack area. The critical condition for crack extension, as first defined by Griffith, corresponds to the maximum in the total energy against crack-area function. To carry out this analysis, first, the different contributions to the total energy that change as a function of crack area are determined and summed, i.e., strain and surface energies of the body and the potential energy of the load. The condition for crack extension is then found by determining the maximum in the total energy against crack-area function. For the needs of the present analysis, the analysis can be simplified by choosing a crack and loading system in which all of the required functions, except the one associated with the stress-induced transformation, are already known. The penny-shaped crack under an applied tensile load first analyzed by Sack [3] was chosen for this analysis.

Fig. 1 illustrates a section of the cracked body under tensile load which contains a uniform dispersion of untransformed inclusions of volume-fraction, V_i. It is assumed that the stress-field associated with the crack-front has caused inclusions to transform. As the crack extends and the stresses within the previously transformed zone decrease, inclusions that have lost some constraint by being either traversed by the crack or in close proximity to the new fracture surfaces will remain in their transformed state. This process leads to a transformation zone which surrounds the crack,

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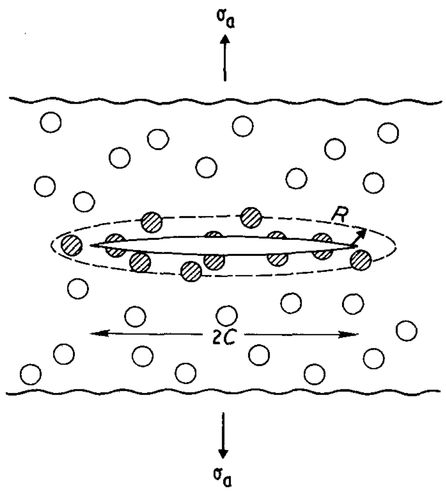

Figure 1 Section of a penny-shaped crack of radius c within a stressed composite containing inclusions. The shaded inclusions have been transformed during crack extension.

as shown in Fig. 1. Only those inclusions which remain transformed will contribute to the non-recoverable work done by the loading system to stress-induce the transformation. Since the inclusions must lose constraint to remain in their transformed state once the stress field of the crack moves, the size of the transformed zone, R, is approximately equal to the inclusion size, D.

Following the solution of Sack [3] to this same problem without the transformation phenomena, the increase in free energy of the body due to new crack surfaces, U_s, is

$$U_s = \pi c^2 G_0, \tag{1}$$

where C is the crack radius and G_0 is the critical strain-energy release rate associated with the formation of new surface. The increase in strain energy due to crack extension, U_{se}, is

$$U_{se} = \frac{8(1-\nu_c^2)\sigma_a^2 c^3}{3E_c}, \tag{2}$$

where σ_a is the applied tensile stress and E_c and ν_c are Young's modulus and Poisson's ratio of the composite material, respectively. The work done by the loading system, W_1, i.e., the decrease in the potential energy of the load, is

$$W_1 = -\frac{16(1-\nu_c^2)\sigma_a^2 c^3}{3E_c}. \tag{3}$$

An additional term arises when the transformation phenomena is included in the fracture process. Recognizing that the volume of the transformed zone is $2\pi R(c+R)^2 \simeq 2\pi Rc^2$, this additional term is the work done by the loading system to form the transformed zone:

$$W_2 = -2\pi Rc^2 WV_i,$$

where W is the work per unit volume of transformed material to induce the transformation. The minimum value of W is determined by

$$\Delta G_{t\rightarrow m} = -\Delta G^c + \Delta U_{se}f - W = 0, \tag{4}$$

where ΔG^c is the chemical free-energy change for the reaction ZrO_2 (tetragonal) → ZrO_2 (monoclinic), ΔU_{se} is the change in strain-energy associated with the transformation and $(1-f)$ is the loss of strain-energy due to the loss of constraint imposed on the inclusions during crack extension. Thus,

$$W = -\Delta G^c + \Delta U_{se}f \tag{5}$$

and*

$$W_2 = 2\pi Rc^2 V_i(|\Delta G^c| - \Delta U_{se}f). \tag{6}$$

Summing Equations 1 to 3 and 6 gives the total energy of the system as a function of crack length:

$$U = \pi c^2 G_0 + 2\pi Rc^2 V_i(|\Delta G^c| - \Delta U_{se}f) - \frac{8(1-\nu_c^2)\sigma_a^2 c^3}{3E_c}. \tag{7}$$

The condition for crack extension is determined by setting $\delta U/\delta c = 0$, which can be used to define the contribution of the stress-induced transformation to either the strength–crack-size relation

$$\sigma_c = \left[\frac{\pi E_c(G_0 + 2RV_i(|\Delta G^c| - \Delta U_{se}f))}{4(1-\nu_c^2)c}\right]^{1/2} \tag{8}$$

or the critical stress-intensity factor

$$K_c = \frac{2}{\pi^{1/2}}\sigma_c c^{1/2} = \left[K_0^2 + \frac{2RV_i E_c(|\Delta G^c| - \Delta U_{se}f)}{(1-\nu_c^2)}\right]^{1/2}, \tag{9}$$

where $K_0 = [(G_0E_c)/(1-\nu_c^2)]^{1/2}$ is the critical stress-intensity factor of the material without the transformation phenomenon.

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*The absolute brackets are used to indicate that the sign of ΔG^c has already been defined as negative in Equation 4 over the temperature range of interest.

3. The approach of Irwin

The same subject can be viewed with the approach of Irwin (4) where a force field is imposed on a stressed crack-tip and the work required to close it by a unit length is calculated. Irwin showed that the work per unit length of crack closure is equivalent to the net work dissipated per unit length of crack extension, $\partial(U_{se} - W_1)/\partial c$, as calculated through the Griffith approach. Fracture will take place when $\partial(U_{se} - W_1)/\partial c \geqslant G_c$, termed the critical strain-energy release rate. The major difference between the two approaches is that, in calculating the net work dissipated, Irwin only needs to consider the stress-field in the vicinity of the crack-tip, whereas the Griffith approach requires complete knowledge of the stress state in the system.

To apply the Irwin approach, let the unit of crack to be considered closed have traversed a transformed inclusion, as shown in Fig. 2a. The work to close this unit of crack can be broken into two parts, one concerned with the transformation, ΔW_t, and one concerned with crack closure, ΔW_c. The first force field applied would revert the fractured inclusion back to its untransformed state, as shown in Fig. 2b. The work performed by this first force field per unit volume of transformed material is

$$W = |\Delta G^c| - \Delta U_{se} f, \tag{10}$$

where $|\Delta G^c|$ is the change in chemical free-energy to revert the ZrO_2 inclusion to its tetragonal structure from its monoclinic structure. ΔU_{se} is the strain-energy associated with the transformation, and $(1-f)$ is that portion of the strain-energy relieved during fracture. The total work done on all inclusions within the volume $2R\Delta c$ per unit crack length is

$$\Delta W_t = 2R\Delta c V_i W = 2RV_i(|\Delta G^c| - \Delta U_{se} f)\Delta c. \tag{11}$$

Once the inclusions have reverted to their untransformed state, the strain energy associated with the inclusions disappears and the crack now looks like any ordinary crack in a two-phase material. At this point, the second force-field can be applied, as defined by Irwin, to close the crack by the unit length Δc, as shown in Fig. 2c. The work performed in this operation is

$$\Delta W_c = G_0 \Delta c, \tag{12}$$

where G_0 is the critical strain-energy release rate for the composite material without the transformation phenomenon.

The total work for crack closure per unit crack length which also reverts the inclusions to their initially untransformed state is

$$\frac{\Delta W}{\Delta c} = \frac{\Delta W_c}{\Delta c} + \frac{\Delta W_t}{\Delta c}$$
$$= G_0 + 2RV_i(|\Delta G^c| - \Delta U_{se} f). \tag{13}$$

Thus, the contribution of the stress-induced transformation to the critical strain-energy release rate of the composite can be expressed as

$$G_c = G_0 + 2RV_i(|\Delta G^c| - \Delta U_{se} f) \tag{14}$$

or expressed as the critical stress-intensity factor

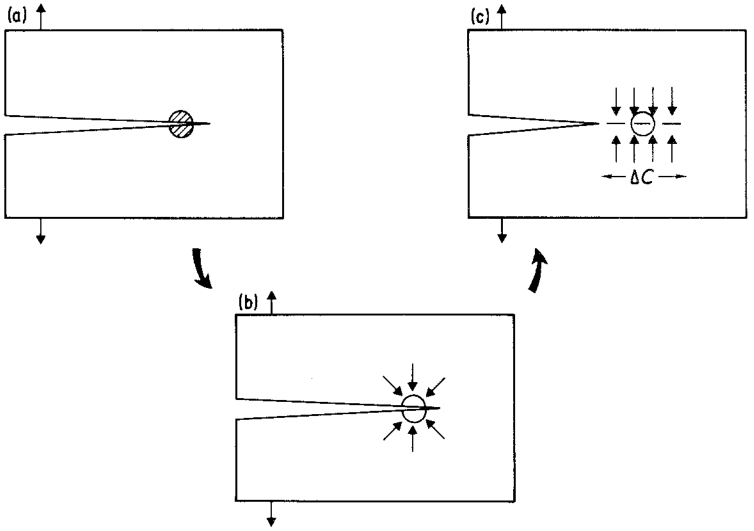

Figure 2 Crack under fixed grip conditions which has (a) intersected a transformed inclusion (shaded). (b) The first force-field reverts the inclusion to its untransformed state and (c) the second force-field closes the crack by a unit length, Δc.

$$K_c = \left[\frac{E_c G_c}{(1-\nu_c^2)}\right]^{1/2} = \left[K_0^2 + \frac{2RV_iE_c(|\Delta G^c| - \Delta U_{se}f)}{(1-\nu_c^2)}\right]^{1/2} \qquad (15)$$

4. Discussion

As expected, both approaches have led to the same expression for the critical stress-intensity factor of a material containing inclusions that can undergo a stress-induced transformation. The expressions show that the contribution of the stress-induced transformation can be maximized by maximizing (a) the volume-fraction, V_i, of inclusions fabricated in their untransformed state, (b) the elastic modulus, E_c, of the composite, (c) the factor $(|\Delta G^c| - \Delta U_{se}f)$ and (d) the size of the transformation zone, R, associated with the propagating crack-front. Each of these factors will be discussed in the following paragraphs.

Maximizing the volume-fraction would result in a single-phase polycrystalline material, e.g., tetragonal ZrO_2. Here, the inclusions could be defined as individual grains, surrounded by neighbouring grains of different misorientations which define the matrix. Each of the neighbouring grains constrain one another from undergoing a stress-free transformation by their anisotropic transformation strains. Thus, a single-phase polycrystalline material can be treated in the same manner as that described above.

The elastic modulus of the composite can be increased by choosing a chemically compatible second-phase with a higher elastic modulus. For the case of ZrO_2, Al_2O_3, with a modulus approximately twice that of ZrO_2, would be a desirable choice. However, adding a second phase to increase the modulus would, at the same time, decrease the volume-fraction, V_i, of the toughening agent. One would, therefore, be concerned with the product of V_iE_c, Equation 15, in optimizing K_c. If it is assumed that the composite modulus is governed by the rule-of-mixtures, $E_c \simeq E_iV_i + E_m(1-V_i)$, then the product would have the form:

$$V_iE_c = V_iE_i[M - V_i(M-1)], \qquad (16)$$

where $M = E_m/E_i$, the ratio of the matrix (m) and the inclusion (i) Young's moduli. Differentiating Equation 16 with respect to V_i gives

$$\frac{\partial(V_iE_c)}{\partial V_i} = E_i[M - 2V_i(M-1)], \qquad (17)$$

which shows that the maximum in the product relation occurs at $V_i = 1$, when $M \leqslant 2$, i.e., the greatest toughness, with other factors constant, should be obtained for a single-phase material. If $M > 2$, the toughness could be optimized when $V_i < 1$. On the other hand, if the objective is to toughen a matrix-phase (e.g., toughening Al_2O_3 with ZrO_2), Equation 16 shows that more toughening is obtained for a given volume-fraction the greater is the modular ratio. That is, small volume-fractions (e.g., $V_i < 0.3$) of the toughening agent will produce greater results the greater is the modulus of the matrix material.

The dependence of fracture toughness on temperatures and alloy content will be governed by the factor $(|\Delta G^c| - \Delta U_{se}f)$. This is because, relative to other factors, the chemical free-energy change, ΔG^c, exhibits the greatest change with temperature and alloying content. For the $ZrO_2(t) \rightarrow ZrO_2(m)$ reaction, $|\Delta G^c|$ decreases with increasing temperature and alloying (e.g., Y_2O_3, CeO_2, etc.) content. Thus, for this transformation, the fracture toughness is expected to decrease with increasing temperature as the factor $(|\Delta G^c| - \Delta U_{se}f)$ decreases to zero. Similarly, K_c will decrease as the alloy content in $ZrO_2(t)$ is increased. That is, fracture toughness will be optimized at the lower temperatures and for the least alloy content. The temperature where the contribution of the stress-induced toughness disappears will depend on the magnitude of $\Delta U_{se}f$. Phenomena that help relieve strain-energy during the fracture, e.g., twinning, will decrease the value of f and thus increase the temperature at which the contribution of the stress-induced toughness disappears.

The major assumption used in the model to derive the K_c-expressions was that the size of the transformation zone, R, was determined by the close proximity of the inclusions to the free surface formed during fracture. That is, inclusions transformed by the stress-field would only remain in their transformed state once the stress field of the crack passes, if much of their constraint was lost during crack extension. This assumption leads to the hypothesis that the zone-size would be directly related to the inclusion size, D such that $R \simeq D$. It is therefore, hypothesized that K_c will increase with increasing inclusion size.

It can also be argued that if inclusions remote from the surface of the crack were to remain in their transformed state, their residual strain-energy would be greater relative to that of those adjacent to the crack surface. Thus, the work-loss to the fracture process for remote inclusions would be less than that for inclusions adjacent to the crack surfaces; that is, adjacent inclusions would contribute more to the fracture toughness than would remote inclusions.

Acknowledgements

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