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Elastic anisotropy and the grain size dependence of ceramic fracture energies

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A literature review of fracture energy (γ)–grain size (G) trends of cubic ceramics, and an analysis based on adaptation of a model for thermal expansion anisotropy effects are made to evaluate effects of elastic anisotropy (EA) on γ. Although the model does not give the specific, typically limited, γ–G dependences suggested by experimental data, it does predict the level of the γ maxima indicated at intermediate G in some materials, and the lower γ values at large against small G. Further, both of these deviations from constant γ are shown to be dependent on crack size and hence consistent with their being more frequently and extensively seen with notch beam (NB) as against most other measuring methods.

1. Introduction

Fracture energies of ceramics show substantial variations which need to be understood in order to better apply fracture mechanics and develop improved materials. An earlier survey [1] indicated and recent experimental evidence [2] shows substantial depedence of fracture energy, γ, on grainsize, G, in noncubic materials. The experimental data, as well as modelling [3], show γ relatively constant at fine G, then rising to a maximum at intermediate G values, e.g. $G \sim 0.25\,G_s$, then subsequently decreasing, so $\gamma \to 0$ as $G \to G_s$ where G_s is the grain size above which spontaneous cracking occurs due to thermal-expansion anisotropy (TEA) stresses. These effects are attributed to microcracks being generated at $G < G_s$ owing to the combined effects of TEA stresses and concentrated applied stress in the vicinity of the crack.

Similar effects might be expected due to elastic anisotropy (EA), which occurs in all materials, even those of cubic structure. This paper summarizes experimental γ–G data for cubic materials, i.e. those not complicated by TEA effects. Then the modelling approach used for TEA effects [3] is applied to EA. Although involving definite uncertainties, both data analysis and modelling indicate that effects due to EA occur, but generally on a scale less than TEA effects (as assumed in developing the model for TEA-γ effects).

2. Experimental data review

Two experimental observations suggest that EA can have detectable effects on the fracture energy of cubic materials. First, Wu *et al.* [4], in a study of the microstructural nature of crack propagation, observed microcracking, or crack branching quite possibly due to microcracking, in the close vicinity of crack tips in cubic materials, and indicated a possible relation of this to EA. Second, a survey [1] and an analysis [5] of γ–G data show that while γ variations with G in cubic materials are generally negligible in comparison with the G-dependence of γ in noncubic materials, there may be some γ–G variations in cubic materials, but commonly on the scale of the data scatter.

The first γ–G variation suggested by a review of data for cubic materials is a limited rise of γ as G increases to intermediate values, then a decrease at larger G in some cubic materials. Thus, for example, Monroe and Smyth [6] have reported γ of Y_2O_3 rising from $4.6 \pm 0.5\,\mathrm{J\,m^{-2}}$ at fine G, to $5.1 \pm 0.5\,\mathrm{J\,m^{-2}}$ at $G \sim 25\,\mu$m and then decreasing to $3.8 \pm 0.4\,\mathrm{J\,m^{-2}}$ at $G > 90\,\mu$m. γ–G of various investigators for SiC, although more scattered, also suggest a possible limited rise and then subsequent decrease with increasing G^2 (e.g. Fig. 1). Most other γ data for cubic materials are too limited to detect such a trend, e.g. $MgAl_2O_4$ data could be consistent with such a limited maximum or being

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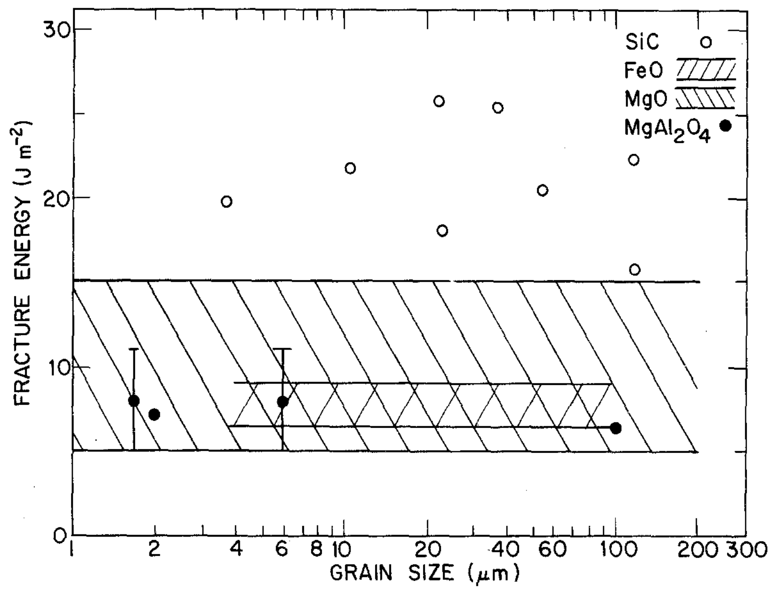

Figure 1 Summary of some of the data on the fracture-energy–grain-size relations at room temperature.

completely independent of G [2, 5] (Fig. 1). Mendelson and Fines' [7] Wustite data show no dependence of γ on G (Fig. 1). However, the easy plastic deformation in this material could well mask any possible effects of EA, due to the mismatch strains being relieved by local slip. At fine G there is more grain-boundary area in the high-stress concentration of the crack tip for significant EA mismatch strains than at large G, while slip is more restricted by finer G. This trade-off between grain boundary area and ease of slip may balance out any possible differences between finer and larger G bodies. γ–G for MgO [2, 5], which might also have variations limited by slip, is too scattered to detect any effects on the scale suggested by the above Y_2O_3 and SiC data.

The second, and more extensively suggested, γ–G variation in cubic materials is a limited decrease of γ at large G relative to that at fine G. Such decreases were often not statistically significant for any one material. However, all of the cubic materials surveyed, whether they suggested an intermediate maximum or not, showed evidence of such a decrease except FeO and MgO (where again local plastic flow could eliminate such effects) [2, 5]. Other factors may cause, or be involved in, these indicated decreases, e.g. impurities, porosity, and stoichiometry second phases have been suggested, at least for the more extreme decreases [2]. However, results of this work suggest that EA can be a factor in such decreases.

3. Model development and evaluation

3.1. Microcracking additions to γ

The approach used by Rice and Freiman [3] for modelling TEA effects will now be applied to EA. This approach is based upon Davidge and Green's [7] model for formation of spontaneous cracks around second-phase particles in a ceramic matrix. Their explanation for a critical particle size for such cracking was predicted on a balance between: (a) the surface-area requirements of fracture energy to form a crack part of, or all, the way around a particle, and (b) the volume dependence of strain energy in a particle and the surrounding matrix due to the presence of the particle.

Although Davidge and Green's model was originally applied to essentially dilute concentrations of second-phase particles and associated mismatch stresses, it has been shown to be applicable to the high concentration of TEA of phase transformation mismatch stresses around grains in single-phase bodies [9] and hence should also be applicable to the treatment of elastic anisotropy. Using the simplest form of this model, i.e. assuming that the differences of Poisson's ratio, ν, are negligible and that, for simplicity, a single average value of $\nu = 0.25$ can be used, the condition for the spontaneous formation of a microcrack is:

$$\sigma = \left(\frac{9E\gamma_B}{G}\right)^{1/2} \qquad (1)$$

where σ is the stress causing the microcrack, E is the average (polycrystalline) Young' modulus, γ_B is the fracture energy for forming the microcrack (generally along the grain boundary), and G is the grain size.

The first of three steps in deriving a model of γ utilizing Equation 1 is to assume that an applied stress can add to the local grain boundary mismatch stresses from EA to possibly cause microcracking in a region (i.e. process zone) around a stressed crack. Such microcracking will limit the stress across this zone to an approximately average value, σ_z, i.e. the applied stress mutliplied by the average stress concentration over the microcracking zone. Microcracks will thus form when the resolved values of σ_z normal to the boundary combined with mismatch stresses, $\Delta\sigma_z$, due to EA reach σ of Equation 1 (typically, only $\Delta\sigma_z > 0$ should cause microcracking); i.e.

$$\sigma \leqslant \sigma_z + \Delta\sigma_z. \tag{2}$$

This inequality arises because σ_z values will be lower owing to boundaries not being oriented at or near normal to σ_z and the maximum of $\Delta\sigma_z$ is 40% of σ_z [7].*

$\Delta\sigma_z$ is readily approximated by the following equation:

$$\Delta\sigma_z = E(\Delta\epsilon) \tag{3}$$

where $\Delta\epsilon$ is the mismatch strain across a grain boundary. Since the strain, $\epsilon_i = E_i$, where $i = 1$ or 2 to represent strains and Youngs' moduli perpendicular to the boundary between two grains:

$$\Delta\epsilon \sim \frac{\sigma_z}{E_1} - \frac{\sigma_z}{E_2} = \sigma_z\left(\frac{\Delta E}{E_1 E_2}\right). \tag{4}$$

On the average $E_1 = E - \overline{\Delta E}$, and $E_2 = E + \overline{\Delta E}$, where $\overline{\Delta E}$ is the average of the absolute $E - E_i$ differences,† so:

$$\overline{\Delta\epsilon} = \frac{\sigma_z\overline{\Delta E}}{E^2 - (\overline{\Delta E})^2} \sim \sigma_z\frac{\overline{\Delta E}}{E^2} \tag{5}$$

where $\overline{\Delta\epsilon}$ = the average of the positive (tensile) strain mismatches. Using this in Equation 3 gives the average zone-mismatch stress:

$$\overline{\Delta\sigma_z} \sim \frac{\sigma_z\overline{\Delta E}}{E} \tag{6}$$

The second step in the fracture-energy model is to calculate the fracture-energy contribution due to microcracking as the product of the number of microcracks formed per unit area of macrocrak propagation, N, times the average energy, W, that each microcrack absorbs from the applied stress field. In direct analogy with the TEA model development:

$$N = \frac{\alpha\overline{\Delta\sigma_a}}{2G^2\sigma_\alpha} = \frac{\alpha}{2G^2}\left(\frac{\overline{\Delta E}}{E}\right) \tag{7}$$

where α is a proportionality constant. The factor 2 in the denominator reflects the fact that on the average only approximately half the grains have $\Delta\sigma_z > 0$ to microcrack. Also, in direct analogy with the previous work [1], the strain energy associated with the formation of each microcrack around a grain is taken as the strain within a volume $\sim 2G$ in diameter. In the present case, the stress associated with microcracking is simply $\sigma_z + \Delta\sigma_z$, so:

$$W = \frac{(\sigma_z + \overline{\Delta\sigma_z})^2 2\pi G^3}{3E}. \tag{8}$$

Then the fracture energy due to microcracking is:

$$\gamma_\mu = \frac{\alpha}{E}\left(\frac{\overline{\Delta E}}{E}\right)\frac{\pi}{3}(\sigma_z + \overline{\Delta\sigma_z})^2 G. \tag{9}$$

Eliminating the unknowns σ_z and $\Delta\sigma_z$, by the use of Equations 1 and 2, assuming for the present that Equation 7 is an equality, gives:

$$\gamma_\mu = \frac{9\alpha\gamma_B(\overline{\Delta E})}{(E)} \sim \frac{9\gamma_B(\overline{\Delta E})}{E} \tag{10}$$

since $\alpha \sim 1$ [1].‡

Equation 10 clearly satisfies a fundamental requirement for the dependence of microcracking on EA, namely that $\gamma_\mu = 0$ when $\Delta E = 0$. On the other hand, Equation 10 gives γ_μ as independent of G, inconsistent with the limited experimental evidence discussed earlier. This discrepancy is attributed to the more limited stresses from EA complicating the modelling based on TEA stresses. While these differences cannot be handled quantitatively, the qualitative differences can be seen.

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*Note that microcracking will prevent $\sigma_z + \Delta\sigma_z$ from exceeding σ of Equation 1.

†Note that $\overline{\Delta E}$ thus depends not just on the maximum E against average E values, but on the complete distribution of E values.

‡In terms of [3], $\alpha = \alpha_1$ and $M = \alpha_1\alpha_2 = 2.5 = \alpha_1 2\pi/3$, so $\alpha_r = \alpha \sim 1$. Also, note that the same functional form of Equation 10 would be obtained if one assumed that $\gamma_\mu = N\Gamma$ where Γ = the total fracture surface energy consumed in generating a microcrack part or all of the way around a grain, since $r\alpha 4\pi G^2\gamma_B$.

TEA microstructural stresses are commonly $\geqslant$ applied stresses and are independent of the applied stress and hence exist throughout the body even in the absence of the applied stress. This typically makes the assumption of $\sigma_z \sim$ constant in the process zone more reasonable and Equation 2 an equality. On the other hand the maximum $\Delta\sigma_z$ is only 40% of σ_z, and as noted earlier depends directly on the applied stress. Since the EA stresses occur only at and near grain boundaries it can be seen that at fine G the stress concentration may not be sufficient to cause spontaneous cracking because the stress for this increases inversely with G (Equation 1). Therefore Equation 2 may often be an inequality rather than an equality at finer G as discussed earlier. This would reduce the contribution of microcracking to γ at fine G. At large G grain boundary cracking is easier (Equation 1), so Equation 2 should be an equality. However, the spatial extent of the stress concentration relative to G is significantly reduced. Thus, the actual total area of microcracking and hence the contribution of microcracking to fracture energy should be reduced at large G. The reduction of EA microcracking at fine and large G would thus support a rise in fracture energy as G increases, going through a maximum and then decreasing with continued increase of G.

While the rise and fall of fracture energy cannot be quantitatively addressed by the simple mathematical development of this model, i.e. by Equation 10, this equation should be a reasonable approximation for the relative maximum of fracture energy expected. For most cubic materials, $\overline{\Delta E}$ will typically be $< 25\% E$, and γ_B will typically be 1/3 to 1/20 of the fine-grain polycrystalline fracture energy (γ_{pc}). Thus, γ_μ would typically be expected to be of the order of $0.5\gamma_{pc}$ or less, which is consistent with the data, i.e. possible changes suggested by Y_2O_3 and SiC are of the order of 20% and 50%, respectively, of γ_{pc}, which is taken as the fracture energy at fine G. One can look at this somewhat more quantitatively in the case of SiC. The elastic anisotropy, i.e. $\overline{\Delta E}/E$, is ~ 7 and 20% respectively for β^{10}- and α^{11}-SiC ($\gamma - G$ data are for bodies of α-* or β-SiC, or both), and the single-crystal fracture energy (γ_c) is ~ 6 J m^{-2} [12]. Since γ_B should be 50 to 100% of γ_c, the maximum of γ_μ should be between 2 and 12 J m^{-2}, i.e. ~ 10 to 50% of γ_{pc} which is in reasonable agreement with the data. Reported elastic anisotropies of $\sim 7\%$ for $MgAl_2O_4$ and UO_2 [10] would indicate limited effects. Only $\sim 2\%$ anisotropy for MgO [10] could be another reason, besides local plastic deformation [4] for no indication of changes of γ with G.

Unfortunately, more detailed evaluation is limited not only by the lack of experimental $\gamma - G$ data, but also by the limitation of the elasticity data. Elastic moduli have been tabulated for a number of materials along their major crystal axes [10]. However, this covers only a small fraction of ceramic materials. Further, the maximum and minimum elastic moduli do not necessarily lie along these principal axes so such tabulations can under- or overestimate the amount of elastic anisotropy. Even less is known about the ratio of $\Delta E/E$, e.g. if this ratio either remains constant or shows no dependence on E itself, γ_μ will show no dependence on E. If for example, ΔE were a function of E, then there should be a dependence of γ_μ on E, which could be explored as an added test of the model.

3.2. Evaluation of γ trends

Next, consider the third step in the model: determining the total fracture energy, γ, i.e. the fracture energy due to the propagation of a macrocrack plus any effects of microcracking. γ_μ accounts for additive effects of microcracking. However, there are some negative effects, namely that some of the macrocrack propagation occurs by its linking with some microcracks, hence reducing the energy for actual propagation of the macrocrack itself below the fracture energy in the absence of microcracking, γ_{pc}. The ease and extent of linking of a macrocrack with microcracks should increase with G owing to the increase in size and density of microcracks with G. Thus, as with analysis for noncubic materials [3],

$$\gamma \sim \gamma_{pc}(1 - G/G_s) + \gamma_\mu \qquad (11)$$

where G_s is the grain size for spontaneous fracture. The concept of spontaneous fracture is not as precisely applicable to EA as to TEA. The idealized end point of such fracture, i.e. where the body is totally microcracked so that no energy is required to propagate the macrocrack and $\gamma = 0$ at $G = G_s$,

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*α-SiC has very low thermal-expansion anisotropy [10] which may add to the possible variation of γ with G, but should not necessarily dominate these variations.

cannot be achieved since cracking from EA always requires some application of stress and hence finite external energy for crack propagation. However, what is of interest is the effect of significantly increased microcracking for which Equation 11 should be suitable.

Equation 11 clearly shows that γ would decrease with increasing G, since the earlier analysis shows γ_μ to be either constant, or, more likely, to pass through a maximum.* It is thus useful to evaluate G_s to obtain some idea of the G range over which γ would decrease, and to compare this with indications of decreasing γ with increasing G noted earlier.

From Equations 1, 2 and 6 we obtain

$$G_s \sim \frac{9E\gamma_B}{(\sigma_z + \overline{\Delta\sigma_z})^2} = \frac{9E\gamma_B}{\sigma_z^2\left(\dfrac{\overline{\Delta E}}{E}\right)^2}. \qquad (12)$$

Since

$$\sigma_z = K\sigma_f \qquad (13)$$

where σ_f is the fracture stress and K is a proportionality constant, i.e. typically the average stress concentration in the microcracking zone, and

$$\sigma_f = Z\left(\frac{2E\gamma}{C}\right)^{1/2} \qquad (14)$$

where C and Z are respectively the flaw (crack) size and geometry factor, Equation 12 becomes:

$$G_s \sim \frac{9\gamma_B C}{2K^2\gamma Z^2}\left(\frac{E}{\overline{\Delta E}}\right)^2 \qquad (15)$$

Since Z^2 ranges from ~ 0.5 (slit crack) to 1.25 (half-penny crack) [13], γ_β/γ is typically 1/3 to 1/20, and $K \leqslant 1.4$, G_s will be of the order of $0.1C\ (E/\overline{\Delta E}^2)$. For $\overline{\Delta E}/E \sim 10\%$, as with materials considered here, this means G_s would be of the order of $10C$, i.e. ~ 10 times the crack size. Unfortunately, crack sizes are often not given in such tests as the NB test. (Other factors such as the notch depth–width ratio may also be important.) However, Equation 15 and the above estimates do indicate that there could be important differences in the tests used. Thus, double cantilever beam (DCB) and double torsion (DT) tests, which typically have C much larger than in the NB test, may show significantly less variation of γ with G than does the NB test. This is consistent with the data since NB tests show more decrease of γ at larger G for any single body than do DCB tests.

4. Summary and conclusions

The effects of EA on γ cannot be modelled by the method used for TEA in as much detail as effects of TEA. This is attributed to greater sensitivity of EA to local stress concentrations. However, overall trends of the model are consistent with data, showing that effects of EA are generally substantially less than those of TEA. The model also shows that when γ is effected by EA, these effects will vary with the crack size and hence the test method.

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*In analogy with TEA effects, such a maximum would be expected to be at $\sim G_s/4$.