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Metallurgical Aspects of the Toughness of Engineering Alloys [and Discussion]

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Metallurgical aspects of the toughness of engineering alloys

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The paper treats micro-mechanical modes of crack extension, classed as 'cracking' and 'rupture' processes. In 'cracking', a cleavage crack nucleus propagates when a critical local tensile stress is attained, the magnitude of the stress being determined by the microstructure. Models for crack propagation from carbides and from martensite/bainite 'packets' are discussed. The 'rupture' processes involve the initiation and growth of voids, centred on second-phase particles. Coalescence may arise from 'internal necking' or 'fast shear' and the factors associated with these two modes are described. Consideration is also given to the ways in which microstructure may produce scatter in toughness values and in growth-rates under fatigue loading, where both cyclic and monotonic failure modes are significant.

Introduction

The techniques of fracture mechanics are proving to be of great value when used, on the macroscopic scale, to assess the safety of engineering structures. Initial crack sizes of interest in practice are usually above the (ultrasonic) non-destructive testing inspection limit, typically greater than 2 mm. For applications involving ultra-high strength marageing steels or powder-formed nickel-based superalloys, however, the crack sizes may be as small as 0.2 mm. The interaction of fracture mechanics with the micro-mechanisms of fracture in metallic alloys is twofold. On the one hand, a detailed understanding of micro-mechanisms provides the metallurgist with a scientific basis, not only for producing alloys of high toughness, but also for reducing the scatter in properties, so that 'risk' analyses can be made with increased confidence. On the other hand, most of the models of fracture processes on the microscopic scale employ continuum (fracture) mechanics, treating the microstructure as a 'micro'-engineering structure. The crack sizes now lie, roughly, in the range 0.2–20 μm, so that the scale is some two to three orders of magnitude smaller than that for conventional fields of application.

The microstructure of interest is that immediately ahead of a crack, which is produced by fatigue in a toughness test-piece, but which arises from a variety of causes in actual structures. Two main points should be appreciated. First, the micro-mechanisms of fracture operate in a region in which there is a steep strain gradient and a substantial hydrostatic stress field, which can produce, in strongly work-hardening material, tensile stresses four to five times as high as the yield stress, in the presence of small plastic strains. Fracture in uniaxial tensile tests is then often irrelevant to fracture behaviour in the crack tip region. Secondly, a crack in service may not end randomly in the microstructure, but may be associated with regions of poor toughness. To give two examples: a shrinkage cavity in a casting or in weld metal may have sharp protrusions, following weak inter-dendritic regions, which were the last to solidify; a stress-corrosion crack in alloy steel may be confined to segregated grain boundaries, which have low toughness. Fracture toughness values obtained in laboratory tests should therefore always be examined critically with respect to their use in any particular application.

In the present paper, the basic tenet is that it is possible to produce a sharp crack in a manner that is non-selective with respect to the microstructure and which does not influence the subsequent fracture process, other than through effects of geometry, strain gradient or triaxiality. Initially, it proves convenient to examine two extremes of fracture behaviour, which may be classed as 'cracking processes' and 'rupture processes'. The former is typified by the cleavage fracture of low-strength structural steels, the latter by fibrous fracture in soft alloys that contain a high volume fraction of non-metallic inclusions.

Cracking processes

Until about 15 years ago, models for the formation of a cleavage crack treated the material as an homogeneous continuum and postulated that the crack was nucleated by a single pile-up of dislocations (Stroh 1957), intersecting dislocations (Cottrell 1958) or intersecting twins (Hull 1960). The material's grain size was incorporated by equating the pile-up length to the grain diameter. From the observation that cleavage fracture occurred more readily in notched bars than in smooth tensile specimens, Cottrell (1958) emphasized the point that the critical stage in the process must be the growth of the cleavage crack nucleus under the action of the applied tensile stress. This view was subsequently confirmed and quantified (Knott & Cottrell 1963; Knott 1966). A detailed analysis of the energy terms involved in propagating a cleavage crack nucleus (Smith 1966; Smith & Barnby 1967*a*) showed that the experimental observation that cleavage fracture was controlled by a critical tensile stress could be reconciled with theory, only if the 'effective surface energy' of the fracture process increased at some stage as the crack length increased.

McMahon & Cohen (1965) demonstrated that cleavage cracks in normalized or annealed mild steel tensile specimens were nucleated in grain boundary carbide films. The fracture behaviour of steels of identical grain size and flow properties was then controlled simply by the carbide thickness, because thicker carbides produced larger crack nuclei. They treated the propagation as a simple Griffith crack under the influence of an applied tensile stress; in essence, employing linear elastic fracture mechanics for mode I, plane strain, to 'pre-existing' (carbide) cracks of lengths in the range 1–10 μm.

Smith (1966) subsequently improved the model to include the effect of the stress field from the dislocation pile-up needed to nucleate the crack, obtaining the following criterion for fracture in a microstructure of grain size d, containing carbides of thickness C_0:

$$(C_0/d)\sigma_F^2 + \tau_{\text{eff}}^2\{1 + (4/\pi)\,(C_0/d)^{\frac{1}{2}}\,\tau_i/\tau_{\text{eff}}\}^2 > 4E\gamma_p/\pi(1-\nu^2)d. \tag{1}$$

Here, σ_F is the tensile stress required to propagate the nucleus, τ_{eff} is the 'effective' shear stress (applied shear stress, τ_{app}, reduced by the friction stress, τ_i), E is the Young modulus, ν is the Poisson ratio, and γ_p is the 'plastic work' involved in propagating the nucleus into the ferrite matrix, i.e. the 'fracture toughness' of the matrix. The carbide itself is supposed to fracture in a brittle manner, so that its work of fracture is less than γ_p. This provides the increase in γ with crack length required by energetic calculations to justify a growth-controlled fracture criterion.

If τ_{eff} in (1) is written as $k_y^s d^{-\frac{1}{2}}$, where k_y^s is the slope of the Petch (1953) relation (in shear), it appears that the equation fails to predict any effect of grain size on cleavage resistance, contrary to experimental observations (Knott 1978). However, Curry & Knott (1978) have shown that in low-carbon steels that have been simply cooled from the normalizing or annealing temperature, there is a progressive increase of carbide thickness with grain size. Taking C_0 as the 'coarsest observed' carbide thickness or the 'thickest 5%' thickness, they were able to demonstrate reasonable agreement between (1) and experimental results in steels of different grain size, if γ_p was taken as 14 J m^{-2} (within a scatter band of γ_p = 11–17 J m^{-2}). Further, in steels containing spheroidized carbides, the same value of γ_p was shown to be consistent with measured fracture stresses, if the carbide size was taken as the 95th percentile radius, and the fracture process was modelled in terms of a 'penny-shaped' Griffith crack. This value of γ_p also appeared to hold for transgranular cleavage fracture in a 0.6% carbon steel subjected to a '350 °C embrittlement' treatment (King *et al.* 1978).

The value of γ_p is not only greater than the work of fracture in the carbide, it is also some seven times greater than the surface energy of iron (2 J m^{-2}), which is usually equated to the elastic work of fracture. Clearly, some local plasticity is involved, even in spreading a micro-crack from a carbide into the matrix. A general criterion (Kelly *et al.* 1967; Rice & Thomson 1974) suggests that cracks *either* propagate in a brittle manner (e.g. in diamond) *or* blunt by the emission of dislocations from the crack tip (e.g. in f.c.c. metals). Iron is found to be a borderline case, in which it is not easy to predict whether a crack will propagate or blunt. It has been suggested (Knott 1978) that, in this case, the generation and *limited movement* of dislocations at the crack tip may be a necessary part of the separation process. The usual criterion for fracture is that the stress on the atomic bond just at the crack tip must be equal to the theoretical strength, say, $0.1E$. Certainly, if the bond were loaded simply as a pair of atoms in free space, any increase in separation would produce catastrophic failure, because the curve of bond-strength against displacement beyond the theoretical strength possesses negative stiffness. This is equivalent to the fracture of a uniaxial tensile specimen at the u.t.s. in a load-controlled testing machine. In the crack tip region, however, the bond is surrounded by a 'cage' of other bonds that all possess positive stiffness. This is equivalent to a tensile bar in a hard, displacement-controlled machine. Fracture demands the complete separation of two surfaces, necessitating displacements of order b, the lattice spacing, whereas 'theoretical strength' (the point of inflexion in the energy–displacement curve) is associated with displacements only of order 0.25–$0.4b$. The movement of dislocations may then be necessary to make the crack tip region sufficiently 'sloppy' to accommodate the extra displacement, between 0.25–$0.4b$ and b. A dislocation of Burger's vector b, moving a distance b under a stress of approx. 0.1μ (where μ is the shear modulus) does work of magnitude $0.1\mu b^2$ per unit length of dislocation. If this work has to be done by one dislocation on either side of the crack tip moving through $3b$, for each increment of crack area, $b \times 1$, the total work per unit area is $0.6\mu b$. Taking μ = 75 GPa and b = 0.25 nm gives 11 J m^{-2}, which, when added to the 2 J m^{-2} surface energy, would agree with the experimental value of γ_p. Such small displacements are confined to the 'end-region' at the crack tip, and the dislocations might not be visible on the fracture surfaces if the image forces were sufficient to remove them, once the applied stresses were reduced to zero by crack propagation. The contribution to γ_p could well be independent of temperature at low temperatures, because 0.1μ is such a high stress that its value is unlikely to be reduced significantly by (low levels of) thermal activation.

The sharp increase from the surface energy of a brittle carbide to 'γ_p' in the ferrite matrix is not the only way in which the effective surface energy experienced by a growing cleavage crack may increase with crack length. Cracks may arrest at grain boundaries, as commonly

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observed in tensile specimens of mild steel at low temperatures (Hahn *et al.* 1959), although this behaviour is seen infrequently in notched or pre-cracked test-pieces, unless the load can relax as the piece begins to crack. The nature of the work that needs to be expended in propagating the crack from grain to grain in mild steel has not been fully explored, although it appears to involve some 'internal necking' between microcracks in adjacent grains (Cottrell 1963).

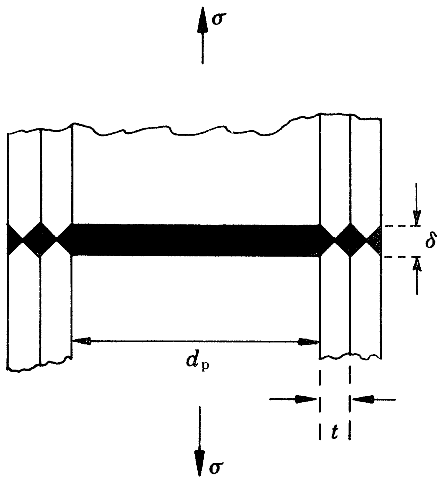

FIGURE 1. Schematic model for the propagation of a cleavage microcrack from one bainitic 'packet' to another. The laths in the second packet are considered as necking to points by slip on 45° slip-lines.

A similar situation involves bainitic or auto-tempered martensitic structures in quenched and tempered structural steels such as HY80 or A533B (Dolby & Knott 1972; Naylor 1976; Brozzo *et al.* 1977). Such microstructures are likely to be found in heat-affected zones or even in thick, quenched plate. On transformation, austenite grains are split up into 'packets' of sympathetically nucleated laths; the largest packet may be as much as half the austenite grain size. In such microstructures, it appears that the lath size determines the yield stress, but that the packet size controls the cleavage fracture resistance. It is observed that a cleavage crack will run in a smooth, brittle fashion across one packet, but will then change to a much rougher path across the next packet. A model of the process is shown in figure 1, and an estimate of the fracture stress, σ_f, involved may be made by assuming that propagation occurs when the displacement, δ, at the tip of a crack equal in length to a pocket diameter, d_p, is sufficient to cause perfect ductile fracture, by internal necking on 45° planes, across a lath of thickness t. Taking the crack as through-thickness, plane strain, we have (Rice 1973)

$$\delta = K^2/2\sigma_y E; \tag{2}$$

$$\sigma_f = (4E\sigma_y t/\pi(1-\nu^2)d_p)^{\frac{1}{2}}. \tag{3}$$

Typical values for A533B at moderately low temperatures might be: E = 200 GPa, σ_y = 600 MPa, t = 0.3 µm, d_p = 12 µm. This gives a value for σ_f of 2050 MPa, which is reasonably in accord with experimental values (Knott 1978; Green 1975; Parks 1976).

In C–Mn weld deposits, a variety of microstructures is often seen, comprising coarse pro-eutectoid ferrite or ferrite 'side-plates' (an upper-bainite-like ferrite–carbide mixture) at prior austenite grain boundaries and fine, interlocking, 'acicular ferrite' within the grains (Widgery 1976). This appears to nucleate heterogeneously on intragranular deoxidation products or other inclusions during cooling, hence the fine distribution of nuclei. Preferential directions for ferrite growth give an overall 'crystallographic' appearance to the microstructure, but the boundaries between individual grains in the 'basket-weave' appear to be high-angle. It is found that the highest resistance to cleavage in C–Mn deposits is given by a large proportion of acicular ferrite. Cracks clearly initiate and run easily in the coarse pro-eutectoid and side-plate ferrite, but whether the good resistance of acicular ferrite is due to the high-angle boundaries, or to the fact that intergranular carbides are very thin, has not been determined.

In forging steels (low alloy steels containing approx. 0.3% C), two microscopically brittle modes of fracture may be observed. Transgranular cleavage may involve different critical events: propagation from packet to packet in the as-quenched state, propagation from interlath cementite when tempered at approx. 350 °C, propagation from ferrite grain to ferrite grain, when tempered at approx. 600 °C, propagation from spheroidal cementite or alloy carbide when spheroidized for a long period at 700 °C. Additionally, if a steel contains trace impurity elements, such as phosphorus, tin or antimony, these may segregate to prior austenite grain boundaries, reduce intergranular cohesion, and produce grain boundary fractures. These fractures again appear to be controlled by growth, under the action of a critical tensile stress (Ritchie *et al.* 1973*a*; Kameda & McMahon 1980) and it is possible to relate the decrease in 'γ_p', for the grain boundary path, to the amount of segregation of trace impurity elements at the boundary, measured, for example, by Auger analysis on fractured samples.

Fracture toughness (cracking processes)

It is possible to use the microscopic fracture models to attempt to predict the macroscopic fracture toughness, K_{Ic}, at least for those situations in which the critical event is propagation from a cracked carbide into a ferrite matrix. The initial problem is that K is a stress *intensity*, with dimensions (stress) × (length)$^{\frac{1}{2}}$, rather than a stress, so that it is necessary to specify not only a critical stress for a process, but also the distance at which it must be attained. A completely analogous situation arose in the derivation of the Petch (1953) relationship for the propagation of yield from grain to grain, although this employed a simple, elastic, stress analysis. Here, a slip-band in a grain of diameter d was modelled as a freely slipping crack (of length $2a = d$) under the action of an effective shear stress, $\tau_{eff} = (\tau_{app} - \tau_i)$. The shear stress at a distance r ahead of the crack is then given by

$$\tau = K_{II}(2\pi r)^{-\frac{1}{2}} = (\tau_{app} - \tau_i)(d/4r)^{\frac{1}{2}} \tag{4}$$

or

$$\tau_{app} = \tau_i + \tau(4r)^{\frac{1}{2}}\, d^{-\frac{1}{2}}. \tag{5}$$

From this, a critical value of $\tau_{app} = \tau_y$ could be derived, but only when a critical value had been assigned, *both* to τ (a dislocation generation stress) *and* to r (the distance to the nearest dislocation source).

For fracture ahead of a pre-existing fatigue crack, we envisage a 'crack-tip' microstructure composed of already-cracked carbides. Catastrophic propagation is supposed to occur when the applied stress has been raised to a level such that the *local stress at a cracked carbide* is sufficient to give local cleavage fracture (i.e. that (1) or its equivalent is satisfied). Ritchie *et al.* (1973*b*) used a full, elastic–plastic stress analysis to predict results for mild steels possessing microstructures of ferrite grains and grain-boundary cementite films. The predicted trend was of the right form and agreement with results was close if the 'critical distance' (that to the 'nearest', 'significant', carbide) was taken as two grain diameters, although it was pointed out that a description of the distance in terms of 'grain diameters' did not rest on a physical argument. Later, Curry & Knott (1976) showed that the critical distance bore no unique relation to the grain diameter, and argued that the problem resolved itself into the probability of finding a carbide of given thickness ahead of the crack.

Table 1. Carbide size distribution and calculation of toughness (after Curry & Knott 1979)

carbide radius, r_0/µm	fracture stress, σ_f/MPa	probability, $P_{r=r_0}$	$10^6 \times$ partial failure probability, $P_{r=r_0}\{X_0/(K/\sigma_y)^2\}^2$
0.22	4746	0.458	0
0.33	3875	0.204	0.204
0.44	3356	0.155	0.82
0.55	3001	0.079	1.53
0.66	2740	0.052	2.26

The statistics of carbide distributions in ferrite–cementite-film microstructures are complicated, and Curry & Knott (1979) applied the probability argument to steels containing a distribution of spheroidal carbides. For convenience, the distribution of carbide radii was represented as a histogram, as in table 1. By using $\gamma_p = 14\,\mathrm{J\,m^{-2}}$, it was possible to calculate the value of failure stress, σ_f, for each carbide size, and, from this, the corresponding area $M(X_0/(K/\sigma_y)^2)^2$ in which a stress equal to, or greater than, σ_f could be obtained: here, X_0 is distance and M is a geometrical factor. The partial failure probability is given by the product of the probability of finding a particle of radius r_0 and the probability of σ_f being able to propagate a crack from that particle. A total failure probablity of unity gives complete failure of the test-piece. Good agreement with experiment was obtained, for a value $M = 3$: this value is arbitrary, but a single figure appears to hold for a number of steels and the limits to M, which can be argued on a physical basis, lie reasonably above and below the assumed value.

There is, then, the beginnings of a microstructural theory for the fracture toughness of steels containing a distribution of spheroidized carbides. More microstructural information is required before the same approach can be applied in a fully quantitative fashion to the ferrite–grain-boundary carbide type of microstructure, although encouraging quasi-quantitative agreement is already apparent. The 'packet' type of microstructure, again, should not require fundamentally different treatment, but the meaning of the 'critical distance' for intergranular fracture is more difficult to comprehend, unless it can be shown that the critical event is one of propagation from grain-boundary carbides. The very fine grains of acicular ferrite in C–Mn weld metals will also be intriguing to study, particularly because Curry (1978) has suggested that there may be a minimum ferrite grain size below which the toughness begins to decrease.

A major point concerns the large values of energy absorption associated with a fracture toughness test. Even a K_{Ic} value as low as 32 MPa $\mathrm{m^{\frac{1}{2}}}$ implies an energy of 4.5 kJ $\mathrm{m^{-2}}$, compared with a surface energy of 2 J $\mathrm{m^{-2}}$ or a 'γ_p' value of 14 J $\mathrm{m^{-2}}$. It should be appreciated that this energy is expended primarily *before* the critical event, in establishing a plastic zone and stress distribution sufficient to produce the critical local tensile stress at a carbide crack nucleus.

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Rupture processes

As the test temperature is raised, a steel's yield stress decreases, so that the maximum tensile stress ahead of a sharp crack, developed by the hydrostatic component, also decreases. To attempt to meet any cleavage propagation criterion, it is then necessary to work-harden the matrix. The strains involved in this work-hardening may be sufficient to initiate fibrous fracture at the crack tip before cleavage nuclei can propagate ahead of the crack tip. In metals with an f.c.c. matrix, cleavage fracture does not occur and K_{Ic} can only be controlled by fibrous processes. High-strength alloys, such as marageing steels, some quenched and tempered low-alloy steels and aluminium alloys, may fracture in a small testpiece under 'valid' K_{Ic} test conditions, but many lower-strength materials are so ductile that small test-pieces undergo general yielding before the fracture initiates. In these cases, and more generally, it is convenient to discuss fibrous fracture in terms of the crack opening displacement (c.o.d.), δ, which may be related to the stress intensity, under small-scale yielding conditions, using (2).

The classic mode of fibrous separation is by the internal necking of ligaments between voids formed around non-metallic inclusions. In low-strength steels, these are usually manganese sulphide or silicates, which are so poorly bonded to the ferrite matrix that no plastic strain for void initiation need be considered. Under these conditions, it would be expected that the critical crack opening would be a simple function of inclusion spacing, and Rice & Johnson (1970) have indeed calculated the variation of initiation c.o.d., δ_i/X, with X/R, where X is the spacing and R is the radius of the inclusions. The value of δ_i/X ranges from less than 1 for X/R less than 10, to approx. 2.5, for X/R of order 80. Initiation, at δ_i, is defined as the stage at which the blunting crack tip first coalesces with an expanding void ahead of the tip. Experimental results for a number of steels of high work-hardening capacity follow the general form of the predictions, but a number of metallurgical factors can lead to lower toughnesses than predicted (Knott 1980).

Even the apparently good agreement needs careful examination, because the model is based on plane strain deformation in a material containing a uniform distribution of (infinitely long, cylindrical) inclusions of uniform size. In practice, a material is likely to contain near-spherical inclusions and the distribution may not be uniform. Initiation then becomes difficult to define, if the crack can tunnel forward along part of its front. Either a statistical definition, based on microscopic examination, will be required, or it may be possible to circumvent the statistics by using macroscopic examination of fibrous thumbnail length and extrapolating the c.o.d. back to zero crack length (Smith & Knott 1971).

Recently, el Soudani has been able to obtain quantitative information on the growth of voids from inclusions, by propagating fatigue cracks in stainless steel weld metal under controlled combinations of (constant) alternating stress intensity, ΔK, and (constant) maximum stress intensity, K_{max}. The fatigue essentially sections the voids at the appropriate stage of growth and it is possible to make quantitative metallographic measurements on large areas of fracture surface, failing under constant conditions. Representative results are shown in figure 2, where it can be seen that the mid-thickness void diameter increases with K_{max}, independently of ΔK. Void growth near the edges of the specimens, where the triaxiality is low, was negligible. The voids increase in diameter by a factor of somewhat more than 2 and rapid growth begins when $K_{max} = 40$ MPa m$^{\frac{1}{2}}$, i.e. with the use of (2) and taking $\sigma_y = 400$ MPa as an appropriate flow stress, when the c.o.d. is 10 μm. At this stage, the number of voids per unit area, N_A, was measured as 0.022 μm^{-2}, giving an average spacing, 0.5 $N_A^{-\frac{1}{2}}$, of 3.4 μm. Coalescence clearly occurs by internal necking between the voids, but the details do not conform with the plane strain model, which proposes that rapid growth occurs when an inclusion is 'enveloped' by the high strain region ahead of the crack tip, which implies a spacing of $1.9\delta = 19$ μm for the stainless steel weld metal.

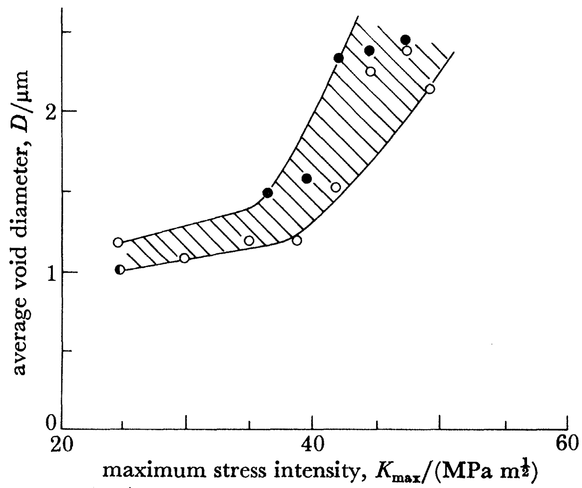

FIGURE 2. Variation in void diameter with maximum applied stress intensity, K_{max}, in a 316-stainless steel weld metal (courtesy S. M. el Soudani). Key: ○, $\Delta K = 22.5$ MPa m$^{\frac{1}{2}}$; ●, $\Delta K = 36$ MPa m$^{\frac{1}{2}}$; ◐, $\Delta K = 40$ MPa m$^{\frac{1}{2}}$.

The general internal necking mechanism is, however, useful in demonstrating that small inclusion spacings can lead to lower toughness in ductile metals. Examples are to be found in weld deposits, where deoxidation products are closely spaced; in castings, where inter-dendritic particles can give 'easy' paths for linkage, and in aluminium alloys, which contain a fine dispersion of intermetallics (Knott 1978). Other reductions in toughness may occur, however, even for widely spaced inclusions, if the matrix does not exhibit its full ductility.

FAST SHEAR

Voids may link by a highly localized 'fast shear' mechanism, involving small tensile displacements, in a number of situations. Forging steels and hardenable structural steels often have low work-hardening capacity and flow localizes in the ligament between crack-tip and void, as the strain is increased. The fine-scale linkage follows the appropriate macroscopic slip-line field (derived for rigid/perfectly plastic material), but, in detail, it runs from carbide to carbide. It seems that the critical event, leading to a catastrophic fast shear between voids, occurs when the carbide/matrix interface decoheres, primarily under the influence of the local stress fields produced by dislocations tangling around the particles, but perhaps also under the influence of the applied tensile stress (Knott 1980). A uniform array of pile-ups, each of length d, piled-up on particles of radius c, produce fracture when (Smith & Barnby 1967b)

$$nb = 2\sqrt{2}(d(1-\nu^2)\gamma_i/\pi E)^{\frac{1}{2}}(d/c)^{\frac{1}{2}}, \quad (6)$$

where n dislocations of Burger's vector b are in each pile-up. Substituting figures of $c = 0.175$ μm, $d = 3.5$ μm, which are typical for tempered carbides in a forging steel, and taking γ_i, the interfacial bonding energy, as $1.35\ \mathrm{J\ m^{-2}}$ (somewhat less than the $2\ \mathrm{J\ m^{-2}}$ for the surface energy of iron), we obtain $nb = 33$ nm, which implies a shear strain of order 0.1 in the particle. It has further been shown (King 1979) that segregation of impurity elements, which could reduce the bonding energy by an estimated factor of 4, reduces the value of δ_i for ductile fracture by a factor of 2.2, in reasonable agreement with (6).

Prevention of localized shear clearly depends on the ability to continue to spread strain, but there is no clear parameter that will represent this matrix flow property. The work-hardening exponent, N, has been used with some success for aluminium alloys (Garrett & Knott 1978), but does not help to explain the decrease of toughness with increase in yield stress in quenched and tempered steels. Here, Slatcher (1979) has pointed out the importance of carbide morphology and local (transformation) dislocation stress fields in producing easy crack nucleation.

Table 2. Effect of pre-strain on δ_i

nominal prestrain (%)	δ_i (HY 80) / mm	δ_i (En32B) / mm
0	0.12	0.09
10	0.08	0.05
20	0.04	0.02

HY 80 results from Clayton & Knott (1976); En32B results from Willoughby (1979).

It is important to realize that improper heat-treatment, as in adventitiously non-stress-relieved heat-affected zones, can strongly affect the crack-tip ductility of weldable steels. In A533B, for example, a '350 °C embrittlement' sequence of heat-treatment (austenitization at 1200 °C, followed by quenching, and tempering at 350 °C) can produce 'nearly valid' behaviour in a 25 mm test-piece at room temperature, giving a K_{Ic} of approx. 140 MPa $\mathrm{m^{1/2}}$. For a design stress of two-thirds of the parent plate yield strength (500 MPa), this gives a critical (edge crack) defect size of approx. 45 mm compared with approx. 75 mm if the toughness were 180 MPa $\mathrm{m^{1/2}}$, which is a conventional lower bound for fully stress-relieved plate.

Cold-work is a second factor that can decrease the value of δ_i for a ductile fracture, and the effect of cold-work will be particularly serious if it is associated with a stress-concentrator, as when a hole is reamed or cold-punched. Table 2 shows the effect of uniform prestrain in two structural steels: in both cases, δ_i is reduced to about one-third of its value in non-cold-worked material. Cold-work can also increase the propensity to low-strain cleavage fracture, particularly if strain-ageing is significant.

A final, important and unexplored factor is that of neutron irradiation. Not only does this increase the yield stress, by point-defect hardening, and hence promote cleavage fracture, but the work-hardening rate is markedly reduced, because flow can channel. No effects on c.o.d. have been reported, but the 'upper shelf' in impact tests is lowered significantly in irradiated specimens (Druce & Eyre 1978) and strong effects would be expected. If irradiation were equivalent to 20% pre-strain, δ_i could be reduced from 0.18 mm (Clark *et al.* 1978) to 0.06 mm (cf. table 2). Clearly, such effects warrant further investigation.

Scatter in results

From the previous discussion, it is apparent that a material's fracture toughness is dependent on the probability of there being a particularly coarse carbide, large bainitic 'packet', or weakly bonded inclusion, in the immediate vicinity of the crack tip. From this it follows that even if the microstructure were completely random, there would be a distribution about the mean for any toughness value. The fact that standard test-pieces are thick tends to reduce the standard deviation, because a large thickness ensures that the volume of material sampled by the high stress or strain region is also large. In practice, it is often assumed that K_{Ic} values follow a normal distribution, with standard deviation of order 10 % of the mean. Such distributions are then used to calculate the distribution of critical defect size, for use in probability analysis. Any metallurgical justification for truncation of the 'tail' of the critical defect size distribution at low values would be of great assistance in establishing lower probabilities of failure.

The assumption of a normal distribution has not, however, been substantiated in all cases and it is not clear that a single distribution would be expected for a material with a mixed, segregated or textured microstructure. Examples of bimodal toughness values in impact tests have been quoted (Wilshaw & Pratt 1965) and recent experiments carried out by Hagiwara have shown that K_{Ic} and c.o.d. values in HY80, heat-treated to give varying proportions of upper bainite and martensite, vary between upper and lower limits equivalent to those for 100 % martensite and 100 % bainite respectively. Here, attempts are being made to explain the variation in toughness for a given proportion of upper bainite in terms of the probability of finding a bainitic region at the crack tip.

Scatter may also be obtained in fatigue-crack propagation rates. Generally, it is quite small but some alloys show more pronounced variation than others, and the rates are also sensitive to the mean stress level. Ritchie & Knott (1973) were able to show that such effects were confined to materials of low *monotonic* toughness and that the cracks propagated by a combination of striation growth (controlled by ΔK) and monotonic growth (controlled by K_{max}). An example has already been given in figure 2 for void growth in stainless steel, but more marked effects are observed if the monotonic mode is cleavage or intergranular.

The area fraction of cleavage facets, A_c, is a monotonic, nearly linear, function of K_{max} (Beevers *et al.* 1975), and el Soudani has shown that the area fraction of voids varies with K_{max} in a similar manner (Knott 1980). If cleavage occurs in a single cycle, the growth rate at a given R ratio, $(\mathrm{d}a/\mathrm{d}N)_R$ would be greater than that at $R = 0$, $(\mathrm{d}a/\mathrm{d}N)_0$, by a factor $(1-A_c)^{-1}$. At high K_{max} values, approaching K_{Ic}, a linear variation of A_c with K_{max} gives $(1-A_c) = k(K_{Ic}-K_{max})$, where k is a constant. The enhancement factor then becomes of the form $k^{-1}(K_{Ic}-K_{max})^{-1}$, which is similar to that used empirically to explain effects of mean stress on growth rate (McEvily 1977). A close study of 'combined mode' fatigue-crack growth therefore appears promising and has application not only with respect to variable loading, but also to weldments, where residual stresses give rise to variations in mean stress. In general, the gaining of a quantitative understanding of fracture mechanisms in welded configurations and associated microstructures represents the main aim for micro-mechanical work in the future.

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PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

Discussion

S. G. Druce (*Metallurgy Division, A.E.R.E. Harwell, Oxon., U.K.*). I should like to ask Dr Knott if he expects the observation that prestrain reduces the ductile initiation toughness by promoting shear localization to be of relevance to the apparent toughness of material suffering repeated loadings? In particular, if a ductile material is loaded to some point on the resistance curve beyond initiation and then unloaded, where, with respect to this point, does initiation occur on reloading?

J. F. Knott. It is important here to distinguish between *uniform* strain, given to the specimen before the notch, slot or pre-crack is put into it, and the establishment of the strain distribution that is necessary to accommodate the c.o.d. in non-prestrained material. The former reduces crack-tip ductility by preventing the spread of strain into regions remote from the 'localized shear' fracture path: the latter is essential, to allow crack-tip strains to be increased up to the point of fracture, by void coalescence, fast shear or whatever. On a single unloading and reloading, I would expect crack growth to continue just as if there had been no unloading: the 'new' 'δ_i' would, however, be generally less than the 'original' δ_i, because the strain profile established ahead of the crack tip during growth means that the further increment required to produce fracture would be smaller. For void coalescence, if the inclusion spacing were X_0 the 'new' 'δ_i' would be approx. $(\mathrm{d}\delta/\mathrm{d}a)X_0$.

D. Tabor, F.R.S. (*Cavendish Laboratory, Madingley Road, Cambridge, U.K.*). I found Dr Knott's presentation extremely interesting and persuasive, but I am concerned over his values of surface energy. He quotes a true value for iron of about 2 J m^{-2} and derives a value of 14 J m^{-2} from his theory. He then goes on to suggest that the discrepancy may be due to the presence of long-range forces that are ignored in the determination of the true value. I do not see how such additional terms could arise, but even if they could the metallic bond operates over an extremely short range, so that once it is 'broken' there is virtually nothing left. If one allows for van der Waals forces the energy involved is only of the order of one-tenth of that arising from the metallic bond itself. I can draw only two conclusions from the discrepancy that he quotes: either there is some plastic work involved, or his theory is too crude and he must accept a sevenfold error as the price. I would welcome his comments.

J. F. Knott. I had certainly intended to convey, in my paper, the belief that some plastic work would be involved in the crack-spreading process in iron. A first point is whether this work is associated with dislocations operated from sources relatively remote from the crack tip or with dislocations generated at the crack tip. The temperature-independence of the local fracture stress, σ_f, and hence the apparent surface energy, γ_p, tends to favour the second situation, in which the shear stresses at the crack tip are so high (approx. one-tenth of the shear modulus) that thermal activation, at low temperatures, would not significantly reduce their value and permit easier dislocation movement. I put forward the suggestion that, in iron, which lies very much on the border-line between inherently 'brittle' and 'ductile' behaviour, in the Kelly, Tyson and Cottrell sense, it might be important to think of the critical fracture stage not just as the achievement of the force-maximum in the atomic-force–displacement curve (although this is clearly necessary, it may not be sufficient), but as the physical separation of atoms to distances such that they were truly 'separated' (i.e. to somewhere of order 1–2.5 spacings rather than half a spacing). In this sense, the local crack-tip dislocation movement might be necessary to achieve the required separation, involving plastic work of the order estimated by the crude calculation in my paper. The experimental values of σ_f give γ_p as 14 J m^{-2} only in a 'common-sense' manner, i.e. for the '5% thickest' grain-boundary carbides or the 95th percentile radius of spheroidal carbides, but they are consistent from one geometry of crack nucleus to another (plates to spheroids) and, whereas I would accept somewhere between, say, 11 and 17 J m^{-2} as possible bounds to γ_p, I do not think that the sevenfold error exists. A second point is that γ_p for the ferrite matrix must be greater than the surface energy of the cementite nucleus, or else fracture is nucleation controlled, not growth controlled, and the strong effects of notches on brittle behaviour cannot be explained. (The point is implicit in the energetics of crack growth treated in Smith's paper.) If the iron were breaking in a purely brittle manner, no increase in 'γ' would be experienced. To summarize, therefore, I am claiming that plastic work *is* involved, but I suggest that this could result from dislocations generated (athermally) from the crack tip, which in a 'borderline' material such as iron actually assist in the 'brittle' fracture process by enabling the crack-tip region to accommodate the fracture displacement of atoms across the cracking plane.

P. Hancock (*Department of Materials, Cranfield Institute of Technology, U.K.*). The work that Dr Knott has presented demonstrates very elegantly that in structural steels local discontinuities are present, or developed, during plastic deformation, at the tip of the crack, and this will produce scatter in the measured fracture properties.

However, when we start considering cracks present in individual grains produced by dislocation mechanisms, I should like to ask how can we justify treating the material as a continuum and applying levels of stresses and material properties that are average values measured in the bulk material.

J. F. Knott. Professor Hancock's point is well taken, and, of course, arises in any attempt to predict macroscopic properties from micro-mechanical models. Although, on the one hand, it might be argued that models such as that due to Hall and Petch have indeed enabled us to understand the benefits of fine grain size with respect to yield strength, the contrary argument is presumably that fracture models are in some sense different, because flow represents a statistical average, whereas fracture is a statistical extreme. The calculations and models in question for cleavage fracture refer to the propagation of a crack nucleus in a carbide situated within a yielded region. Although I have used Smith's model for propagation, because it is the best that there is, it turns out that for most of the microstructures for which the results have been analysed, the dislocation contribution is rather small (approx. 10%) compared with that of the applied stress and that the details of the dislocation configurations within the grains have therefore only second-order importance. Provided that the grain size or carbide spacing is relatively small (say, less than 1%) of the test-piece thickness, there will be a number of positions ahead of a notch or a pre-crack in which the conditions for fracture are almost, but not quite, equivalent to the worst possible. In a single crystal of iron, the Young modulus and Poisson ratio vary with orientation, but in a grain surrounded by fourteen others (for a tetrakaidecahedral shape), the effective energy release is, to a large extent, likely to be a compromise, probably close to that calculated from bulk values of the elastic constants. This would not be so, of course, for textured material; an interesting exercise, possibly of some relevance with respect to controlled-rolled steels, or weld metals, would be to investigate the behaviour of a single microstructure with different crystallographic textures, if these could be developed.