DISLOCATION-THEORETICAL APPROACH TO THE BRITTLE-TO-DUCTILE TRANSITION IN METALS

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The Bilby-Cottrell-Swinden model for a crack in a ductile material will be modified by introducing a dislocation free zone at the crack tip. A condition for the activation of dislocation sources will be explicitly taken into account. An energetic fracture criterion will be applied in order to derive expressions for the plastic work and the fracture toughness as functions of the material parameters for the case of small plastic zones. The temperature dependence of the fracture toughness will be briefly discussed.

INTRODUCTION

The fundamental criterion for unstable fracture of a cracked stressed solid is that the elastic energy stored in the specimen and the loading system be sufficient to supply the energy needed for the increase in the area of the crack. For the limiting elastic case Griffith (1) identified that energy with the surface free energy or ideal work of fracture $\gamma.$ Within linear-elastic fracture mechanics an expression for the fracture toughness in terms of material parameters can be derived on the basis of this criterion. For deformable solids such as metals Orowan (2) modified the Griffith criterion by the addition of a plastic work term $\gamma_{\rm D}$ to γ in order to take account for inelastic modes of energy dissipation during crack extension, the most important of which is plastic deformation. Thereby it was implicated that $\gamma_{\rm D}$ is a material parameter in the same sense as γ , independent of crack geometry and loading configuration.

In this paper we develop a dislocation-theoretical crack model, which will be used to justify the Orowan hypothesis for the case of small plastic zones at the crack tip. For the well-known dislocation crack model of Bilby, Cottrell and Swinden (3) it can be shown that the release of elastic energy during crack extension is totally cancelled by the work of plastic deformation, a result which holds for any size of the plastic zone (4). As a consequence, it is impossible to fulfill the fundamental fracture criterion even for small plastic zones within this model. We have, therefore, extended the BCS-model by introducing a dislocation-

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free zone at the crack tip, which has been directly observed during in situ electron microscope experiments by Kobayashi and Ohr (5), and, the size of which we connect with the condition for the activation of dislocation sources. On the basis of the fundamental fracture criterion expressions for the plastic work γ_p and the fracture toughness are derived, which turn out to be functions not only of the elastic and plastic material parameters, but also of the ideal surface energy γ itself.The consideration of the temperature dependence of the material parameters leads to a qualitative understanding of the brittle-to-ductile transition and the high values of the fracture toughness above the transition temperature.

ENERGETIC CONSIDERATIONS FOR THE BCS-MODEL

For the application of an energetic fracture criterion it is necessary to calculate the energy change &E of the solid accompanying the crack extension. A continuummechanical calculation of this energy change for the Dugdale or Bilby-Cottrell-Swinden (BCS) model of a crack in a ductile material has been done by Yokobori and Ichikawa (4). We will show here that their results can easily be derived by dislocation-theoretical means. In what follows we consider a crack in an infinite solid disc under uniform shear stress at infinity, assuming that the results are at least qualitatively applicable to other loading modes.

The distribution of crack and crystal dislocations $\rho\left(x\right)$ for an elastic-plastic crack of length 2c (Fig. 1) and plastic zone size a-c is given by (3)

$$\rho(x) = \frac{2(1-v)\tau_{F}}{\pi\mu b} \left\{ \operatorname{arcosh} \left| \frac{m}{c-x} + n \right| - \operatorname{arcosh} \left| \frac{m}{c+x} + n \right| \right\}$$
 (1)

with $m=(a^2-c^2)/a$ and $n=\frac{c}{a}=\cos(\frac{\pi}{2}\frac{\tau}{\tau_F})$. Here, μ is the shear modulus, ν Poisson's number, τ the shear stress at infinity, τ_F the critical shear stress and b the absolute value of the Burgers vector. $\rho(x)$ turns out to be a solution of the singular integral equation

$$\frac{\mu b}{2\pi (1-\nu)} \int_{-a}^{a} \frac{\rho(x') dx'}{x - x'} + P(x) = 0$$
 (2)

with
$$P(x) = \tau$$
, $|x| \le c$
= $\tau - \tau_F$, $c < |x| \le a$.

Using this equation it can easily be shown (6) that the elastic energy stored in the stress field of the dislocation distribution, U, is connected with the work of the loading system on the dislocations, W, by the equation

$$U = -W/2$$
 (3)

This leads to a general relation for the change of the total elastic energy with crack length given by

$$\delta (U+W) = -\frac{d}{dc} \left(\frac{1}{2} \int_{-a}^{a} \tau \Phi(\mathbf{x}) d\mathbf{x}\right) \delta c$$
 (4)

with
$$\Phi(\mathbf{x}) = b \int_{\mathbf{x}}^{a} \rho(\mathbf{x'}) d\mathbf{x'}$$
.

Inserting Eq.(1) into Eq. (4) one obtains

$$\delta (U+W) = \frac{8(1-v)\tau_F^2}{\pi \mu} \quad (lnsec \theta - \theta tg \theta) \delta c$$
 (5)

with
$$\Theta = \frac{\pi \tau}{2\tau_F}$$
.

On the other hand, the work of plastic deformation, $\delta\Gamma$, which has to be performed during crack extension is given by (7)

$$\delta \Gamma = \left(2\tau_{F} \int_{C}^{a} \frac{\partial \Phi(\mathbf{x}, \mathbf{c})}{\partial \mathbf{c}} d\mathbf{x}\right) \delta \mathbf{c}$$
 (6)

with $\Phi(\mathbf{x},\mathbf{c})$ defined in Eq. (4). The integration of Eq. (6) leads to the remarkable result

$$\delta \left(\mathbf{U} + \mathbf{W} + \mathbf{\Gamma} \right) = \mathbf{O} \tag{7}$$

which means that the elastic energy, which is released during the extension of an elastic-plastic crack described by the BCS or Dugdale model, is totally cancelled by the plastic work, and this, independent on the size of the plastic zone. As a consequence, it is not possible to fulfil a fracture criterion, since there is no energy left to supply the energy needed for the increase in the area of the crack.

MODIFIED CRACK MODEL WITH DISLOCATION-FREE ZONE

The plastic zone ahead of the crack tip arises either by activation of neighbouring Frank-Read sources or by new dislocations being punched out of the tip of the crack into the surrounding good crystal. The spontaneous emission of dislocations, which has been treated in detail by Rice and Thomson (8), is possible in high stress fields which are not shielded by neighbouring dislocations. We expect, therefore, this mechanism to work in dislocation free solids, e.g. semiconductors, or in metallic solids with low dislocation density. On the other hand, the Frank-Read sources in the dislocation network of metals under normal conditions are activated by rather low stresses of the order of the critical shear stress. If we identify the critical shear stress τ_F with the resistance against dislocation glide, the condition for this activation is that the local stress at the site of the source exceeds τ_F by an amount τ_O which is given by

$$\tau_{O} \approx \frac{\mu b}{k_{O}}$$
 (8)

Here, $\ell_{\rm O}$ is the length of a dislocation line of the source lying between two nodes, typical values of which for the dislocation networks of metals are of the order 10^{-6} - 10^{-5} m (9). With beginning external loading the Frank-Read sources just ahead of the crack tip, where the stress is high enough, are activated to send dislocations into the surrounding crystal. We allow for this activation process by assuming a dislocation-free zone with a size of the order of $\ell_{\rm O}$ lying between the crack tip and the plastic zone and, in which the local stress is not less than $\tau_{\rm F}+\tau_{\rm O}$ (Fig. 2). This assumption leads to a modification of the distribution of crack and crystal dislocations in comparison with the BCS model which will allow to fulfil the energetic fracture criterion and to derive an expression for the fracture toughness. To this end, we start with an integral equation for the dislocation density $\rho(x)$,

$$\frac{\mu \ b}{2\pi (1-\nu)} \int_{-a}^{a} \frac{\rho (x') dx'}{x-x'} + P(x) = 0$$
with
$$P(x) = \tau , |x| \le c$$

$$= \tau - \tau_{F} - \tau_{O}, c < |x| < c + \ell_{O}$$

$$= \tau - \tau_{F}, c + \ell_{O} \le |x| \le a,$$

the solution of which is given by

$$\rho \left(\mathbf{x} \right) \; = \; \frac{2 \left(1 - v \right)}{\pi \mu b} \; \left\{ \; \tau_{\mathrm{F}} \; g(\mathbf{x}, c) \; + \; \tau_{\mathrm{O}} \left(g(\mathbf{x}, c) \; - \; g(\mathbf{x}, c + \ell_{\mathrm{O}}) \right) \right\}, \tag{10}$$

where

$$g(x,y) = \operatorname{arcosh} \left| \frac{m}{y-x} + n \right| - \operatorname{arcosh} \left| \frac{m}{y+x} + n \right|$$

with $m = \frac{a^2 - y^2}{a}$ and $n = \frac{y}{a}$.

Moreover, we set $\rho(x)=0$ for c < |x| < c + ℓ_O to take account for the dislocation free zone. The condition for the size of the plastic zone turns out to be

$$\frac{\pi}{2} \tau - \tau_F \arccos \frac{c}{a} - \tau_O \left(\arccos \frac{c}{a} - \arccos \frac{c + \ell_O}{a}\right) = 0. \tag{11}$$

Eqs. (9) - (11) reduce to the corresponding BCS equations in the limit $\ell_O=0$. Eq. (9) is only an approximation to the exact integral equation incorporating directly the dislocation free zone (10). The advantage of eq. (9) lies in the fact that its solution for $\rho(x)$ may be treated analytically in order to calculate elastic and plastic energies according Eqs. (4) and (6). Moreover, the activation condition (8) has been directly taken into account, and we suppose the error to be small by setting $\rho(x)=0$ within the dislocation free zone.

In what follows, we restrict ourselves to the case of small plastic zones, i.e. a-c << c or $\tau << \tau_F^{}$, which is interesting

for the calculation of a fracture toughness. On the other hand, the size of the plastic zone must still be large compared with ℓ_0 since otherwise the concept of a continuous density of dislocations makes no sense. Solving Eqs. (4) and (6) for the change of the elastic and plastic energies during crack extension and taking into account the terms of lowest order in τ/τ_F only, one obtains

$$\delta (U + W + \Gamma) =$$

$$-\frac{4(1-\nu) \ell_O \tau_F^2}{\pi \mu} (1 + \frac{\tau_O}{\tau_F}) \ln \left(\frac{2c}{\ell_O} \left(\frac{\pi \tau}{2\tau_F}\right)^2\right) \delta c.$$
 (12)

With the aid of the fracture criterion

$$\delta \left(U + W + \Gamma + 4\gamma \delta c \right) = 0 \tag{13}$$

Eq. (12) leads to expressions for the fracture toughness, K $_{\rm C}$ = $\tau_{\rm C}/\pi{\rm C}$, and for the effective work of fracture, $\gamma_{\rm eff}$ = γ + $\gamma_{\rm p}$, according to Orowan's hypothesis. The results are

$$K_{C} = \tau_{F} \sqrt{\frac{2\ell_{O}}{\pi}} \exp \left(\frac{\pi \mu \gamma}{2(1-\nu)\tau_{F}(\tau_{F}+\tau_{O})\ell_{O}} \right)$$
 (14)

and

$${}^{\gamma}\text{eff} = \frac{2(1-\nu)\ell_0\tau_F^2}{\pi \mu} \exp\left(\frac{\pi \mu \gamma}{(1-\nu)\tau_F(\tau_F + \tau_0)\ell_0}\right). \tag{15}$$

On the basis of the known temperature dependence of the material parameters $\mu,~\gamma,~\tau_F,~\tau_o$ and ℓ_o , these results make it possible to discuss the temperature dependence of K_C or $\gamma_{\mbox{eff}}$ above the transition temperature T_o . Since for metals there is only a weak temperature dependence for $\mu,~\gamma$ and $\ell_o,~$ and τ_o is small compared with $\tau_P,~$ the change of K_C with temperature is mainly determined by the temperature behaviour of $\tau_F.$

Within our model there is a relation between the transition temperature T_0 and the size of the dislocation-free zone, ℓ_0 . Under the condition that the local stress in this zone is not less than $\tau_F + \tau_0$ one obtains in the limit of disappearing plastic zone for which a-c is of the order ℓ_0

$$\tau_{\mathbf{F}}(\mathbf{T}_{0}) + \tau_{0} \approx \tau_{\mathbf{F}}(\mathbf{T}_{0}) = \frac{K_{CO}}{\sqrt{2\pi\lambda_{0}}}.$$
 (16)

Here ${\rm K}_{\infty}$ is the brittle fracture toughness of the same material below ${\rm T}_{\rm O}$ given by

$$K_{CO} = \sqrt{\frac{4\mu\gamma}{1-\nu}}$$
 (17)

Typical values for K_{CO} and $\tau_F(T_0)$ confirm the order of magnitude for ℓ_0 to be 10^{-6} – 10^{-5} m. Connecting Eq. (16) with (14) one obtains an equation for the ratio K_c/K_{CO} which, to demonstrate the results, is shown in Fig. 3 together with the critical shear stress τ_F for Fe single crystals (11) as a function of temperature. Thereby, the material parameters have been chosen to be $\mu=6.92\cdot10^4$ MPa, $\gamma=1.975$ J/m², $\nu=0.291$ and $\ell_0\approx10^{-5}$ m. The results clearly demonstrate the strong enhancement of K_C with beginning plastic deformation. For deep temperatures the values of K_C approximate the brittle fracture toughness value, K_{CO} , the transition temperature lying at about 150 K. The limitations of the model, however, lead to a too rapid rise of K_C with increasing temperature. Hardening effects, on the other side, reduce the plastic deformation, and thus should lower the values of K_C above the transition point.

SYMBOLS USED

b = absolute value of the Burgers vector

 ℓ_{o} = size of the dislocation-free zone

 K_C = fracture toughness

 ${\rm K_{CO}}$ = fracture toughness below the transition temperature

U = elastic energy stored in the specimen

W = elastic energy of the loading system

 $T_{O} = transition temperature$

 γ = surface free energy

 γ_{D} = critical plastic work

 γ_{eff} = effective work of fracture

Γ = plastic work

μ = shear modulus

ν = Poisson's number

τ = shear stress

 τ_F = critical shear stress

 τ_{o} = stress, necessary to activate dislocation sources

REFERENCES

- Griffith, A.A., 1921, Phil. Trans. Roy. Soc, A221, 163
- Orowan, E., 1949, Rep. Progr. Phys, 12, 185
- Bilby, B.A., Cottrell, A.H. Swinden, F.R.S. and K.H., 1963, Proc.Roy.Soc, A272, 304
- 4. Yokobori, T., and Ichikawa, M., 1966, Rep. Res. Inst. Strength and Fract. of Mat., Tohuko University, Sendai, 2, 21
- 5. Kobayashi, S., and Ohr, S.M., 1980, Phil. Mag. A, 42, 763
- 6. Pfuff, M., 1982, GKSS-Bericht, 82/E/11
- Goodier, J.N., and Field, F.A., 1963, Fracture of Solids, Wiley, New York
- 8. Rice, J.R., and Thomson, R., 1974, Phil. Mag, 29, 73
- 9. Friedel, J., 1964, <u>Dislocations</u>, Pergamon, London
- 10. Chang, S.-J., and Ohr, S.M., 1980, "Dislocation Modelling of Physical Systems", Proceedings of the International Conference, Gainsville, Florida, USA
- 11. Seeger, A., 1958, "Kristallplastizität". Handbuch der Physik, Springer, Berlin-Göttingen-Heidelberg.

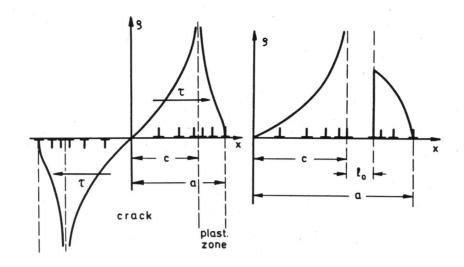


Figure 1 Dislocation distribution for the BCS model

Figure 2 Modified BCS model with dislocation free zone

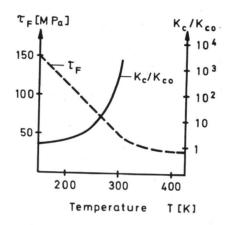


Figure 3 Critical shear stress and fracture toughness according to Eq. (14) for Fe single crystals