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A SIMPLE ELASTIC CELL MODEL OF CLEAVAGE FRACTURE IN THE PRESENCE OF DISLOCATION PLASTICITY

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Abstract—The current analysis is prompted by the recent recognition that an elastic core embedded about the crack tip in a plastic medium affords a mechanism for cleavage-type crack growth with significant plastic dissipation [Beltz *et al.*, *Acta metall. mater.*, submitted (1995)]. We build upon recent notions that recognize the large disparity between relevant length scales involved in plastic flow processes around cracks in metals and on metal–ceramic interfaces. A simple, continuum-based model that assumes the presence of a dislocation-free core of dimension R_c is used. The crack tip is assumed not to emit dislocations. The core size is chosen in a self-consistent manner by identifying a maximum equivalent stress in the plastic zone with that predicted by the phenomenological hardening law having the form $\sigma_{flow} = \alpha Eb/R_c$. When the inner elastic stress field is matched with the approximate stress field within the plastic zone, it is found that the applied energy release rate needed to initiate crack extension is several orders of magnitude greater than the ideal work of fracture. This apparent shielding of the crack tip is found to strongly depend on the ideal work of fracture, indicating a possible mechanism for segregation-induced interfacial embrittlement.

Résumé—Notre analyse se base sur la récente reconnaissance du fait qu'un noyau élastique inclus autour de la tête de fissure dans un milieu plastique permet un mécanisme pour une propagation de fissure de type clivage, avec une dissipation plastique significative [Beltz *et al.*, *Acta metall. mater.*, soumis à publication (1995)]. Nous démarrons à partir des idées récentes qui reconnaissent la large disparité qui existe entre les échelles de distance impliquées dans les processus d'écoulements plastiques autour des fissures dans les métaux et aux interfaces métal–céramique. Nous utilisons un modèle simple, basé sur l'idée d'un continuum, qui suppose la présence d'un noyau sans dislocation, de dimension R_c. La tête de fissure est supposée ne pas émettre de dislocation. La taille du noyau est choisie d'une manière autocohérente, en identifiant une contrainte équivalente maximum dans la zone plastique avec celle prédite par la loi phénoménologique de durcissement ayant la forme $\sigma_{flow} = \alpha Eb/R_c$. Lorsque le champ de contrainte élastique intérieur est rattaché avec le champ de contrainte approximatif de la zone plastique, il apparaît que le taux de restitution d'énergie appliqué nécessaire pour amorcer l'extension de la fissure est supérieur de plusieurs ordres de grandeur au travail de rupture idéal. Cette apparante protection de la tête de fissure apparaît dépendre fortement du travail de rupture idéal, ce qui indique la possibilité d'un mécanisme de fragilisation interfaciale induite par ségrégation.

Zusammenfassung—Die vorliegende Analyse wurde durch die Erkenntnis stimuliert, daß ein elastischer Kern, der im plastischen Medium um eine Rißspitze eingebettet ist, einen Mechanismus für spaltartiges Rißwachstum mit signifikanter plastischer Dissipation bietet [Beltz *et al.*, *Acta metall. mater.*, eingereicht (1995)]. Aufbauend auf neuen Konzepten, die die großen Unterschiede zwischen den relevanten Längenskalen in plastischen Fließprozessen in der Umgebung von Rissen in Metallen oder an Metall-Keramik-Grenzflächen anerkennen, wird ein einfaches kontinuumsmechanisches Modell verwendet, das das Vorhandensein eines versetzungsfreien Kernes der Dimension R_c annimmt. Es wird angenommen, daß von der Rißspitze keine Versetzungen ausgehen. Die Kerngröße wird in einer selbstkonsistenten Prozedur ausgewählt, indem eine maximale äquivalente Spannung in der plastischen Zone mit derjenigen Spannung identifiziert wird, die durch das phänomenologische Härtungsgesetz $\sigma_{flow} = \alpha Eb/R_c$ vorhergesagt wird. Wenn das innere elastische Spannungsfeld mit dem genäherten Spannungsfeld in der plastischen Zone in Übereinstimmung gebracht wird, findet man, daß die für Rißvergrößerung benötigte Energiefreisetzungsrate um mehrere Größenordnungen größer ist als die ideale Brucharbeit. Es ergibt sich, daß diese offensichtliche Abschirmung der Rißspitze stark von der idealen Brucharbeit abhängt, was auf einen möglichen Mechanismus für seggregationsinduzierte Grenzflächenversprödung hindeutet.

1. INTRODUCTION

The ductile versus brittle behavior of metals and semiconductors is among the least understood of the fundamental mechanical phenomena in the field of materials science. Much attention in the past few decades has been devoted to understanding the factors that affect ductile–brittle behavior within either continuum or atomistic frameworks. However, recent work has suggested that the interaction between processes occurring over length scales ranging from atomistic to macroscopic may be critical to quantitative understanding of fracture behavior. We are presently interested in the fracture process in which nominally brittle fracture occurs concomitantly with plasticity in such a manner that the apparent toughness is much greater than the energy required to simply create new fracture surfaces.

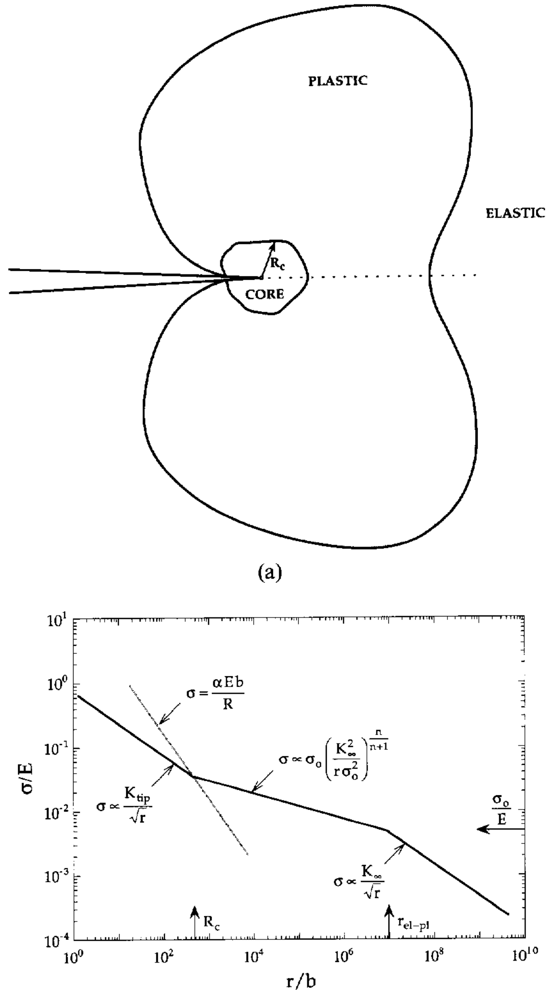
Early fracture models tended to draw a sharp distinction between "brittle" and "ductile" fracture. The treatment of brittle fracture is epitomized by Griffith's classical argument based on the balance between the elastic energy stored in a cracked body (and its surrounding loading system) and the energy associated with the newly created fracture surfaces [1]. By contrast, fully plastic fracture is typically characterized by crack tip blunting and hole growth [2, 3]. The first break with this tradition came with Orowan's assertion that the Griffith criterion for brittle fracture be modified to include the plastic work dissipated in the crack tip process zone [4]. A significant advance in the understanding of brittle fracture was Rice's recognition that the amount of plastic work dissipated during the fracture process has a strong functional dependence on the surface (or Griffith) energy itself, a phenomenon referred to as the "valve" effect [5]. The importance of plasticity in brittle fracture processes is especially evident in problems of segregation-induced interfacial embrittlement in metals and metal–ceramic couples [6, 7]. Such problems are characterized by a dramatic reduction in the apparent toughness associated with the introduction of small amounts of impurities at grain boundaries or bimaterial interfaces. Previous attempts at quantifying the valve effect, notably those by Thomson [8], Suo *et al.* [9] and Jokl *et al.* [10], have identified the existence of the inherently non-linear coupling between the crack tip and the surrounding plastic zone. However, these models fall short of a self-consistent description of the fracture process in terms of known or measurable material parameters. Here, we present a simple analysis that allows the coupling between the Griffith energy and the plastic work to be expressed analytically and self-consistently in terms of the relevant material parameters.

2. THE MODEL

We build our conceptual model on a framework first proposed by Thomson [8] and more recently extended by Rice and coworkers [9, 11, 12]. Figure 1 conveys the essential physical motivation for the following discussion. A body containing a sharp crack is loaded by remote tractions. The material around the pre-existing, sharp crack is allowed to plastically deform and strain harden, following the large-strain limit of the generalized Ramberg–Osgood constitutive law:

$$\bar{\sigma} = \sigma_0\left(\frac{E\bar{\varepsilon}_p}{\beta\sigma_0}\right)^n, \tag{1}$$

where $\bar{\sigma}$ is the effective stress (defined as $\sqrt{\frac{3}{2}s_{ij}s_{ij}}$, where s_{ij} is the stress deviator), σ_0 is the uniaxial yield stress, $\bar{\varepsilon}_p$ is the effective plastic strain (defined as $\sqrt{\frac{2}{3}\varepsilon_{ij}\varepsilon_{ij}}$), E is Young's modulus, n is the work-hardening exponent, and β is an empirical prefactor of order unity ($\beta = 3/7$ in the original Ramberg–Osgood for-



(b)

Fig. 1. Schematic illustration of the elastic core concept. (a) The plastic zone surrounding a remotely loaded, sharp crack. The discrete nature of the dislocation distribution within the plastic zone gives rise to a net dislocation-free elastic region immediately surrounding the crack tip. The size of the elastic core is stochastic, and is related to the local dislocation density near the crack tip. (b) Idealized stress distribution ahead of the crack tip, showing the two elastic regimes (elastic core and far-field K-dominant region) and the plastic regime. Stress continuity is enforced at the elastic–plastic boundaries in accordance with the flow stress at the outer surface of the elastic core.

Table 1. Selected values of f_n and I_n under plane strain and plane stress conditions [27]

	Plane strain		Plane stress	
n	f_n	I_n	f_n	I_n
0.0	1	3.7	1	2.5
0.1	0.67	4.5	1.00	3.0
0.2	0.46	5.0	0.99	3.4
0.3	0.30	5.4	0.98	3.8
0.4	0.18	5.7	0.98	4.0
0.5	0.09	5.9	0.97	4.2

mulation [13]). We assume for simplicity that the crack is loaded in opening mode. The asymptotic crack tip stress field within the plastic zone can be obtained from numerical solutions (HRR) presented by Hutchinson [14] and Rice and Rosengren [15]. The effective stress directly ahead of the crack tip ($\theta = 0$) is:

$$\bar{\sigma} = f_n \sigma_0 \left(\frac{\xi}{\beta I_n} \frac{K_{\mathrm{I},\infty}^2}{r \sigma_0^2} \right)^{n/(1+n)}, \tag{2}$$

where r is the distance ahead of the crack tip and $K_{\mathrm{I},\infty}$ is the applied, or far-field, stress intensity factor that characterizes the elastic field well beyond the plastic zone. (We assume small-scale yielding, wherein the plastic zone remains small in relation to other length scales in the problem.) The parameter ξ characterizes the state of constraint, taking on the value 1 for plane stress and $1 - v^2$ for plane strain, where v is Poisson's ratio. The factors f_n and I_n are weak functions of the work-hardening exponent and are determined numerically in the HRR solution (Table 1).

To this point, the crack tip has been tacitly assumed to be stable against dislocation emission. This assumption was invoked in the work of Thomson [8], Rice [11] and Beltz *et al.* [12], who have proposed the existence of a dislocation-free core immediately ahead of the crack tip [Fig. 1(a)]. The core size, R_c, scales approximately as the inverse root of the local dislocation density (i.e. the mean dislocation spacing) near the crack tip. The stress field inside the core retains an elastic singularity described by a crack tip stress intensity factor, K_{tip}. (Note that the assumptions just made rely on the additional condition that the elastic core remain large enough compared to atomic dimensions for continuum elasticity theory to be valid.) Thus, the effective stress directly ahead of the tip ($\theta = 0$) is given by:

$$\bar{\sigma} = \lambda \frac{K_{\mathrm{I,tip}}}{\sqrt{r}}, \tag{3}$$

where $\sqrt{2\pi}\lambda$ is unity for plane stress and $1 - 2v$ for plane strain.

A final constraint on the stress field is taken from a standard correlation in crystal hardening theory, originating from the fundamental work of Taylor [16], that relates the flow stress to the dislocation spacing (or dislocation cell size):

$$\bar{\sigma}_{\mathrm{flow}}^{\max} = \frac{\alpha E b}{R_c}, \tag{4}$$

where b is the magnitude of the Burgers vector. In equation (4), $\bar{\sigma}_{\mathrm{flow}}^{\max}$ can be thought of as the maximum effective flow stress to which the material has hardened; in a work-hardening material, this is expected to occur directly at the interface between the elastic core and the surrounding plastic zone. The parameter α is an experimentally measurable material constant that reflects the strength of interaction between moving dislocations in a plastically deforming body [17]. The formation of cellular dislocation structures has been associated with values of α in the range 5–10 [18–20], whereas random dislocation distributions lead to αs as low as 0.3 [21, 22].

Having described the form of the stress fields ahead of the crack tip [see Fig. 1(b)], it remains to determine the conditions for fracture initiation. At the point of incipient fracture, the crack tip stress intensity reaches its critical value:

$$K_{\mathrm{I,tip}} \rightarrow \sqrt{\frac{1}{\xi} \mathscr{G}_c^{\mathrm{tip}} E}, \tag{5}$$

where $\mathscr{G}_c^{\mathrm{tip}}$ is the inherent Griffith toughness. The value of $\mathscr{G}_c^{\mathrm{tip}}$ is simply the work of adhesion, W_{ad}, of the solid–solid interface—a material parameter that can be calculated from atomistic models or estimated using various experimental techniques. We are interested in calculating the shielding ratio afforded by the plastic zone as a function of the Griffith fracture energy. We do so by enforcing stress continuity at the elastic core boundary, $r = R_c$, using equations (2)–(4). After rearrangement, the shielding ratio—defined as the ratio of apparent toughness to the work of adhesion—is recovered in simple analytical form:

$$\frac{\mathscr{G}_c^{\infty}}{W_{\mathrm{ad}}} = \beta I_n \left(\frac{\lambda^2}{\xi f_n^{1+n}} \right)^{1/n} \left(\frac{W_{\mathrm{ad}}}{\alpha b \sigma_0} \right)^{(1-n)/n}. \tag{6}$$

Figures 2(a)–(c) show the dependence of the shielding ratio on the work of adhesion for selected values of α and the work-hardening exponent, n (note that n typically ranges from 0.1 to 0.3 for metals).

Combining equations (3) and (4), we can also solve for the self-consistent elastic core size at the initiation of fracture:

$$R_c = \frac{\xi}{\lambda^2} \frac{E(\alpha b)^2}{W_{\mathrm{ad}}}. \tag{7}$$

Figure 2(d) shows the corresponding dependencies of the elastic core size on the work of adhesion.

3. DISCUSSION

It is evident from equations (6) and Figs 2(a)–(c) that very small excursions in the work of adhesion can lead to dramatic changes in the apparent toughness. This prediction is consistent with recent observations of the dependence of toughness on small amounts of segregants at metal grain boundaries and metal–ceramic interfaces. In experiments on copper

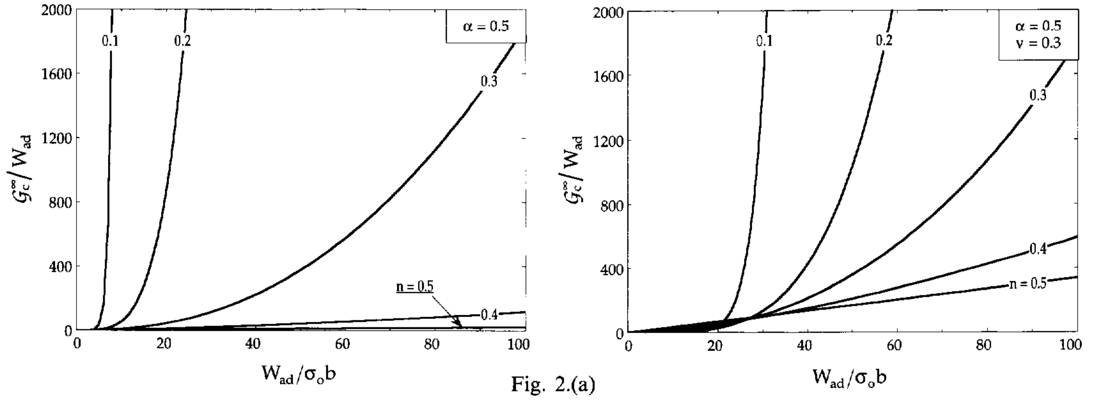


Fig. 2.(a)

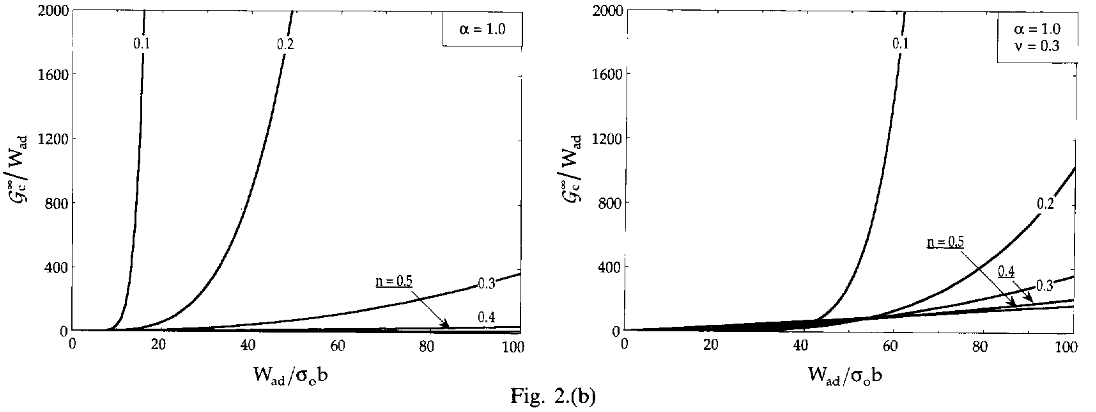


Fig. 2.(b)

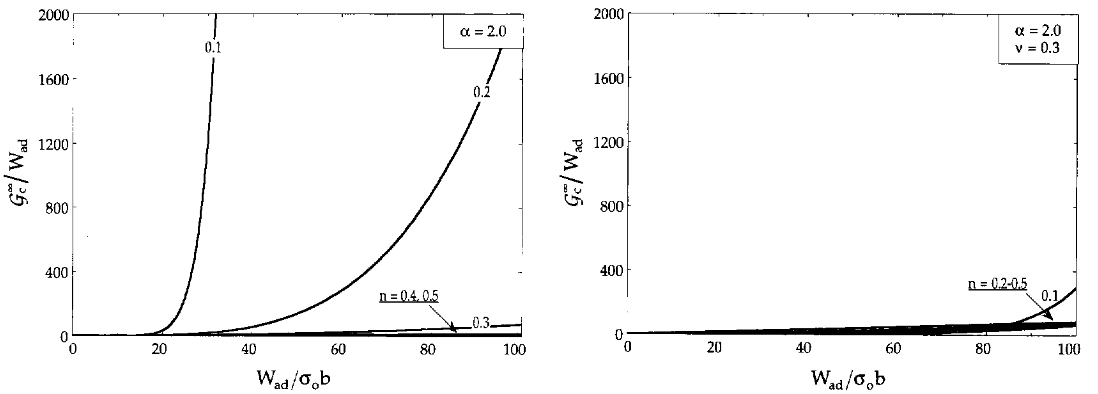


Fig. 2.(c)

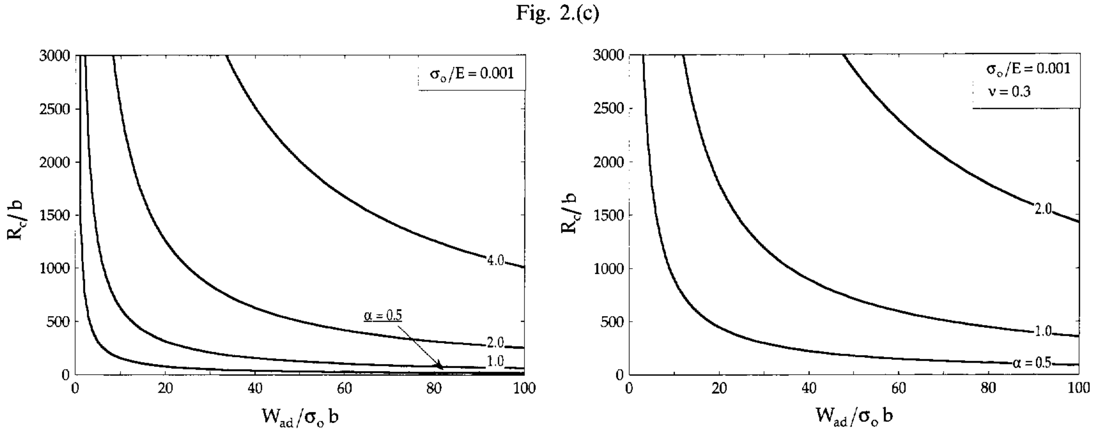


Fig. 2.(d)

Fig. 2. The variation of shielding ratio with the work of adhesion and work-hardening exponent for (a) $\alpha = 0.5$, (b) $\alpha = 1$ and (c) $\alpha = 2$. (d) Corresponding dependence of the elastic core size on the work of adhesion. Figures on left correspond to plane stress solutions, while those on the right were calculated for plane strain conditions with $\nu = 0.3$.

bicrystals with interfacial bismuth [23] and niobium–sapphire interfaces with phosphorous and sulfur segregants [24], marked reduction in the fracture toughness was noted over the pristine compositions. Most recently, Lipkin *et al.* have attempted to quantify the embrittling effects of interfacial carbon on the gold–sapphire system [25]. Preliminary results have shown that a carbon-induced decrease in the interfacial work of adhesion from 0.6 to 0.3 J/m^2 leads to a ten-fold drop in the fracture toughness, from 190 to 16 J/m^2. Current work on the effects of carbon segregation in this system is expected to provide the first quantified validation of the valve effect.

The segregation-induced change in work of adhesion can be predicted using well-established thermodynamic relations [26]. For the case of fracture at fixed segregant composition (e.g. if the segregant is immobile during separation):

$$W_{ad} = W^{o}_{ad} - \int_{0}^{\Gamma} [\mu_b(\Gamma_b) - \mu_s(\Gamma_s/2)]\, d\Gamma, \quad (8)$$

where W^{o}_{ad} is the work of adhesion for the pure interface, Γ is the surface excess of the segregant, and $\mu_b(\Gamma_b)$ and $\mu_s(\Gamma_s/2)$ are the boundary and surface adsorption isotherms, respectively. By definition, normal segregants have a lower chemical potential at a free surface than at an internal boundary, rendering the integrand in equation (8) positive. The consequential reduction in the work of adhesion, coupled with the associated decrease in the plastic dissipation given by equation (6), is believed to lead to the dramatic changes in fracture behavior observed in segregation-embrittled systems.

4. SUMMARY

We have shown that the segregation-induced embrittlement observed in a number of metals and metal–ceramic interfaces exhibiting nominally brittle fracture can be explained in terms of the coupling between the plastic deformation and the crack tip (Griffith) fracture energy. The amount of shielding afforded by plastic dissipation is calculated using a dislocation-free elastic core model. The shielding is expressed in terms of the two continuum plasticity parameters: yield strength and work-hardening exponent. The elastic core sizes are self-consistently determined and are found to be two to three orders of magnitude times the size of the Burgers vector, in agreement with the postulate that the elastic core must scale approximately with the dislocation spacing or dislocation cell diameter in hardening metals.

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