Fracture 1977, Volume 3, ICF4, Waterloo, Canada, June 19 - 24, 1977

NONLINEAR LATTICE THEORY OF FRACTURE*

E. R. Fuller, Jr. and R. Thomson**

INTRODUCTION

In recent theoretical literature [1, 2, 3] regarding fracture in atomic lattices some questions have arisen regarding the fundamental role of the surface energy in brittle fracture. This paper represents an attempt to clarify some of these basic ideas. Hsieh and Thomson [1] have shown that in a two-dimensional lattice containing a crack there is a range of applied stress for which the crack is mechanically stable, and accordingly, is "trapped" by the lattice. This lattice trapping regime is bounded by a regime of fast fracture for stresses larger than an upper critical stress, σ_+, and by a spontaneous crack healing regime for stresses smaller than a lower stress, σ_-. These stress boundaries were found to vary as the inverse square root of the crack length, a,

$$\sigma_{\pm} = \sqrt{Y\gamma_{\pm}/a} \ , \tag{1}$$

in precisely the same manner as in the continuum theory of Griffith [4]. Y is a constant of proportionality. The effective surface energy densities, γ_+ and γ_-, in this Griffith-like expression define the limits of the lattice trapping regime. When the macroscopic surface energy, γ_o, as defined by one-half the area under the cohesive force law curve, is compared with γ_+ and γ_-, it is found that γ_o lies between these two limits. This result is then used as a basis for constructing a theory of subcritical crack growth, or healing, when the stress is either above, or below, the Griffith stress $\sigma_o = \sqrt{Y\gamma_o/a}$. These general ideas have been picked up and expanded by Lawn [2] in a self-consistent and straightforward manner to form a basis for subcritical crack growth in the presence of an external atmosphere.

However, a recent paper by Esterling [3] has indicated that when a more realistic cohesive force law is used in a lattice theory, the macroscopic surface energy, as defined above, no longer lies within the lattice regime. A Griffith thermodynamic surface energy can be defined by the condition where thermal fluctuations cause a crack to advance and recede at equal rates. If this definition of surface energy corresponds to γ_o, the subcritical crack growth theory loses its basis since thermodynamic equilibrium occurs in a regime where the crack is mechanically unstable towards spontaneous healing. Since these ideas are considered to be basic to the fracture process in general, and to subcritical crack growth in particular, this paper will reinvestigate the relationship between the surface energy and fracture with particular attention to the subcritical crack growth regime.

** Physical Properties Section, National Bureau of Standards, Washington, D. C. 20234, U. S. A.

ONE-DIMENSIONAL LATTICE MODEL

The quasi-one-dimensional lattice model of a crack to be considered here is similar to that of Thomson et al [5]. The model consists of two semi-infinite chains of atoms that are bonded with two types of interactions, Figure 1. These interactions are modeled as bendable (horizontal) spring elements and stretchable (transverse) spring elements. The free ends of the chains are subjected to equal and opposite vertical opening forces P at the zeroth atoms. All displacements are assumed to be vertical with the displacement of the jth atom from its equilibrium separation, c, being denoted by u_j. The stretchable elements up to the nth atom are considered to be stretched beyond their range of interaction, or "broken", thus forming a crack of finite length.

The total potential energy of this system consists of three contributions: the change in potential energy of the external loading system (the negative of the work done by the external force); the strain energy of the bendable bonds; and the strain and/or surface energy of the stretchable bonds across the crack plane. The potential energy of the external loading system is given simply by $U_{ext} = -W_{ext} = -2\,P\,u_o$. The interaction of the bendable spring element is modeled as a second-neighbour interaction between atoms at j-1 and j+1 that resists flexure about their common nearest neighbour at j. The strain energy of this interaction about atom j is given by

$$\frac{1}{2}\beta\,[(u_{j-1}-u_j)-(u_j-u_{j+1})]^2 = \frac{1}{2}\beta\,[u_{j+1}-2u_j+u_{j-1}]^2\ , \qquad (2)$$

where β is the spring constant for this interaction. The total strain energy of the bendable spring elements, U_{bend}, is twice the summation of these contributions for atoms j = 1, 2, ... (one contribution for each side of the crack). The strain energy contained in the interaction of the jth stretchable spring element across the crack plane can be written as $2\gamma(u_j)c$, where $\gamma(u_j)$ is defined as the density of the surface energy assigned to each surface of the chains of atoms [6]. This surface energy per unit length of surface is given by

$$\gamma(u_j) = \frac{1}{2c}\left[2\int_0^{u_j} f_j(u)\,du\right]\ , \qquad (3)$$

where $f_j(u_j)$ is the cohesive force of the jth stretchable bond which has been extended a distance $2\,u_j$ from its equilibrium separation. A finite range of interaction is assumed for this nonlinear cohesive force, so that elements which are stretched beyond a critical separation, $c + 2\,u_c$, are taken to be "broken". The surface energy for the "broken" spring element (j = 0 to n - 1) is given by one-half the area under the cohesive force law curve, $\gamma_o c$. The strain (and/or surface) energy contained in the nonlinear element at the "crack tip" is $2\gamma(u_n)c$, and represents the nonlinear *elastic* energy of that bond. All stretchable elements beyond j = n are assumed to be linear elastic, $f_j(u_j) = \alpha(2\,u_j)$ for j = n + 1, ... The spring constant, α, is the linear part of the nonlinear force law, $\alpha = [df_j/d(2\,u_j)]$ at $u_j = 0$. The total energy of the stretchable bond elements, $U_{stretch}$, is given by the summation of these contributions for j = 0, 1, ...

Combining these potential energy terms, the total potential energy of the system is given by

$$U = -2Pu_o+\beta\sum_{j=1}^{\infty}(u_{j+1}-2u_j+u_{j-1})^2+2\gamma_o nc+2\gamma(u_n)c+2\alpha\sum_{j=n+1}^{\infty}u_j^2. \qquad (4)$$

For a given applied force P and crack length a = nc, necessary conditions for equilibrium configurations of the crack are $(\partial U/\partial u_j) = 0$, for j = 0, 1, ... These equations of stability give an infinite set of fourth-order difference equations which can be solved analytically for the displacements u_j. The solutions for j = 0, 1, ..., n - 1 are

$$u_j = [\xi+(n-j)c]u_n/\xi + P(n-j)[2n^2+3n(\xi/c)+1-j(j+n)]/6\beta \qquad (5)$$

and for j = n +1, n + 2, ... (i = 1, 2, ...) are

$$u_{n+i} = \left[u_n\cos(\eta i)-(Pn/2\beta\sinh\lambda)\,\frac{\sin(\eta i)}{\sin(\eta)}\right]e^{-\lambda i} \qquad (6)$$

where

$$\cosh(\lambda) = 1/\cos(\eta) = \sqrt{1+(\alpha/8\beta)} + \sqrt{\alpha/8\beta}$$

and ξ is a length defined by the spring constant ratio, β/α, according to $\xi = c/\tanh(\lambda)$, or equivalently, $(2\beta/\alpha) = \xi^2(\xi^2-c^2)/c^4$. The displacement of the nth atoms, which interact through the nonlinear cohesive force $f(u_n)$, is determined from the nonlinear coupling equation, $(\partial U/\partial u_n) = 0$

$$\frac{P(nc+\xi)}{2\alpha u_c\xi} = \Psi(u_n) = \frac{f(u_n)}{\alpha(2u_c)} + \left(\frac{\xi-c}{2c}\right)\left(\frac{u_n}{u_c}\right). \qquad (7)$$

The solution for u_n, from which the other displacements can be determined by equations (5) and (6), can be illustrated graphically. Consider an idealized nonlinear atomic force law and its corresponding surface energy density, as plotted in Figures 2a and 2b, respectively. A graphic solution of equation (7) for this nonlinear stretchable force law is shown in Figure 3 for three ratios of bendable to stretchable force constants, β/α. For given elastic properties (i.e., β/α) and a given position of the nonlinear, stretchable spring element (i.e., n), there exist a range of applied loads P, over which equation (7) has three solutions for u_n. The first and third solutions, denoted on the figure by u_n (1) and u_n (3), respectively, correspond to stable equilibrium configurations for cracks of length a = nc and a = (n+1)c, respectively. For the first solution, the crack-tip bond is just beginning to see the influence of the nonlinear elastic region; whereas, for the third solution, the crack-tip bond is linear elastic by assumption, and the last broken bond has started to heal nonlinearly. Viewed in multi-dimensional configuration space, the total potential energy as a function of displacements, $U = U[n, u_o, u_1, \ldots u_j, \ldots]$, has a relative minimum at configurations corresponding to both u_n (1) and u_n (3). Topological arguments require that at least one saddle point exists between these two minima. Since the configuration corresponding to u_n (2) is the only possible candidate for an extremum, this configuration is the required saddle point.

Unstable bond rupture occurs when the applied force P is increased to a critical value P_+, so that solutions u_n (1) and u_n (2) coalesce to give $\Psi_+ = \Psi[u_n\ (1)] = \Psi[u_n\ (2)]$. Spontaneous bond healing occurs when the applied force is decreased to a critical value P_- so that solutions u_n (2) and u_n (3) coalesce. In the intermediate regime of applied force, $P_- < P < P_+$, the crack is lattice trapped. As noted by Thomson et al [5], increasing the ratio of β/α (that is, "stiffer" bendable spring elements and/or "softer" stretchable spring elements) results in a decrease in the lattice trapping regime. In constast to their model, however, lattice trapping will vanish for some critical *finite* ratio of spring constants, β/α (the upper curve in Figure 3). Thus, the existence of lattice trapping depends on the elastic properties of the solid. In general, the nonlinear nature of the crack-tip bond tends to decrease the range of lattice trapping in comparison to their "bond-snapping" model.

ONE-DIMENSIONAL CONTINUUM MODEL

In order to compare these results with the macroscopic surface energy γ_o, it is necessary to obtain a continuum model for the same type of crack. The simplest approach is to take the linear-elastic continuum limit of the total potential energy of the system, and use the Griffith approach. The potential energy of the system can be calculated by substitution of equations (5) and (6) into equation (4). The energy contained in the bendable and stretchable bonds is given by

$$U_{bend} + U_{stretch} = Pu_o + 2\gamma_o nc + [2\gamma(u_n)c - u_n f(u_n)] \ . \qquad (8)$$

For linear elasticity, the term in square brackets vanishes, yielding the usual fracture mechanics relationship that the strain energy in the bendable and unbroken stretchable bonds is equal to one-half the work done by the external force, $W_{ext}/2$, or $-U_{ext}/2$.

To obtain the one-dimensional continuum model, the limits as $n \to \infty$ and $c \to 0$ is taken in such a manner that $nc \to a$, and βc^3 and α/c remain constant. [The bendable spring constant β must scale as c^{-3} (stiffen) in order to maintain a finite displacement at the zeroth atom for an infinite number of small spring elements. For this stiffening, the stretchable elements must soften proportional to c to maintain a non-zero crack-tip displacement.] Taking this limit and setting $(\partial U/\partial a) = 0$, gives the continuum relationship,

$$P(a+\xi) = \sqrt{2\beta c^3 \gamma_o} \ , \qquad (9)$$

which is analogous to the force-crack length relationship for the double cantilever beam. Since equation (7) has the same form as equation (9), effective surface energy densities $\gamma_\pm$ can be defined from equation (7) for the discrete lattics model, analogous to equation (1).

DISCUSSION

When a crack is lattice trapped, thermally activated subcritical crack propagation, or crack healing, is possible [1, 2, 7]. Previous treatments used a modified continuum model to predict the character of the thermally

activated crack growth. Since the present model predicts the configuration of the saddle point, it is possible to calculate the forward and backward activation energy barriers within the framework of the model. The forward activation barrier is given by $\Delta U_+ = U[\ldots u_n\ (2)\ldots] - U[\ldots u_n\ (1)\ \ldots]$; and the backward barrier is given by $\Delta U_- = U[\ldots u_n\ (2)\ldots] - U[\ldots u_n\ (3)\ldots]$. When the applied force is P_+, the forward barrier vanishes and catastrophic rapid fracture ensues. Similarily, spontaneous crack healing occurs at P_-. The equilibrium thermodynamic (Griffith) condition corresponds to an applied force P_G at which the forward and backward energy barriers are equal. Since P_G is always bounded by P_+ and P_-, the Griffith thermodynamic condition must always lie within the rapid fracture and spontaneous healing limits. The regime of applied forces for thermally activated subcritical crack growth is between P_G and P_+, where rapid fracture occurs.

The result obtained by Esterling [3], $\gamma_o < \gamma_-$, implies, therefore, that the macroscopic thermodynamic surface energy, γ_o, is not related to the microscopic thermodynamic surface energy, γ_G. This apparent "paradox" is best illustrated by two examples: for the cohesive force law plotted in Figure 2, $f(u_n) = \alpha(2\ u_n)(1-u_n/u_c)^2$, equation (7) with $\xi = 3c/2$ (or $\beta/\alpha = 45/32$) gives the central curve of Figure 3. The lattice trapping regime is given by

$$\gamma_+/\gamma_o = 6/5 > 1 \qquad \text{and} \qquad \gamma_-/\gamma_o = 250/243 > 1 \ .$$

Thus, for this choice of nonlinear cohesive force law the macroscopic surface energy density γ_o is not bounded by the lattice trapping limits γ_+ and γ_-, similar to the findings of Esterling [3]. However, the present model is not self-consistent for this force law and choice of elastic constants. This inconsistency is easily seen from Figure 3. As previously mentioned, u_n (3) is the solution for the displacement of the nonlinear atom at n which is one atomic spacing behind the crack tip at n + 1. Using u_n (3) the crack-tip displacement can be calculated from equation (6). For self-consistency this displacement should correspond to solution 1 of equation (7), u_{n+1} (1), when the nonlinear spring element is assumed to be at n + 1. This is not possible in general, since there is no "weakly interacting" nonlinear spring element one lattice spacing behind the nonlinear atom at n + 1. That spring element has been assumed to be "broken". In order to reduce this inconsistency for an arbitrary nonlinear cohesive force law, additional nonlinear interactions must be included (i.e., a larger crack-tip cohesive region). The feasibility of this extension is presently under investigation.

A second example more clearly illustrates that this inconsistency in the present model is the probable cause of the macroscopic surface energy density lying outside the lattice trapping regime. A cohesive force law (see Figure 4) is chosen so that the conditions previously mentioned are self-consistent. For this nonlinear cohesive force law,

$$P/P_o = \Psi/\sqrt{\Psi_+ \Psi_-}$$

where

$$\Psi_+ = \left(\frac{\xi+c}{2c}\right)\left(\frac{u_m}{u_c}\right) \qquad \text{and} \qquad \Psi_- = \left(\frac{\xi-c}{2c}\right).$$

Thus,

$$\gamma_+/\gamma_o = \Psi_+/\Psi_- > 1 \qquad \text{and} \qquad \gamma_-/\gamma_o = \Psi_-/\Psi_+ < 1 \ .$$

For a given nonlinear bond at n, calculation of the applied force P_G when the forward and backward activation barrier are equal gives $\gamma_G/\gamma_o = (P_G/P_o)^2 = 1$. Thus, in this case, not only does γ_o lie within the lattice trapping range, but it is also equal to γ_G.

CONCLUSIONS

It appears that the result obtained by Esterling, $\gamma_o < \gamma_- \leq \gamma_G \leq \gamma_+$, for some nonlinear cohesive forces might be due to an assumed linearity of atomic interactions beyond the crack-tip bond, which is not necessarily a self-consistent assumption. In one case where the assumption of linearity was forced to be satisfied in the present model, not only was the macroscopic surface energy density bounded by the lattice trapping limits, but it also was equal to the Griffith thermodynamic value. This explanation, however, requires further investigation, since the possibility exists that the microscopic and macroscopic thermodynamic surface energies are not equivalent.

It is interesting to note that the model is self-consistent as a stress corrosion model. A two step process is required to advance the crack by one atomic spacing. The crack-tip bond is first broken by a thermally activated process. The activation energy barrier for this process, ΔU_+, is easily calculated within the framework of the present model. Now, the strong linear bond which was originally one lattice spacing ahead of crack-tip is partially exposed to the corrosion environment and can be corroded by a chemical activation process to return the crack-tip status to its original configuration with the crack length advanced by one lattice spacing.

REFERENCES

1. HSIEH, C. and THOMSON, R., J. Appl. Phys., 44, No. 5, 1973, 2051.
2. LAWN, B. R., J. Mater. Sci., 10, 1975, 469.
3. ESTERLING, D. M., J. Appl. Phys., 47, No. 2, 1976, 486.
4. GRIFFITH, A. A., Phil. Trans. Roy. Soc., (London), A221, 1920, 163.
5. THOMSON, R., HSIEH, C. and RANA, V., J. Appl. Phys. 42, No. 8, 1971, 3154.
6. BLEKHERMAN, M. Kh. and INDENBOM, V. L., Phys. Stat. Sol. (a), 23, 1974, 729.
7. TYSON, W. R., CEKIRGE, H. M. and KRAUSZ, A. S., J. Mater. Sci., 11, 1976, 780.

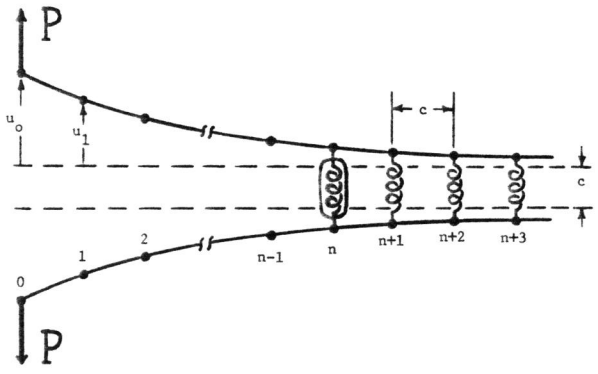

Figure 1 Quasi-One-Dimensional Lattice Model of a Crack

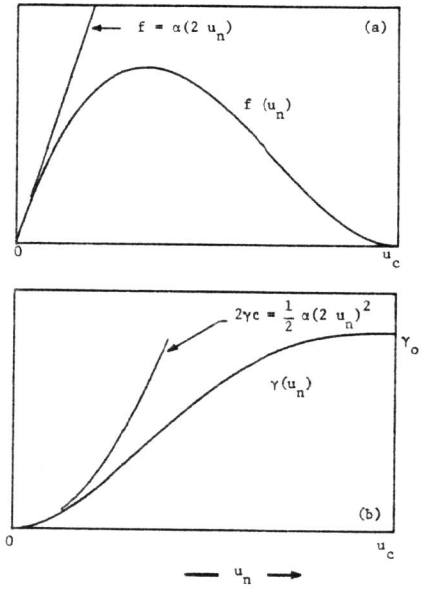

Figure 2 (a) Idealized Atomic Force Law
(b) Corresponding Surface Energy Density
Also Plotted are the Linear Elastic Relations

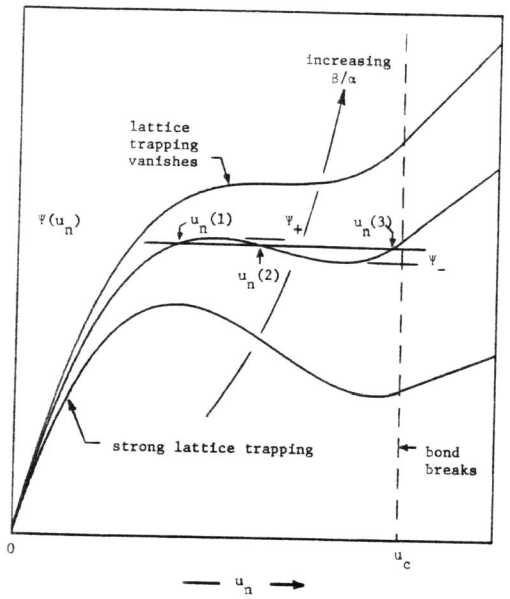

Figure 3 Graphic Solution of equation (7) for the Cohesive Force Law in Figure 2. The Three Ratios of β/α Vary Between Strong and Vanishing Lattice Trapping

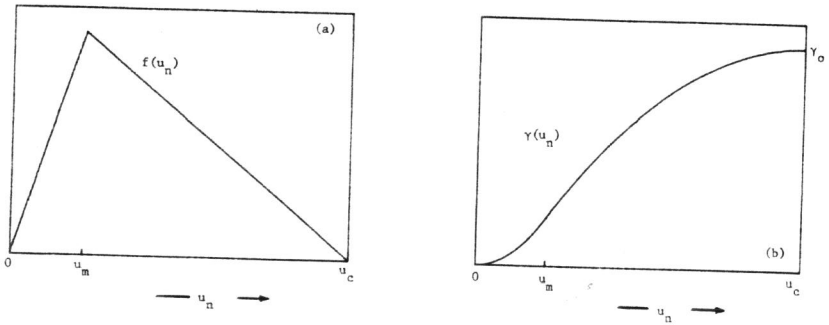

Figure 4 (a) Cohesive Force Law
(b) Corresponding Surface Energy Density