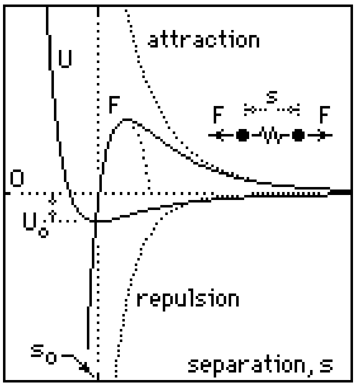
Crack growth kinetics

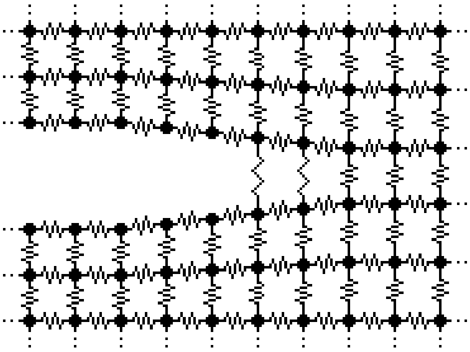
It was stated that Fracture Mechanics leads to a better understanding of the crack propagation mechanism than conventional fatigue arguments can provide, and without the need for the latter's empiricism. The preceding discussion has borne this out, but some aspects remain which were not explained satisfactorily :

- the rate and temperature dependency of fracture toughness
- the sigmoidal shape of the fatigue velocity curve which requires Paris' empiricism
- the effect of corrosion in exacerbating crack formation and early growth . . . etc.

Greater appreciation of crack growth will follow from examination at the atomic scale, as, when all said and done, it is at this level that temperature effects for instance make themselves felt.



The simplest model at the atomic level involves an isolated pair of interacting atoms which behaves as a non-linear spring. The force between the atoms, F, is the net effect of an attraction and short range repulsion, while the interaction energy, U, is represented by the area under the F-s characteristic (dU = F.ds). The force and energy vary with atom separation, s, as shown. At the *equilibrium* spacing, s_o, the net force vanishes and the energy exhibits a stable minimum, U_o - the work required to break the bond between the atoms, ie. to separate them to infinity.



A very simple model of a material's microstructure is a static lattice of such atom pairs, in which the influence of adjacent atoms only is recognised. ***Crack advance demands progressive breaking of the inter-atomic bonds*** and the formation of two free surfaces. An atom on such a surface has no neighbours on one side, and, as bond energies are negative, its energy exceeds that of interior atoms by U_o.

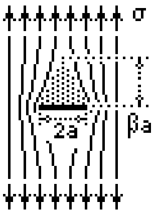
A sinusoidal approximation to the F-s characteristic near equilibrium is indicated on the sketch above. Since the stress and strain in the loaded material are $\sigma = F/s_o^2$ and $\varepsilon = (s-s_o)/s_o$, the stress/strain behaviour may be taken as : $\sigma = \sigma_{max} \sin(E\varepsilon/\sigma_{max})$ to ensure an initial slope of E. The energy density on each of the two surfaces of a crack - the surface tension, γ - is given by :

$$2\gamma = U_o/s_o^2 = (1/s_o^2)\int_{s_o}^{\infty} F\,ds = s_o\int_0^{\infty} \sigma\,d\varepsilon \approx 2s_o\sigma_{max}^2/E \quad \text{from this sinusoid.}$$

Rearranging this equation gives the fracture stress according to the model as $\sigma_{max} = \sqrt{(\gamma E/s_o)}$ - of the order of E/10 since γ is around $Es_o/100$ for many materials. Experimental values are often a couple of orders of magnitude below this, indicating severe shortcomings in this simple model.

In an attempt to explain this disparity, Griffith argued from an energy viewpoint, recognising that the impetus for crack extension is the energy balance between that absorbed in creating new surfaces and the elastic potential released by a larger crack. Thus, if a through-crack of length 2a occurs in a large plate of unit thickness, transverse to a background load, σ, then lines of force suggest that two triangular areas become stress-free, as indicated by the sketch. Letting the triangles' height be βa, then for half the crack :

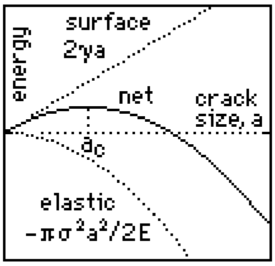
gain in surface energy = surface tension ∗ crack surface area = γ.2a
loss in elastic energy = specific elastic energy ∗ stress free area = $(\sigma^2/2E).\beta a^2$



A more sophisticated analysis reveals that β = π in plane stress. The net energy available for driving the crack is just the difference between these energy transfers - which depend on crack size as shown.

The net energy exhibits an unstable equilibrium at a certain critical crack size, a_c, given by :

$$d(2\gamma a - \pi\sigma^2 a^2/2E)/da = 2\gamma - \pi\sigma^2 a_c/E = 0 \quad \text{ie} \quad \pi\sigma^2 a_c = 2\gamma E.$$

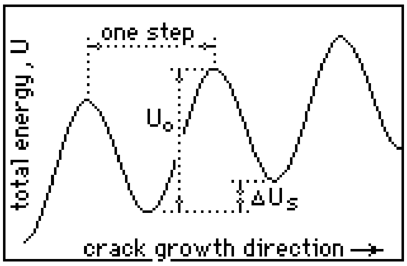


Cracks larger than the critical will grow out of hand, to reduce the system energy. The critical stress predicted by this equation is $\sigma_{max} = \sqrt{(2\gamma E/\pi a_c)}$ which is much more realistic than that of the static lattice model above, since $a_c >> s_o$. Despite the neglect of plasticity in this Griffith model (though plastic energy may be incorporated at the cost of extra complication), its focus on energy, rather than on 'elastic' phenomena at the crack tip, is of great significance.

Further modelling realism can be gained by reverting to the lattice above, but recognising that it is not static since all atoms are in continuous motion with random vibrations about their mean lattice positions. Concentrating on an isolated atom pair at the crack tip for simplicity, we have :

(**6**) $U = H + W$

where H is random vibrational energy which is perceived macroscopically as thermal energy,
W is energy due to work done by external loading on the pair, and
U is the total energy of the pair - clearly this also varies randomly.



As changes in vibrational amplitude sweep through the material with wavelike motion, sooner or later the atoms at the crack tip will be host to a crest which is large enough to result in U attaining a value of U_o, whereupon the bond breaks and the crack advances by one step, that is, by s_o. Diagrammatically, for the crack tip region, crack advance by one step needs sufficient energy to be input to hoist the total energy over the hill of height U_o into the next stable energy valley, where the energy level is increased by the energy inherent in the newly created free surfaces, ΔU_s.

One fundamental aspect of atomic behaviour is the possible reversal of processes, given appropriate directions and magnitudes of the random vibrations. Thus a pair of well separated atoms may be juxtaposed to create a bond and the crack is partially healed. Whilst this rebonding occurs on an atomic scale, macroscopic crack healing is uncommon (for reasons given below) though not unknown under controlled conditions.

These concepts may now be extended from the simple, essentially one-dimensional near-tip system consisting of a few isolated atom pairs, to the real three-dimensional lattice. It is possible to describe such a large multi-body system only in probabilistic terms, ie via statistical mechanics.

Rate theory, as used to describe transport processes - heat, mass and momentum transfer for example - is applicable also in the present context. The following account makes no claims to rigour, for this the literature must be consulted.

A crack advances by a series of steps; its average velocity may be expressed as :

$v = \lambda/\tau$

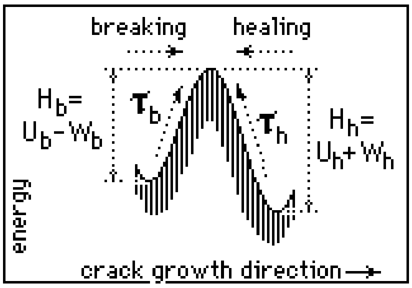
where λ is the average step length, an integral number of atomic distances, s_o
τ is the average waiting time between successive steps - in the literature, its inverse is referred to as a 'rate constant'.

One of the prime aims of fracture kinetics is to identify and quantify the individual processes which control any particular crack's behaviour. This is accomplished by evaluating the velocity peculiar to each process - one velocity might appertain to crack growth in a certain corrosive environment, another to a particular crack advance mechanism, and so on - then combining the velocities in a manner appropriate to the sequence of the processes, be they simultaneous, or sequential, or whatever. Since energy fluctuations govern any transport process at the atomic level, the corresponding waiting time must be dependent on and described statistically in terms of thermal energy, thus for the i'th process

(**7**) $\tau_i = (h/kT)\exp(H_i / kT)$

where k, h are Boltzmann's, Planck's constants ($1.38 * 10^{-23}$ J/K, $6.62 * 10^{-34}$ Js) respectively,
T is the absolute temperature (K), and
H_i is the thermal energy (J) level necessary to activate the i'th process.

It is apparent that temperature effects, which have been noted previously as playing a major role in fracture, are automatically included in (**7**). Further analysis demonstrates that temperature, in the usual range encountered, is significant only in the exponential term - variations of the (h/kT) premultiplier in (**7**) are swamped - and the equation takes Arrhenius' form. But it should be stressed that while Arrhenius equations are empirical, the equations developed here are based upon the known behaviour of real processes.



For bond breaking, ie for the crack growth process, from (**6**) :

$H_b = U_b - W_b$

in which the 'b' subscript refers to the breaking process. For the healing process (subscript 'h'), external work which tends to open the crack will oppose this process, so :

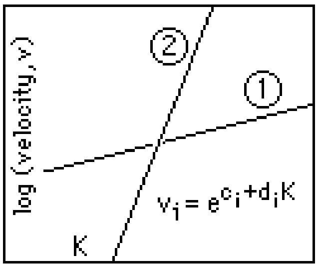
$H_h = U_h + W_h$ (ie. W is negative in (**6**))

The RHS of these last two equations replace H_i in (**7**) applied to the appropriate process. U_i takes the form of a constant energy magnitude representing the total energy crest - again appropriate to the process. W_i expresses the overall loading; in LEFM, this term would be a function of stress intensity, K, while plastic behaviour of the crack would necessitate a function of COD or the J-integral. The breaking and healing processes are shown diagrammatically above. Due to the senses of the work terms and consequent energy crests, breaking is more likely than healing.

Neglecting variations in the premultiplier of (**7**), and taking stress intensity as a measure of loading for example, the waiting time for the i'th process is of the form :

$\tau_i = \exp(a_i + b_i K)$; a_i, b_i being temperature dependent.

Within the context of LEFM therefore, the effects of isothermal crack growth promulgating processes are linear log(velocity) vs stress intensity plots, as shown here for the two separate processes, 1 and 2.



If the two processes are not independent, but interact in promoting growth, then their net effect depends upon whether they act simultaneously (parallel) or sequentially (serial). Thus, given the individual process velocities $v_1 = \lambda_1/\tau_1$, $v_2 = \lambda_2/\tau_2$ the velocity, v, when they act in concert is :

Simultaneous if the waiting period is $\tau = \tau_1 = \tau_2$, then the step size is

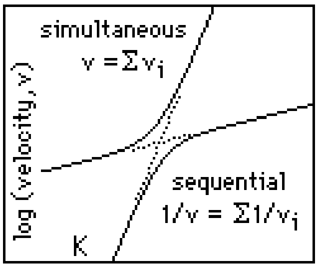
$\lambda = \lambda_1 + \lambda_2 = v_1.\tau + v_2.\tau$ and $= v.\tau$; so

(**8a**) $v = \Sigma v_i$

Sequential if the step size is $\lambda = \lambda_1 = \lambda_2$, then the waiting period is

$\tau = \tau_1 + \tau_2 = \lambda/v_1 + \lambda/v_2$ and $= \lambda/v$; so

(**8b**) $1/v = \Sigma 1/v_i$

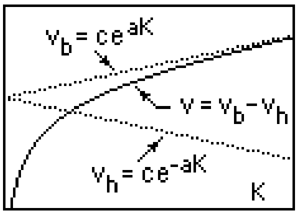


Plots of the velocity due to two interacting processes indicate that the larger of the two velocities controls when the processes are simultaneous; the lesser of the two velocities controls when the processes are sequential. Crack growth mechanisms involving an arbitrary number of known processes, simultaneous and/or sequential, can be described in a similar manner.

Crack growth processes only have just been considered - but what happens when breaking and healing processes act together ? Noting that these processes counteract one another, then, using (**7**), the net velocity is :

$$v \quad = v_b - v_h \;=\; \lambda(1/\tau_b - 1/\tau_h \;) \;=\; \lambda\,(kT/h)\,\{ \exp(- (U_b - W_b)/kT) - \exp(- (U_h + W_h)/kT) \}$$

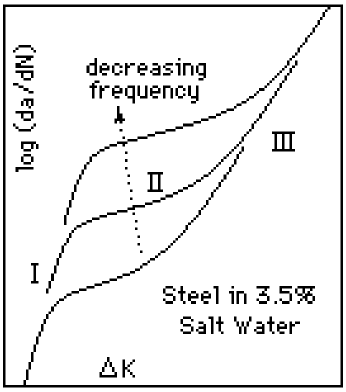
An unloaded crack will not grow. Since it is unloaded, $W_b = W_h = 0$, and the absence of macroscopic growth requires $U_b = U_h$ so that $v=0$. This does not imply that atomic bond breaking does not occur; it does, but bond healing progresses at the same pace, so there is no discernable growth. The sketch illustrates such a situation, with load characterised by stress intensity. As the 'load' grows, by increases in background stress or crack length, the effect of the healing process rapidly diminishes, and the net effect approaches that of a single bond breaking process. Such behaviour is typical at threshold.



An example of the application of fracture kinetics is shown. It involves isothermal fatigue test results of a certain steel in a corrosive environment, at various loading rates. The fatigue mechanism here apparently involves three processes, I, II and III, with I and III being unaffected by loading rate, whilst process II is rate-dependent. Processes I and II appear to be sequential; while processes II and III are simultaneous. The velocity due to the three can thus be formulated variously via (**8**) as :

$$\begin{aligned} v \quad &= 1/(1/v_I + 1/v_{II}) + v_{III} \qquad \text{or} \\ &= 1/(1/v_I + 1/(v_{II} + v_{III})) \;; \quad v_{II} \;=\; \text{function(frequency)} \end{aligned}$$

where each process velocity is of the form $v_i \;=\; \exp(a_i + b_i . \Delta K)$.



This example demonstrates the practical relevance of Fracture Kinetics - by its use it is possible to examine the individual processes involved in any given crack propagation mechanism, and to predict their combined effect. Fracture Kinetics is not merely a curve-fitting exercise, however the reasoned application of the technique will not be explored further here - the literature should be consulted for fuller details.

In conclusion, it has been said before, and is particularly relevant to Fracture Mechanics - a mathematical model is all very well, but engineering judgement remains a sine qua non. Non-mathematical considerations which have not been mentioned here include the very significant implications of metallurgy; the very real possibility of changing crack direction, or of mode or flaw interaction; the limitations of non-destructive testing; the difficulties associated with cumulative fatigue, and so on. For example how would one tackle a situation in which a crack spends its early days in the shadow of a stress concentration due to some geometric feature of the component; but on maturing, the crack's tip emerges from the shade ?