SURVEY OF RECENT WORK ON THE EFFECT OF THE ATOMIC STRUCTURE'S DISCRETENESS ON CLEAVAGE CRACK EXTENSION IN BRITTLE MATERIALS

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I. INTRODUCTION

The excellent pioneering work of Taylor [1], Orowan [2] and Polanyi [3] on the one hand, and Griffith [4] on the other, has led to the acceptance that a crystalline material's mechanical behaviour, and more particularly its plastic deformation and fracture characteristics, are crucially dependent on the mobility of dislocations and cracks in the material. Furthermore, it is also accepted that in developing an understanding of these processes, the simplest approach is to use a theoretical model in which the real material is represented by an elastic continuum. If such a model is used to describe a perfect dislocation, there is no resistance to the dislocation's movement, because in the real situation the crystal structure reverts to its original form following the passage of a perfect dislocation through the crystal. However, as Griffith clearly appreciated, movement of a cleavage crack tip is associated with a finite resistance even with a continuum model, since the original crystal structure is not retained after the passage of a crack tip. This is because atomic bonds break irreversibly, a process that is incorporated into the continuum description through the surface energy term γ; a crack tip is therefore analogous to an imperfect dislocation, with the surface energy corresponding to the fault energy associated with the imperfect dislocation's movement. Moreover, using thermodynamic arguments for a perfectly elastic solid, Griffith [4] showed that with prescribed values of γ and the applied stress σ, there exists a critical crack size below which a crack should contract, and above which it should extend unstably, eventually leading to complete failure of a solid. Thus only a crack having the critical size can be in equilibrium, which is of the unstable type, and the critical instability stress as a function of unstable crack size is shown schematically in Figure 1.

Use of a continuum-type model, as in the preceding discussion, does not really account for the atomic structure's discreteness, since the γ term merely averages out the atomic bond rupture processes, and does not incorporate the interplay between the breaking of individual atomic bonds in the vicinity of a crack tip. This neglect of the atomic structure's discreteness when using a continuum-type model was recognized over thirty years ago by Peierls [5] in the case of a dislocation. Using a model that allows for lattice discreteness within the crystal planes immediately adjacent to a slip plane and their interaction via an appropriate interatomic force law, the remainder of the material obeying the classic laws of linear infinitesimal elasticity theory, Peierls [5] and Nabarro [6] showed that discreteness can have a marked effect on the mobility of a straight dislocation, by virtue of the lattice providing periodic barriers as the dislocation moves from one equilibrium position to the next; the resistance to movement is greater the smaller the dislocation width, i.e. a quantitive measure of the spread of distortion along the slip plane.

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Subsequently, more detailed consideration has been given to the problem, and it is now generally accepted that there is a good correlation between a dislocation's mobility, its width, and also the type of atomic bonding. Thus, if the bonding is non-directional, as in an ideal metal which is less resistant to elastic shear than tension, a dislocation is wide and very mobile, whereas if the bonding is directional, as in a covalently bonded material which is more resistant to elastic shear than tension, a dislocation is narrow and its movement is difficult, being manifested in a high flow stress; these general conclusions are supported by experimental data, which has been admirably reviewed by Kelly [7].

Until quite recently, little consideration has been given to the way in which the discreteness of the atomic structure affects cleavage crack extension in a crystalline material. However, during the last few years, several investigations have led to the very important conclusion that stable crack tip configurations can exist in the sense that, within a range of crack tip stress intensifications, a crack can extend or contract in a stable manner as the stress is raised or lowered. This is because the atomic discreteness provides discrete barriers to a straight crack front as it moves through the crystal lattice, and is a behaviour that contrasts markedly with that of the Griffith-type continuum model in which the solid can sustain only cracks which are in unstable equilibrium. This phenomenon of 'lattice trapping' of a straight crack tip has been the focus of recent investigations, and this paper's purpose is to survey the main conclusions arising from this recent work, particularly with regard to the effect of the nature of the atomic bonding on the magnitude of the lattice trapping effect. It will be shown that lattice trapping is not likely to be responsible for brittle fracture energies, as determined via appropriate cleavage experiments, being very different to values of γ derived with the aid of an appropriate force law; the main significance is that lattice trapping allows a crack to propagate, within a range of crack tip stress intensifications, by a thermally activated process. This effect has been observed experimentally, as will be emphasized in the paper, but more importantly, the lattice trapping models provide a basis for understanding the effect of aggressive environments on cleavage crack extension, a problem that is of considerable technological significance.

II. SURVEY OF RECENT THEORETICAL WORK

The first investigation on the effect of the atomic structure's discreteness on brittle cleavage crack extension (i.e. cleavage without any accompanying plastic deformation in the form of dislocation generation or mobility) was that of Goodier and Kanninen [8]. Using a numerical procedure based on a Peierls-Nabarro type approach which allows for discreteness within the atomic planes bounding the cleavage crack, the remaining material obeying the classic laws of linear infinitesimal elasticity, they investigated a model appropriate for a two-dimensional cubic lattice, and determined the critical crack extension stress for a range of idealized force laws describing the interaction between the atoms across the cleavage plane. They showed, that (a) linear cut-off and sinusoidal force laws are both characterized by the existence of stable cracks which are absent in the Griffith continuum-type model, (b) the critical crack extension stress exceeded that given by the Griffith relation, using a value of γ relevant to the force law. These results provided the first demonstration of lattice trapping and of discreteness having an effect and providing a a resistance to the mobility of a straight crack front.

Thomson, Hsieh and Rana [9] used an analytical procedure to investigate a Peierls-Nabarro type model, and by introducing a series of simplifying assumptions, particularly concerning the crack tip profile, were able to relate the magnitude of the discreteness effect or lattice trapping effect, as reflected in the ratio of the lower and upper critical crack extension stresses (see Figure 2), with a parameter which is representative of the crack front width (i.e. a measure of the spread of distortion along the cleavage plane). This conclusion is analogous to that for a dislocation where the stress, usually referred to as the Peierls-Nabarro stress, to move a dislocation increases as the dislocation width decreases, width in this case being defined as the spread of distortion along the slip plane. Smith [10] has also used a Peierls-Nabarro approach that to some extent circumvents the limitations of Thomson, Hsieh and Rana's investigation; using a simple Mode III model (Figure 3) to simulate the Mode I situation, he systematically related the magnitude of the lattice trapping effect to the crack width, and confirmed Thomson, Hsieh and Rana's conclusions. Smith's approach is applicable for the range of force laws

$$\frac{p}{\mu} = \frac{2(w/a)}{1 + 16m^4(w/a)^4} \tag{1}$$

where p is the stress acting across the cleavage plane, 2w is the relative displacement of adjacent atoms in the two planes bounding the crack, a is the distance between these planes, b is the atomic spacing in the direction of crack propagation (the lattice is assumed to be two-dimensional), μ is the shear modulus, and m is a parameter (Figure 4). Maximum and minimum values of the applied stress σ arise respectively when $\varepsilon = 0$ and $b/2$ (Figure 3), their magnitudes for a macroscopic crack of length 2c being

$$\sigma_{max} = \left[\frac{\mu^2 a}{2m^2 c} \coth\left(\frac{\pi a}{2b}\right)\right]^{1/2} \tag{2}$$

and

$$\sigma_{min} = \left[\frac{\mu^2 a}{2m^2 c} \tanh\left(\frac{\pi a}{2b}\right)\right]^{1/2} \tag{3}$$

whereupon

$$\frac{\sigma_{min}}{\sigma_{max}} = \tanh\left(\frac{\pi a}{2b}\right) \tag{4}$$

Stable equilibrium atomic configurations exist between the stress limits σ_{min} and σ_{max} and the ratio $\sigma_{min}/\sigma_{max}$ may be regarded as a measure of the lattice trapping effect, i.e. the effect is large when this ratio is small and small when the ratio approaches unity. Furthermore, the instability condition associated with a purely continuum model, and which corresponds to the Griffith relation, is

$$\sigma_{GRIFF} = (4\mu\gamma/\pi c)^{1/2} \tag{5}$$

where the surface energy γ relevant to the range of force laws (1) is

$$\gamma = \int_0^\infty pdw = \frac{\pi\mu a}{8m^2} \qquad (6)$$

It must be remembered that expressions (2) - (5) refer to a Mode III model, and μ should be replaced by $\mu/(1 - \nu)$ when they are applied to the Mode I situation, ν being Poisson's ratio. The crack front width is defined to be that distance from the crack tip along one of the bounding planes where the displacement is a half of the crack tip value. This width is calculated to be 15a/16, whereupon expressions (2) and (4) show that the magnitude of the lattice trapping effect and the critical crack extension stress both increase as the crack front width decreases. These conclusions and indeed those of Thomson, Hsieh and Rana are applicable only for a specific range of force laws (see Figure 4 in the case of Smith's analysis); consequently such analyses are somewhat limited in their scope, particularly if the effect of force law and the type of atomic bonding on the lattice trapping effect are to be assessed. To attain this objective the approach must be broadened, and as a first step useful conclusions may be reached merely by using very simple physical reasoning procedures [11]. As already indicated, dislocation width can be correlated with the type of atomic bonding, a relation that may be seen by examining an idealized model of an edge dislocation. In Figure 5b where the material's elastic shear resistance is low and the planes normal to the slip plane are flexible, the dislocation is wide, while in Figure 5a where the elastic shear resistance is high and the planes normal to the slip plane are not so flexible, the dislocation is narrow. Similar simple physical arguments may be used for a crack, by removing the associated extra half-plane of atoms associated with the dislocations in Figure 5. Thus if the elastic shear resistance is low, the atomic planes parallel to the crack are flexible and the crack front width is small, while if the elastic shear resistance is high, these planes are fairly rigid and the crack front width is large. Taken together with the correlation of the lattice trapping effect with crack front width arising from the Peierls-Nabarro type analyses [9, 10], these simple arguments suggest that the trapping effect is greatest when a material's elastic shear resistance is low and least when this resistance is high.

It is obviously desirable to confirm this viewpoint using more rigorous methods, and with this in mind, Thomson, Hsieh and Rana [9] examined a very simple model (Figure 6), which is similar to the Frenkel-Kontorova model [12] of a dislocation; the planes bounding a crack are represented by chains of atoms that are linked by two types of spring: lateral bendable springs link the atoms within each chain, while the two chains are attached by transverse stretchable springs, both types of spring being linearly elastic. The transverse springs rupture upon the attainment of a critical displacement or tensile force, while the applied stress is represented by the force P applied to the terminal atoms in the chains, and the crack surface by atoms whose transverse bonds have ruptured; with this model a material's shear and tensile elastic resistances are simulated by respectively the bending and transverse stiffnesses of the two types of spring. Lattice trapping is observed with this model, its magnitude increasing with the ratio stretchable spring stiffness: bendable spring stiffness, in accord with the conclusion reached by simple physical arguments, since the bending stiffness may be associated with a material's elastic shear resistance.

However, with this model, Thomson, Hsieh and Rana did not take the intermediate step of quantitatively correlating the lattice trapping effect with crack front width. Accordingly, Smith [11] considered an even simpler

Frenkel-Kontorova type crack model, which enables the magnitude of the trapping effect, crack front width and the type of atomic bond, as reflected in a material's elastic characteristics, to be systematically related; furthermore, and most importantly, use of such a simple model enables its analysis to be readily extended, without introducing serious mathematical complications, so as to simulate different force laws describing the rupturing of the atomic planes bounding the cleavage crack. With Smith's simulation model (Figure 7), the atomic planes bounding a crack are again represented by two chains of atoms but the major difference as compared with the Thomson, Hsieh and Rana model is that the atoms are constrained to move in the direction of the chains rather than transverse to them; the applied stress is simulated by forces applied to the terminal atoms. Each chain is an aggregate of identical springs having an initial length b, these springs being linearly elastic with a tensile stiffness M. Furthermore, each atom in a chain interacts with its neighbour in the other chain, the two chains are a distance a apart, such that the force tending to restore an atom to its original position is $R(\bar{u}) = L\bar{u}/a$, where $\bar{u}$ is the relative displacement of neighbouring atoms in the two chains; this restoring force is assumed to be operative until the relative displacement attains some critical value beyond which the restoring force is zero, thereby simulating the 'linear bond-snapping' that is characteristic of the Thomson, Hsieh and Rana model [9]. Since the atoms move in the direction of the chains rather than transverse to them, their equilibrium positions are governed by a second order difference equation rather than a fourth order equation, and this simplifies the mathematical analysis in comparison with that of Thomson, Hsieh and Rana. The shear and tensile elastic resistances of the actual material are simulated by respectively the stiffness M of the springs within a chain and the slope L of the linear cut-off force law. Equilibrium of the atomic configuration is shown to be possible when $P_1 < P < P_u$ where

$$\frac{P_1}{\left(\frac{Lq}{2}\right)} = \sqrt{1 + \lambda} - 1 \qquad (7)$$

$$\frac{P_u}{\left(\frac{Lq}{2}\right)} = \sqrt{1 + \lambda} + 1 \qquad (8)$$

whereupon

$$\frac{P_1}{P_u} = \frac{\sqrt{1 + \lambda} - 1}{\sqrt{1 + \lambda} + 1} \qquad (9)$$

where $\lambda = 2Ma/Lb$ and $R(u) = 0$ when $u > qa/2$ with $u = \bar{u}/2$ being the displacement of an atom. It is instructive to relate these results with those obtained by assuming the chains to be continua. In this case it is readily shown that $P_c = qaM/b\sqrt{\lambda}$; Figure 8 shows how P_1, P_u and P_c are affected by the type of atomic bonding, as reflected in the magnitude of λ. Before entering a detailed discussion of these results, however, the critical stresses will be related to the crack front width. Again, defining the crack front width w as that distance from the crack tip at which the displacement is half the displacement at the crack tip, it is found that w is equal to $0.35\ b\sqrt{\lambda}$.

The magnitude of the lattice trapping effect is reflected in the ratio of P_1/P_u, and it therefore immediately follows from the relation $w = 0.35\ b\sqrt{\lambda}$

and relation (9) that if λ is small, w is small and the lattice trapping effect is large, whereas if λ is large, w is large and the lattice trapping effect is small. Consequently, with the real as distinct from the model situation, if the elastic shear resistance of a material is low (reflected in low values of M and λ) the crack front is narrow and the lattice trapping effect is large, while if the elastic shear resistance is high (reflected in high values of M and λ) the crack front is wide and the lattice trapping effect is small. These conclusions are entirely in accord with those arising from simple physical reasoning procedures and also with those obtained by Thomson, Hsieh and Rana for their more sophisticated Frenkel-Kontorova model; as indicated previously, these latter workers correlated a material's elastic shear resistance with the magnitude of the lattice trapping effect but did not develop a quantitative link with the crack front width.

The one-dimensional analyses reviewed to date have used a linear cut-off force law and have therefore simulated 'linear bond-snapping'; it is clearly desirable to extend the discussion to a wider range of force laws with the objective of correlating, in a fairly general quantitative manner, the effect of the non-linear characteristics of the force law with the magnitude of the lattice trapping effect. Smith's one dimensional model is ideal for such a study, in view of its mathematical simplicity. Thus consider the force law for which $R(u) = Lq$ for $qa/2 < u < (q + t)a/2$ while $R(u) = 2Lu/a$ for $0 < u < qa/2$ (Figure 9). Detailed analysis [13] for this force law shows that provided

$$\frac{t}{q} < \frac{2}{\lambda}\left[\sqrt{1 + \lambda} + 1\right] \tag{10}$$

equilibrium of the system is possible when $P_l < P < P_u$ where

$$\frac{P_e}{\left(\frac{Lq}{2}\right)} = \left(1 + \frac{t}{q}\right)\left(\sqrt{1 + \lambda} - 1\right) \tag{11}$$

and

$$\frac{P_u}{\left(\frac{Lq}{2}\right)} = \left(1 + \frac{t}{q}\right)\left(\sqrt{1 + \lambda} - 1\right) + 2 \tag{12}$$

whereupon

$$\frac{P_l}{P_u} = \frac{\left(1 + \frac{t}{q}\right)\left(\sqrt{1 + \lambda} - 1\right)}{\left(1 + \frac{t}{q}\right)\left(\sqrt{1 + \lambda} - 1\right) + 2} \tag{13}$$

and is a measure of the magnitude of the lattice trapping effect. This result clearly shows that the lattice trapping effect becomes more pronounced as the force law becomes sharper (i.e. t/q becomes smaller) and also as λ becomes smaller (i.e. as the ratio stretchable bond stiffness: bendable bond stiffness becomes larger in the actual material). Expression (13) is valid provided the force law is sufficiently sharp that t/q is less than the value given by expression (10); the upper limits of t/q for various values of $\lambda = 2Ma/Lb$ are shown in Table 1, which therefore gives an indication of the range of force laws for which expression (13) is valid. Suppose, for example, that $\lambda = 1$ when the broadest force law for which (13) is valid is that for which t/q = 4.83. At this limit P_l/P_u is equal to 0.54, decreasing to 0.17 when t/q = 0, a decrease that illustrates in dramatic form the effect of force law sharpness in providing a marked

lattice trapping effect. When the inequality sign in (10) is reversed, the situation becomes more complicated, but a detailed consideration of the system's equilibrium again shows that the magnitude of the lattice trapping effect increases (i.e. P_l/P_u decreases) as the force law becomes sharper (i.e. t/q becomes smaller). Indeed, whereas both P_u and P_l increase with t/q, assuming q remains constant, the difference between them is always Lq, as is also evident by examining the detailed results for small t/q values (i.e. those satisfying (10)).

Now consider the force law (Figure 10) for which $R(u) = [Lq/ta][(t+q)a-2u]$ for $qa/2 < u < (q+t)a/2$ while $R(u) = 2Lu/a$ if $0 < u < qa/2$. Detailed analysis for this force law shows that provided relation (10) is satisfied, equilibrium atomic configurations are possible when $P_l < P < P_u$ where

$$\frac{P_l}{\left(\frac{Lq}{2}\right)} = \left(1 + \frac{t}{q}\right)\left(\sqrt{1 + \lambda} - 1\right) \tag{14}$$

and

$$\frac{P_u}{\left(\frac{Lq}{2}\right)} = \left(\sqrt{1 + \lambda} + 1\right) \tag{15}$$

whereupon

$$\frac{P_l}{P_u} = \frac{\left(1 + \frac{t}{q}\right)\left(\sqrt{1 + \lambda} - 1\right)}{\left(\sqrt{1 + \lambda} + 1\right)} \tag{16}$$

an expression which clearly shows that the lattice trapping effect is more pronounced the steeper the descent from the force law maximum, i.e. as t/q becomes smaller, and also as λ becomes smaller. Expression (16) is valid provided the descent from the force law maximum is sufficiently rapid that t/q is less than the value given by expression (10), and again the upper limits of t/q for various values of t/q are shown in Table 1, which therefore indicates the range of force laws for which (16) is valid. At the limits, P_u and P_l are equal and there is no lattice trapping. However, this state of affairs is unique since with t/q values slightly in excess of the critical value, P and P_l are different and there is a lattice trapping effect; the maximum force (P_u) situation is associated with an atom being subject to maximum restraint and another atom with a displacement on the decreasing part of the force law, while the minimum force (P_l) situation is associated with an atom just having lost its restraint with another atom having a displacement on the decreasing part of the force law. As t/q increases, there are other unique values of t/q for which $P_u = P_l$ and there is no lattice trapping; each of these unique situations corresponds to the existence of equilibrium atomic configurations with an atom in the force law maximum position, another having just lost its restraint, and with other atoms having displacements associated with the decreasing part of the force law.

All the models reviewed in this section to date, are idealized to the extent that they are of the Peierls-Nabarro type or are one-dimensional simulation models; such models allow for the atomic structure's discreteness only within the atomic planes that bound a cleavage crack. The simplicity of the models, particularly those of the one-dimensional type, has enabled the

interplay between a variety of factors to be readily appreciated with a minimum of mathematical analysis. The conclusions reached from the simple models are supported by a limited number of investigations of more realistic models. As regards the effect of the shape of the non-linear part of the force law, Esterling [14] has examined the stability of a two-dimensional Mode I crack in a simple cubic lattice within a lattice statics approximation, investigating the effect of various idealized nearest neighbour force laws for the case where Poisson's ratio is zero; Esterling's analysis therefore extends a similar analysis due to Hsieh and Thomson [15], who specifically considered the force law appropriate to linear bond-snapping. Inspection of Esterling's results clearly shows that the lattice trapping effect is more marked the steeper is the descent of the force law from the maximum to the zero restraint position, and this accords with the predictions of the simple one-dimensional simulation model. Moreover, if the maximum is maintained at a constant value, the greatest effect is on the lower limiting crack tip stress intensification, a result which clearly agrees with the predictions of equations (14) and (15).

Sinclair has examined the behaviour of a two-dimensional Mode I (111) cleavage crack in silicon with a straight edge parallel to the [0$\bar{1}$1] direction, using an atomistic computer simulation model. Several non-central interatomic force laws were investigated, all being matched to the elastic constants and the cohesive energy, but varying in shape at long-range; a short-ranged force law gives a more pronounced trapping effect than a long-ranged law. This result agrees with the predictions from Smith's simple one-dimensional model, for if the general force law in Figure 10 is considered for two specific laws characterized by the same areas under the curves, tq has the same value (say ε) for the two laws, if the area under the increasing linear portions is neglected. Consequently relation (13) becomes

$$\frac{P_1}{P_u} = \frac{\left(1 + \frac{t^2}{\varepsilon}\right)\left(\sqrt{1+\lambda} - 1\right)}{\left(1 + \frac{t^2}{\varepsilon}\right)\left(\sqrt{1+\lambda} - 1\right) + 2} \qquad (17)$$

whereupon P_1/P_u decreases with t; thus a short-ranged force law (small t) shows a greater lattice trapping effect than a long-ranged law, which is precisely Sinclair's result.

III. DISCUSSION

As indicated in the Introduction, a particular aim of investigations concerned with the lattice trapping effect is to relate the critical crack extension stress, with discreteness taken into account, to the critical extension stress predicted by the classic Griffith theory, which is continuum based and incorporates the surface energy γ of the particular material under consideration. If this latter procedure is applied to the simple one-dimensional model, the simulated crack extends when the applied force P attains the critical value P_c given by

$$P_c = \sqrt{\frac{\lambda L}{a} \int R(u)\,du} \qquad (18)$$

where R(u) is the force law, and the integration limits are zero and that value of u for which the restraining force becomes zero. For the

force law in Figure 9, it immediately follows that:

$$\frac{P_c}{\left(\frac{Lq}{2}\right)} = \sqrt{\lambda\left(1 + \frac{2t}{q}\right)} \qquad (19)$$

when comparison with expressions (11) and (12) shows that $P_1 < P_c < P_u$ irrespective of the value of t/q; in other words, the Griffith force lies between the force limits within which equilibrium configurations are possible with the discrete atom model. The same conclusion is also valid for the force law in Figure 10, for then

$$\frac{P_c}{\left(\frac{Lq}{2}\right)} = \sqrt{\lambda\left(1 + \frac{t}{q}\right)} \qquad (20)$$

and the conclusion follows by comparison with expressions (14) and (15). Against this background it is worth looking very carefully at the results obtained by Esterling [14]. He showed that the Griffith stress was bounded by the upper and lower critical stresses for only a few of the wide variety of force laws studied; for most laws, the Griffith stress was less than the lower critical stress. The laws for which the Griffith stress is bounded are those where the descent from the force law maximum to the zero restraint position is particularly steep; laws characterized by a tail prior to zero restraint are associated with a Griffith stress which is less than the lower critical value. This suggests that if a force law with a similar tail is used with the simple one-dimensional model, a similar effect ought to be observed. This is indeed the case, since it is easily demonstrated that with the artificial force law shown in Figure 11, with $t/q < 2\,[\sqrt{1+\lambda} + 1]/\lambda$ (i.e. relation (10)), P_1 and P_u have the same magnitudes as for the dotted force law (i.e. the same law as that shown in Figure 10), and these are given by relations (14) and (15); furthermore, for a range of λ values there is a corresponding range of t/q values for which P_c is less than P_1. Thus when the force law has a pronounced tail prior to the zero restraint position, it is possible for P_c to be less than P_1, a result that accords with Esterling's behaviour pattern.

The results from the various investigations reviewed in the preceding section, strongly suggest that for a two-dimensional cleavage crack subject to Mode I loading conditions, the magnitude of the lattice trapping effect, as reflected in the ratio of the upper and lower crack tip stress intensification limits between which stable cleavage cracks can be sustained within a brittle solid, is greater:

(a) the larger is the ratio stretchable bond elastic stiffness: bendable bond elastic stiffness
(b) the narrower is the force law describing the tensile rupturing of atomic bonds across a cleavage plane
(c) the steeper is the descent of the force law from the maximum to the zero restraint position.

In viewing conclusions (a), (b) and (c), it is therefore quite clear that maximum lattice trapping of a straight crack front should be observed with a narrow force law, a steep descent from the maximum to the zero restraint position, and the larger the ratio stretchable bond elastic stiffness: bendable bond elastic stiffness, with the latter parameter likely to be having the dominant effect. However, if a particularly low bendable bond elastic stiffness is the cause of this ratio being large, it will at the same time promote dislocation activity. Whether or not dislocation gener-

ation and mobility does actually occur in the vicinity of a crack tip, is an aspect of the cleavage problem that is beyond the scope of the simple models described in the preceding section; however, it is a most important problem and has received detailed consideration (e.g. [17], [18]), for it is central to the classification [19, 20] of materials into ductile and brittle categories. As an example of a specific study, Gehlen, Hahn and Kanninen [21] have studied the configuration near the tip of a straight {100} cleavage crack in alpha iron using an atomistic computer simulation approach, and showed that the extension stress was appreciably in excess of the Griffith value, with dislocation nucleation being observed.

Because dislocation activity is easy in materials with a low elastic shear resistance (i.e. in the extreme case, those having an ideal metallic bond), it means that where brittle crystalline materials are concerned, very special circumstances indeed are likely to be required to give sufficiently strong lattice trapping of a straight crack front, for it to be reflected in the experimentally measured crack extension stress being markedly in excess of that predicted by the Griffith relation. Accordingly, use of the Griffith approach, based on a continuum-type model and a value of γ relevant to the force law describing the behaviour of the atoms along the cleavage plane, should suffice for most practical purposes.

However, as emphasized in several papers [15, 16, 22, 23], the main consequence of lattice trapping is that it is responsible for what is known as the 'creep mobility of cracks'. Thus, analogous to the behaviour of dislocations, it should be possible for a crack to propagate slowly, with the aid of thermal fluctuations, by the nucleation and movement of kinks along a crack front, rather than by the forward propagation of the entire crack front. Experimental evidence for thermally activated cleavage crack growth is provided by the observations of Wiederhorn, Hockey and Roberts [24] on $\{10\bar{1}0\}$ cleavage cracks in sapphire tested in vacuum. Figure 12 shows the critical stress intensity factor for rapid cleavage fracture as a function of temperature, while Figure 13 shows the stress intensity factor - crack velocity variation at specific temperatures. Such observations clearly suggest that, for sapphire, cleavage cracks can propagate in vacuum by a thermally activated process, and this is powerful support for the existence of lattice trapping. Similar experimental results have been obtained [25] for some glasses, where the degree of local order in the crack tip vicinity is presumed to be sufficient for the processes discussed in this paper to become operative.

The behaviour of a kinked crack front in alpha iron has been investigated via an atomistic simulation approach by Kanninen and Gehlen [23], and in silicon by Sinclair [16], and also via a lattice statics approach by Esterling [14] in a general material for a variety of idealized nearest neighbour force laws. As with a straight crack front, there is a range of crack tip stress intensification within which a crack kink is lattice trapped, but this range is appreciably narrower than the corresponding range for a straight crack front. More importantly, Esterling found that the widths of the ranges in which a crack kink and a straight crack front are lattice trapped increase and decrease together, with the kink limit stresses always lying between the straight crack limit stresses. Thus, although this paper has concentrated on the lattice trapping of a straight crack front in terms of the force law and the nature of the atomic bonding, the conclusions should nevertheless be equally applicable to the trapping of an irregular crack front, and therefore very relevant to thermally activated cleavage crack extension. Interest in this phenomenon is reflected in the recent series [15, 16, 22] of analyses concerned with crack kink kinetics; such analyses have followed similar lines to those used

more than a decade earlier for dislocation kinks. A major reason for this interest is that an understanding of thermally activated cleavage crack growth provides a basis [22] for explaining the effects of aggressive environments on cleavage crack extension in brittle materials, a problem that is of considerable technological importance. It is the author's opinion that this research area will receive extensive study, both theoretical and experimental, in the next few years.

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Table 1 - The Limits of t/q for which expression (13) is valid, for various values of $\lambda = 2Ma/Lb$

λ	t/q
0	∞
0.50	8.89
1	4.83
2	2.73
3	2.00
8	1.00

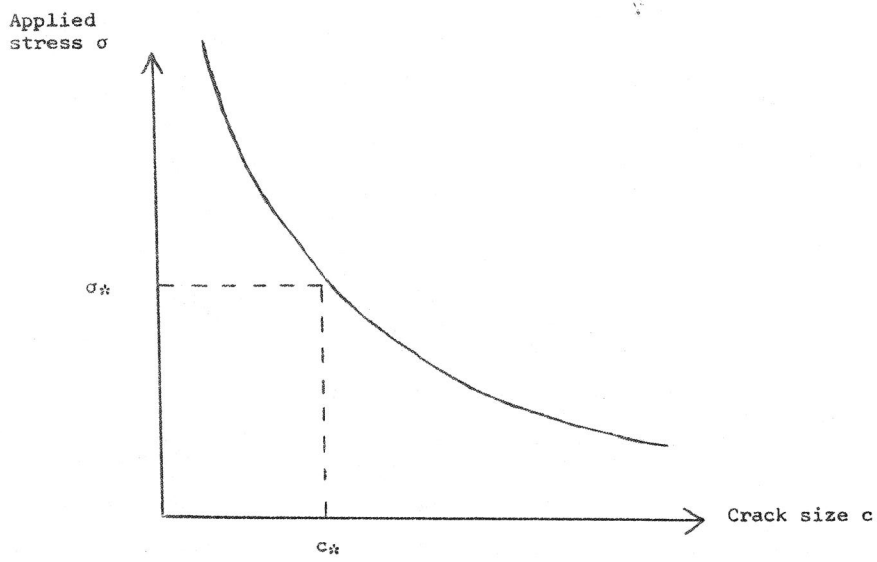

Figure 1 - The relation between the critical applied stress σ required to extend a crack as a function of its length, as predicted via the Griffith continuum-type model; the relation follows a $\sigma \propto 1/\sqrt{c}$ form. For a given applied stress σ_*, a crack of length $c > c_*$ extends, while a crack of length $c < c_*$ contracts.

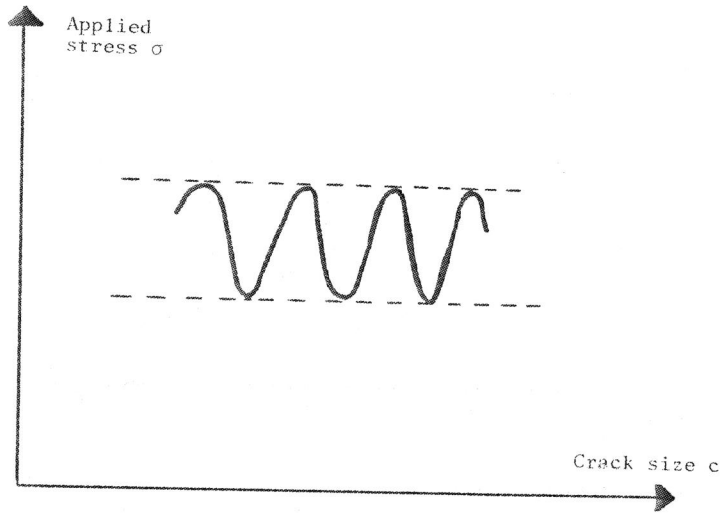

Figure 2 - The schematic relation that exists between the applied stress and stable crack size, when atomic discreteness is taken into account; it is important to note that the distances between the peaks and troughs are of atonic dimensions, which are of course very small in comparison with the macroscopic crack size.

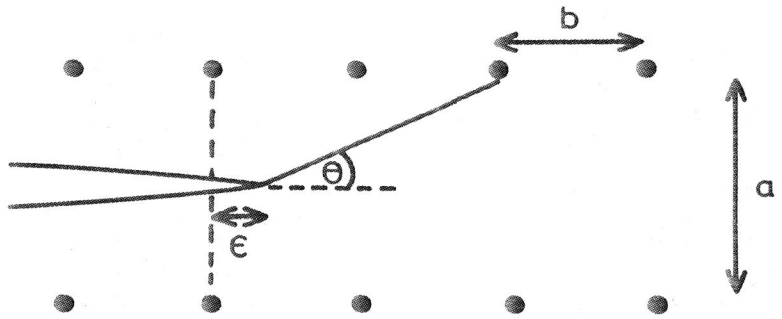

Figure 3 - Discrete atoms in the vicinity of a crack tip in Smith's Mode III Peierls-Nabarro type model. The atoms in the upper plane are displaced with respect to those in the lower plane as the crack tip moves from left to right.

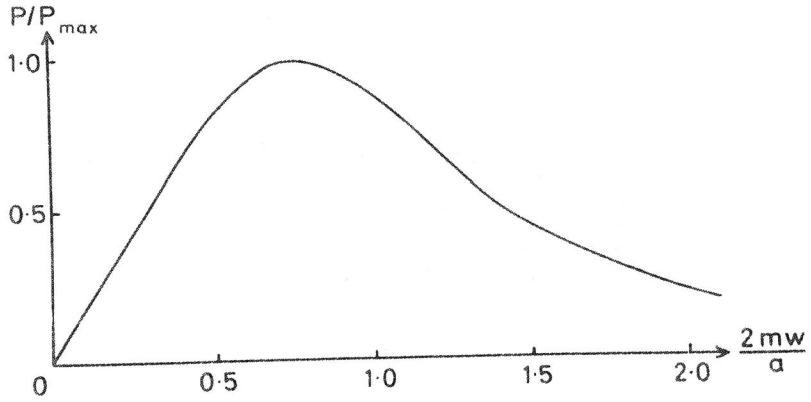

Figure 4 - Force law represented by relation (1) with $P_{max} = (3\mu/4m)(1/3)^{1/4}$

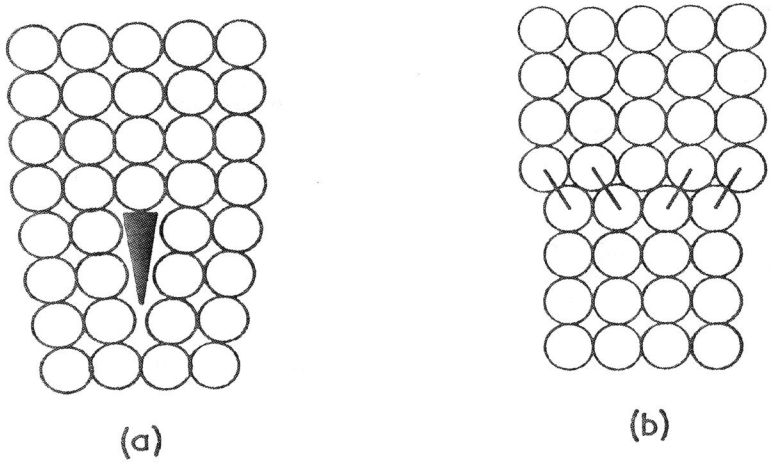

Figure 5 - Idealized models: (a) a narrow edge dislocation, (b) a wide edge dislocation

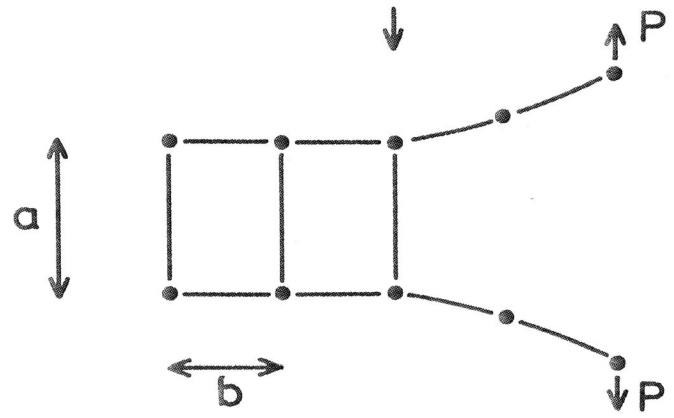

Figure 6 - Thomson, Hsieh and Rana's one-dimensional model [9] of the cleavage process

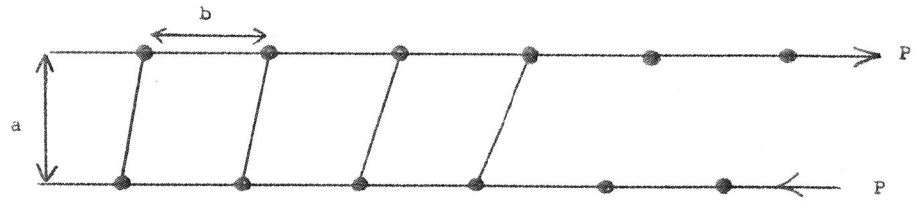

Figure 7 - Smith's one-dimensional model [11] of the cleavage process

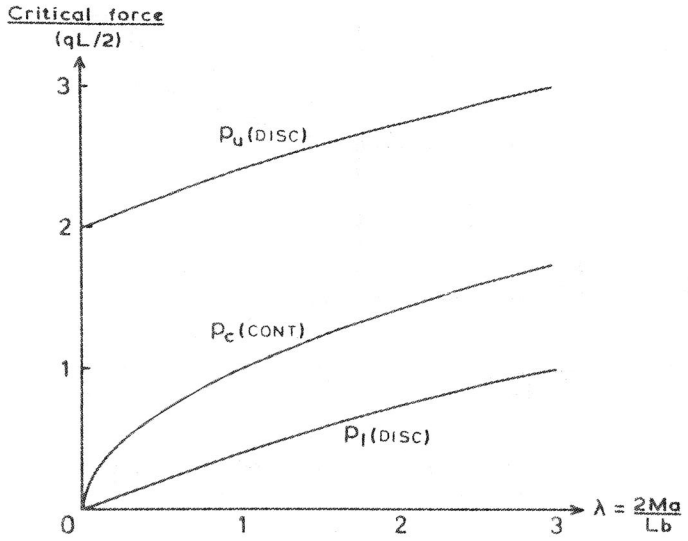

Figure 8 - Upper and lower bounds P_u and P_l for the crack extension force in Smith's one-dimensional discrete atom model, compared with the value P_c for a continuum model; the results are for a linear cut-off force law.

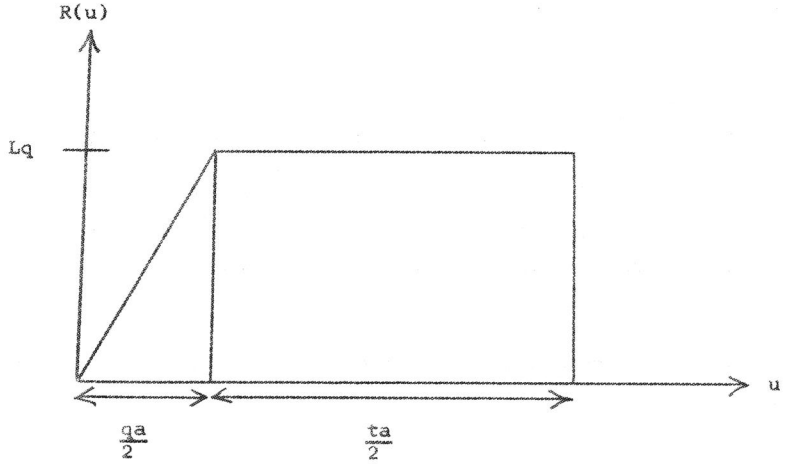

Figure 9 - The force law leading to expressions (11) - (13); u is the displacement of an atom, and R(u) is the restraining force due to its interaction with an adjacent atom in the neighbouring chain

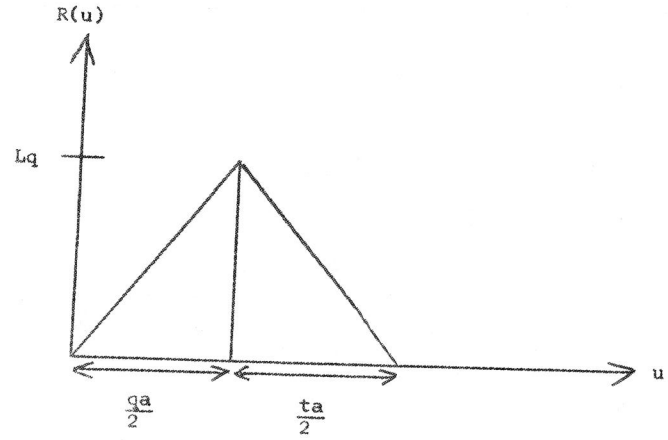

Figure 10 - The force law leading to expressions (14) - (16); u is the displacement of an atom, and R(u) is the restraining force due to its interaction with an adjacent atom in the neighbouring chain

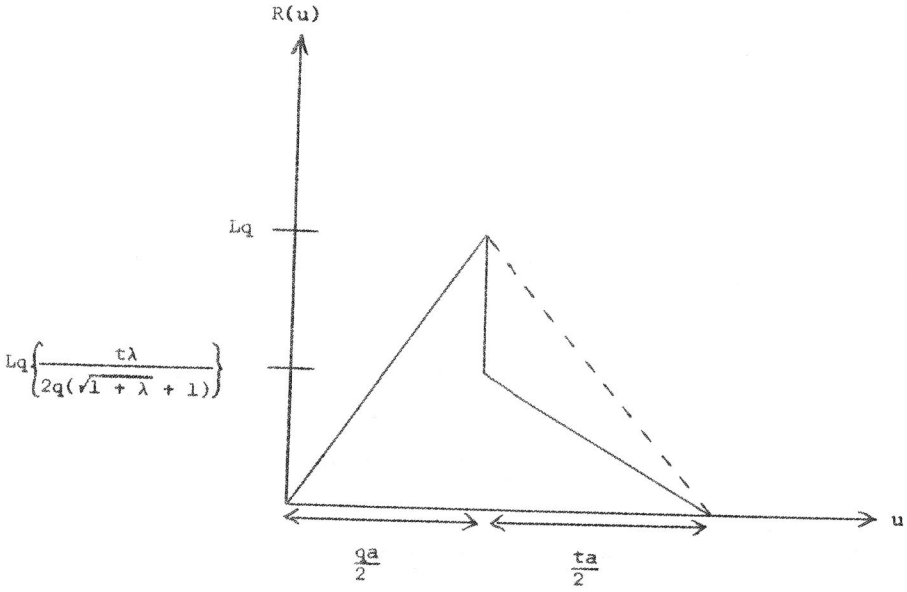

Figure 11 - The force law (full lines) used to show that it is possible for P_c to be less than P_l with the simple one-dimensional model

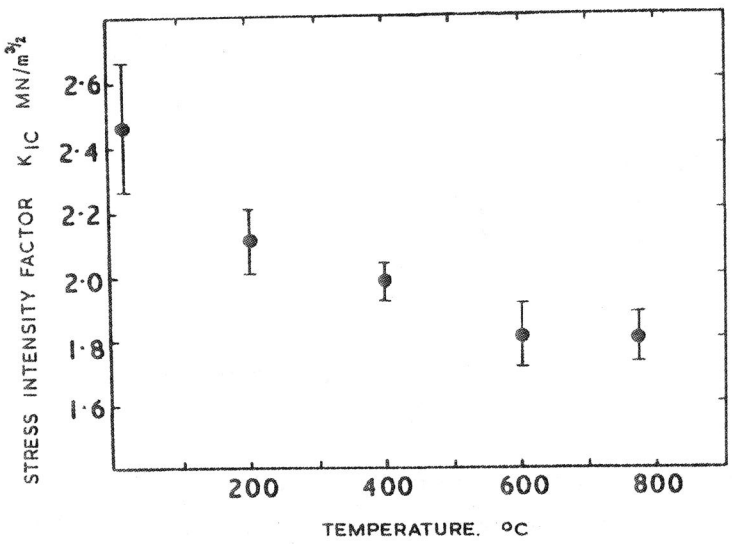

Figure 12 - The critical stress intensity factor for rapid cleavage fracture of sapphire as a function of temperature; the brackets give the standard deviation of the data which was obtained by Wiederhorn, Hockey and Roberts [24].

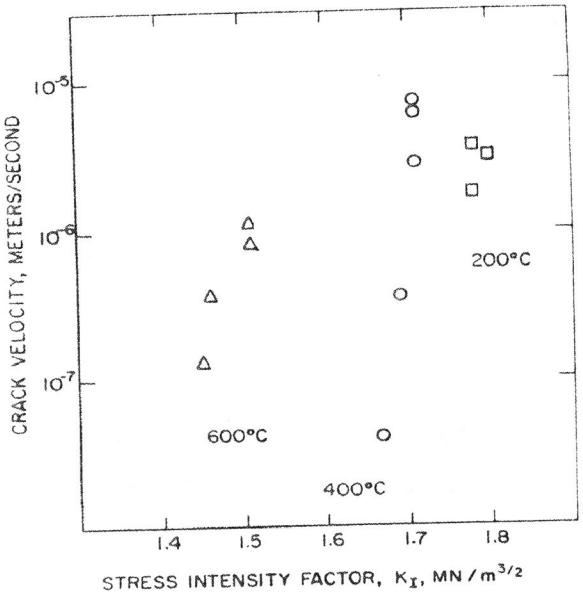

Figure 13 - The stress intensity factor - crack velocity variation for sapphire at specific temperatures [24].