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COMPUTER MODELING OF CRACKS*

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ABSTRACT

The theoretical techniques used in modeling cracks in crystalline lattices are reviewed. It is shown that there is generally a trade-off between sample size and realistic interatomic potentials. Infinite discrete one and two-dimensional lattices can be handled by the methods of lattice statics, but only with simple unrealistic potentials. In the hybrid lattice statics models a very small crystalline region, where the calculations are done with realistic potentials, is imbedded in an infinite elastic continuum. In this approach the boundary matching between the two regions is the difficulty. At the other end of the scale, molecular dynamic techniques can be used on an unconstrained system of a "large" number of atoms interacting with a reasonably realistic interatomic potential (this is the only way dynamic simulations have been done so far). Here, of course, the question is how "large" is large enough to simulate the behavior of the corresponding infinite system.

The results of a recent molecular dynamic study of a two-dimensional triangular Lennard-Jones system of about 10,000 atoms are described. Static calculations on this system show very little lattice trapping in contrast to the often quoted results of lattice statics models. Using molecular dynamics, the properties of the system, with and without a crack, are understood sufficiently quantitatively to allow extrapolation to infinite

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size. At 10,000 atoms size effects are small enough to render the simulation highly reliable. It is also shown that when lattice statics and hybrid lattice statics calculations are performed using realistic, long-range potentials, lattice trapping is small.

Dynamic simulations at constant applied stress show an intricate interplay between brittle crack propagation and the tendency to form dislocations. At low stresses the behavior is brittle while dislocation generation and crack blunting is observed at elevated stresses. The velocity of crack propagation has also been studied using a constant applied strain. A constant velocity is attained relatively soon after the crack has begun to propagate at both constant applied stress or strain. At constant strain, the changes in elastic energy and in the modulus during propagation are in good agreement with a simplified elastic theory for a non-linear solid. The change in kinetic energy during propagation has the functional form suggested by Mott. The credibility of the various models is discussed.

I. INTRODUCTION

Modeling involves two basic steps: 1) the construction of a model incorporating the key physical features of the system, and 2) the calculation, analytically or by computer techniques, of the physical characteristics of interest. If step 2 is carried out to high accuracy, which can now be done with the availability of modern computers, then the limitations of the results are those of the model itself. Modeling can lead to very significant insights, but it is essential to try to determine which parts of the results are (or may be) artifacts of the model and which parts are general and relevant to the real physical system being modeled. There are always simplifying assumptions and constraints in a model which need careful scrutiny.

The description of a crack in a solid with an applied external load or strain is rather simple to envision. One has a semi-infinite periodic three-dimensional array of atoms interacting with one another via an interatomic potential. A crack is inserted in the solid and a load is applied externally to appropriate surfaces. If the load is sufficiently large, the crack grows and the solid ultimately fractures. Why is this phenomenon so much more difficult to treat than other problems encountered in solid state physics? In most fundamental phenomena in solids, the periodicity of the solid is used to reduce the problem to an examination of a simple representative cell or region. Hence, the infinite number of atoms is not a serious problem. In the case of a crack, with its finite extension and the resulting long-range strain field, such reductions are not possible. Hence, one must resort to simplified models to try and gain insight into the role of cracks in brittle fracture.

Fig. 1. Illustration of the various current approaches to the modeling of cracks in crystalline solids.

The various approaches are illustrated in the block diagram of Fig. 1. In each case, some trade off has been made between giving up some aspect of the phenomenon in nature for some simplification that enables one to carry out a quantitative study. As the lattice static methods have been treated in some detail by Thomson¹ in an earlier paper, we shall here try to emphasize the kinds of trade-offs made in each type of model and the physical significance of the simplifying approximations.

In the various approaches illustrated in Fig. 1 different facets of the real phenomena are emphasized. If the semi-infinite periodic nature of the system is the major concern then one is led to the lattice static methods.¹⁻⁴ Cracks in such lattices can be handled by these methods but only for very simple unrealistic interatomic potentials. In the so-called hybrid models⁵⁻⁷ a very small crystalline region, where the calculations are done with realistic potentials, is imbedded in a simplified elastic region. The boundary matching, the above simplification, and the appropriateness of the size of the imbedded region are the important approximations in this technique. If the nature of the atomic forces and of the atomic motions is the main concern one is led to the molecular dynamic approach which can be used on an unconstrained system of a "large" number of atoms interacting with a realistic interatomic potential (this is the only way dynamic simulations can be carried out). Here, of course, the question is how "large" is large enough to simulate the behavior of the corresponding infinite systems.

These are the topics reviewed in this paper. The lattice statics approaches are reviewed rather briefly since they have already been treated at this Conference and since excellent reviews are available in the literature.²⁻⁷ The molecular dynamic simulations, both static and dynamic, are treated in considerable detail since these are rather recent and some of the results discussed here have not yet been published.⁸⁻¹²

II. LATTICE STATICS

1. Outline of the Method

The key feature of the lattice statics is that it treats an infinite number of atoms interacting via some simplified potential.¹⁻⁴ Two lattice statics calculations will be outlined here with emphasis on the simplified forms of the potential. The first is the quasi one-dimensional¹³ model which is commonly used to illustrate the lattice trapping which results from lattice statics calculations. As shown in Fig. 2, two semi-infinite chains of atoms are bonded together horizontally by bendable bonds and vertically by stretchable bonds. The zeroth atoms are stretched apart vertically by the forces σ and the first n

Fig. 2. One-dimensional model of a crack. Two semi-infinite chains of atoms are bonded together horizontally by bendable bonds and vertically by stretchable bonds. The zeroth atoms are stretched apart vertically by the forces σ and the first n vertical bonds are broken. (After ref. 13)

vertical bonds are broken (the transverse springs stretched beyond their limit) forming a crack of finite length. In Fig. 3, the atomic force law is illustrated as a function of the displacement y .¹⁴ The key feature of the force law is the bond snapping property, i.e. the force abruptly goes to zero at some displacement y_0 . It will be shown that bond snapping considerably enhances lattice trapping and indeed may be the largest contribution to lattice trapping. The mathematical details of the lattice statics calculation will be here outlined.¹³⁻¹⁴ The energy u_j in the lateral bond connecting atoms j with $j-1$ is

$$u_j = \frac{1}{2}\beta(\theta_j - \theta_{j-1})^2; \quad j = 1, 2, \dots \quad (\text{II-1})$$

where β is the bendable spring constant. The energy in a stretchable spring is

$$u_j = \frac{1}{2}\gamma(2y_j)^2 \quad j = n, n+1. \quad (\text{II-2})$$

Making the small angle approximation in (II-1), the total energy may not be written

Fig. 3. The assumed force law between the atoms is linear to a displacement of y_0 at which point the bond snaps discontinuously and the force falls to zero. (After ref. 14)

$$u = -2\sigma y_0 + \beta \sum_{j=1}^{\infty} (y_{j+1} - 2y_j + y_{j-1})^2 + 2\gamma \sum_{j=n}^{\infty} y_j^2. \quad (\text{II-3})$$

Inserting the equilibrium conditions $(\partial u / \partial y_j) = 0$, conditions are obtained on a complex vector $\underline{k}$

$$\cos 2\lambda - 2 \tanh^2 \lambda = 1 + \frac{1}{2}k \quad (\text{II-4})$$

$$2 \tan^2 \eta + \cos 2\eta = 1 + \frac{1}{2}k \quad (\text{II-5})$$

where $k = \lambda + i\eta$. The above solution can be used to find the force σ_+ for which the bond snaps. The crack is stable for forces less than σ_+ down to the point where the displacement of atom $n-1$ is equal to the critical value y_0 . At that point, σ_- , the previously broken bond snaps back together and the crack heals. The ratio $R = \sigma_+ / \sigma_-$ is the measure of lattice trapping. As $R \rightarrow 1$ there is no lattice trapping. At $R \gg 1$, lattice trapping becomes quite important. Thomson et al.¹³ give three approximate expressions for R

$$R \rightarrow 1 + 2\lambda \quad k^{1/4} \ll 1 \quad (\text{II-6})$$

$$R = 4.3 \quad k = 1 \quad (\text{II-7})$$

$$R = k+9 \quad k \gg 1 \quad (\text{II-8})$$

2. Major Results

The expressions (II-6 to II-8) predict the conditions for anything from negligible to large lattice trapping depending on the features of the potential. It is unfortunate that in the earliest lattice statics calculation, a numerical error was made in an independent model calculation, which led Thomson et al.¹³ to assume that large lattice trapping was in accord with realistic potentials. To this end, another lattice statics calculation is illustrated, with a different potential used as the interatomic force as shown in Fig. 4. In this calculation the surface energy of the atoms on the crack plane was calculated. The energy was taken to be of the simple form

$$E(n) = \frac{1}{2}E_0 \left(1 - \frac{2}{\pi} \tan^{-1} \frac{n}{\alpha} \right). \quad (\text{II-9})$$

The adjustable parameter α is adjusted to fit the results to the actual shape of the crack and to the force law. α can be thought of as the width of a "core region" of a crack. The key feature of the potential relative to the previous model is that there is no bond snapping in this force law. The parameter α contains both the shape of the crack and how rapidly the energy changes from atom to atom in the vicinity of the crack tip. A simple closed

Fig. 4. Functional form of the surface energy for moving a crack $S(x)$ (plotted on the left axis), and the corresponding force $\sigma = -dS/dx$ (plotted on the right). The dashed line represents the average surface energy used in the continuum approximation. (After ref. 13)

form was obtained for R,

$$R = \frac{1+2e^{-2\pi\alpha}+e^{-4\pi\alpha}}{1-2e^{-2\pi\alpha}+e^{-4\pi\alpha}} \quad (\text{II-10})$$

Thomson et al.¹³ performed one of the most important steps in establishing the reliability of any quantitative, unexpected result for a model, since they did the calculation for a very different model in order to see how the results compare. They determined α from the computer calculations of Gehlen and Kanninen¹⁰ using an empirical force law for iron and the computer positions for the atoms near the tip. Unfortunately they made a numerical error in this comparison. Using the data of Gehlen and Kanninen, $\alpha = 0.524$ and $R = 1.15$ indicating small lattice trapping. Thomson et al.¹³ quote a value of $R = 2.14$ which led them to conclude that lattice trapping is large. Subsequent lattice static calculations, mainly incorporating bond snapping features, yielded large lattice trapping and have led those working in fracture to conclude that large lattice trapping is a consequence of the discrete nature of the lattice. Clearly, the non-bond snapping lattice static calculation, matching realistic potentials, yields negligible lattice trapping and thus lattice trapping is not a consequence of the discrete nature of the lattice but rather a consequence of the displacements of the atoms near a crack top and the way the potential varies in this regime. Later Esterling¹⁵ used similar lattice static techniques and a variety of force laws and observed that crack healing is sensitive to the long-range portion of the cohesive force. Nevertheless Esterling accepts lattice trapping as non-negligible and goes on to treat some of the thermodynamic consequences. The lattice statics practitioners seem not to take seriously some of the concurrent hybrid lattice static calculations of Sinclair⁷ which, prior to Esterling's work, gave evidence that long-range potentials yield little lattice trapping.

3. Credibility of the Results

Thus arises the key problem associated with models and their quantitative results--the credibility of the results. This is the most difficult problem in modeling; how to establish the credibility of a model, and of any unexpected results. There are two general methods to establish credibility: develop a physical picture that explains the results or do other independent model calculations to get confirmation of the results. Both have been tried in lattice statics to confirm the unexpectedly large lattice trapping results obtained. Thomson et al.^{3,13-14} tried both but there seem to be serious objections to both the physical description and to the different models.

For the physical explanation of lattice trapping, Thomson et al. draw an analogy to the Peierls stress for dislocation.

This does not seem to be justified for continuous non-truncated interatomic potentials. If the stress that is applied is less than critical, indeed there will be a stress barrier against the crack propagating. However, there will be no stress opposing the crack healing. Any infinitesimal motion to close the crack will result in a lowering of the free energy; hence there will be no Peierls stress to overcome healing. If the stress is slowly increased and the crack does not propagate it should heal. This should be the case until the maximum or critical stress is applied; at this point a slight increase in stress should result in crack propagation. This is essentially the Griffith¹⁶ picture of fracture. Of course, if a material is not entirely brittle and some deformation can take place, then it is possible that the energy is approximately the same for a range of stresses leading to metastability, i.e. a range of stresses at which a crack neither propagates nor heals. This, however, does not seem to be the origin of the lattice trapping calculated by Thomson et al., particularly since even in their two-dimensional calculation,¹⁴ all motion is essentially transverse to the crack surface (i.e. Poisson's ratio is kept at zero). Hence, the Peierls-like barrier does not seem to be a simple consequence of the lattice periodicity independent of the potential and is not a universal phenomenon which yields lattice trapping as a fundamental property of a periodic array of atoms.

The second way to confirm credibility is by using an entirely different model. This was done by Thomson et al. using a surface-energy summation technique, and if it weren't for the numerical mistake made in evaluating R they would have indeed found little lattice trapping in a system that is meant to model iron. This same procedure was used to find R for the two-dimensional array with a Lennard-Jones potential by Paskin et al.¹² A value of $R=1.02$ was obtained in good agreement with the molecular dynamic results. This suggests that the lattice statics with a realistic value of α , obtained by matching empirical potentials, can give useful insight into the critical properties of fracture. The result also demonstrates the importance of the realistic interatomic potential in any model calculation.

III. HYBRID LATTICE STATICS

1. Outline of Method

The hybrid approach involves separating the infinite solid into two regions. In region I, near the crack tip, both the atomic structure and the atomic interaction are treated explicitly. In region II, the outside region, the force law and also the atomic structure are simplified. In an early Sinclair and Lawn⁵ calculation, region II is treated by the continuum approximation and the boundary between regions I and II is fixed. In a later calculation

by Sinclair,⁷ the I-II boundary is flexible and higher order terms are included in the elastic field equations. In the Sinclair and Lawn hybrid calculations, a suitable semiempirical potential for the diamond-structure crystals was constructed. The atoms were then relaxed within region I in such a way that the total potential energy tended to a minimum. This was systematically done on a computer with the boundary between I and II kept rigid. The boundary was obtained by solutions of the continuum field equations. While the results seem to be reasonable, it is difficult to determine their reliability.

Sinclair⁷ thought that the rigid boundary introduced some error in the hybrid calculations that made them not suitable for a study of the critical conditions for crack extension or closure. The reason is that, if the solutions of the inner region are not compatible or consistent with the solutions of the outer region in the rigid boundary method, no adjustment can be made for this mismatch in forces. The rigid boundary forces a state of stability in the system that may be inconsistent with the local stress fields. If the crack in region I would like to expand (or contract) the rigid boundary prevents this relaxation. The flexible boundary model allows some relaxation of the boundary so as to prevent forces building up at the boundary. Sinclair does this by including higher order terms in the elastic crack-field equations for region II; by suitably adjusting the coefficients of these terms a configuration free of residual forces may be obtained for a given applied stress. The approximation in this procedure is that the forces are calculated correctly in region I but approximately in region II.

2. Major Results

a. Rigid Boundary. The results for the rigid boundary model were mostly qualitative and reasonable. Sinclair and Lawn found that except for very near the crack tip the continuum and atomic relaxation calculations showed close agreement, despite the fact that the elastic nonlinearity and the atomicity render continuum theory strictly invalid throughout the core region. It is not clear how much of this result depends on the use of rigid boundaries matched to continuum solutions. In Fig. 5 the bonds in the vicinity of the crack tip are shown. As illustrated in Fig. 6 the relaxation varies with the size of the atomic region. It is apparent that the continuum solutions are forcing a larger crack to exist than the atomic solutions yield. Thus, in this case the "true" crack is smaller than the "continuum" crack. Unfortunately, it is difficult to estimate the quantitative errors introduced by this procedure.

Fig. 5. Computer-relaxed atomic configuration near equilibrium (111) crack tip in silicon. (After ref. 5).

Fig. 6. Dependence of Si-Si bond-lengths PS, QT, RU on size of relaxed region. As region I is increased from 2 to 4 rectangular shells, the bond QT contracts from the "ruptured" to the "stretched" state, thus closing the crack by one atomic spacing. (After ref. 5)

b. Flexible Boundary. The main results of the flexible boundary hybrid treatment were directed towards examining the effect of various potentials on lattice trapping.⁷ In Fig. 7, the radical component of the force laws used are shown. The important point to note is that potentials I, II and III are quite long range compared to IV, which has the bond snapping character usually used in lattice statics. In table 1, the lattice trapping ratios for these potentials are given. It should be noted that the long-range potentials yield R ranging from 1.13 - 1.45 but the bond snapping force gives $R=7.3$. Thus, the hybrid model clearly demonstrates that bond snapping severely exaggerates lattice trapping, while the long-range potentials yield much more modest lattice trapping.

Table 1. Lattice-trapping ratios for straight $[0\bar{1}1]$ edge cracks.⁷

	Pot I	Pot II	Pot III	Pot IV
R	1.13	1.45	1.41	7.3

Fig. 7. The radial component of the force laws derived from potentials I to IV. (After ref. 7)

3. Credibility of the Hybrid Model

The fact that the hybrid lattice statics are in relatively good qualitative agreement with molecular dynamic calculations (as discussed in section IV) shows that both models are reasonable. What is more difficult to assess is the accuracy of the hybrid model using flexible boundary conditions. It is not easy to see how one can get a quantitative measure of the accuracy of the model. There must be some artificial mismatch at the boundary as the force laws in regions I and II are not the same. A systematic variation of region I and the resulting variation of the thermodynamic properties to enable an extrapolation to the infinite atomic solid, would lend more credibility to the quantitative results. It is difficult to compare the lattice trapping results for the long-range potentials in the hybrid model with those of the molecular dynamic calculations. The potentials used by Sinclair are non-central whereas the molecular dynamic potentials are central. The non-central nature of the forces may allow nonbrittle distortions not contained in the central force treatment. In any event, hybrid lattice static calculations using semi-empirical potentials predict negligible to little lattice trapping, as opposed to the bond snapping force models which yield large ($R > 2$) lattice trapping.

IV. MOLECULAR DYNAMICS - STATIC CALCULATIONS

1. Outline of the Method

The computer simulation of atomic motion in solids by the technique of molecular dynamics has been treated extensively in the literature.¹⁷ Basically Newton's differential equations of motion are solved numerically for a large number of atoms interacting with a given potential. The simulations to be described¹² were carried out on a two-dimensional triangular lattice illustrated in Fig. 8 (half sample). The largest sample consisted of 10704 atoms arranged in 79 rows. Mirror symmetry about the central vertical axis was used to reduce the computation time.

For the atomic interaction the Lennard-Jones (6-12) (L-J) potential was used in the form

$$\phi_{ij}(r_{ij}) = \epsilon_0 [(d/r_{ij})^{12} - 2(d/r_{ij})^6] \quad (\text{IV-1})$$

with all energies measured in units of ϵ_0 , and distances r_{ij} in units of d , the equilibrium spacing. The forces were calculated between atoms which were initially nearest neighbors. After the introduction of the crack, forces were calculated between all atoms within $1.6d$, well beyond the distance $1.11d$ where the interatomic force is maximum and slightly less than the second-neighbor distance. The calculations were performed using the Verlet¹⁸ method for solving Newton's equation of motion. The atomic positions,

Fig. 8. The triangular lattice of 79 rows with a crack of 38 broken bonds. The half sample is shown. The lines represent the bonds between atoms. (After ref. 12).

velocities, forces, total energy, kinetic energy, potential energy, and modulus of elasticity were monitored throughout. For dynamic properties the time step in the calculation gave one part in 10^6 accuracy in the energy. For equilibrium (static) calculations a time step eight times as long was employed to obtain equilibrium by a less costly procedure.

In a static simulation the system was brought to equilibrium under a constant external strain ϵ before inserting the crack. The constant external strain was applied by specifying and maintaining the vertical displacement of the individual atoms in the uppermost and lowermost rows with all other atomic motions free to adjust. Thus, there were no additional constraints on the system. The calculations have also been performed at constant applied stress. This case will be discussed later. Equilibrium was attained (at zero temperature) by inserting critical damping into the equations of motion. A crack was created by cutting some of the bonds across the central rows of the sample (Fig. 8).

2. Major Results

a. Mechanical Properties of the Triangular 2-D Lennard-Jones Solid: The Perfect Solid. The elastic constants of the 2-D triangular L-J solid are well known, i.e. the response to an infinitesimal stress (σ) (or strain, ϵ).^{9,19} In particular, Young's modulus, M , defined as tensile stress over tensile strain, is $83.14 \epsilon_0/d^2$, at an infinitesimal deformation.

As the strain is increased the system shows a highly nonlinear behavior, i.e. M is a function of ϵ , arising from the highly nonlinear forces of the L-J interaction. For a uniform tensile strain one can calculate M directly¹² from a balance of forces on one deformed triangular cell as shown by the sketch of Fig. 9. With $r_1^0 = r_2^0 = 1$ the pertinent equations are

$$\epsilon = \Delta/(\sqrt{3}/2) \quad (\text{IV-2})$$

Fig. 9. Tensile deformation of the elementary triangle.

$$r_1^2 = \frac{3}{4}(1+\epsilon)^2 + \frac{1}{4}(1-\nu\epsilon)^2 \quad (\text{IV-3})$$

$$r_2 = 1 - \nu\epsilon$$

where ν = Poisson's ratio. The tensile force, F , is given by

$$F = \frac{2\sqrt{3}}{2} \frac{(1+\epsilon)}{r_1} \frac{d\phi}{dr} \quad (\text{IV-4})$$

where $\phi(r)$ is the interatomic potential. ν is determined by minimizing the energy with respect to ν , namely

$$2 \frac{d\phi}{dr_1} \frac{dr_1}{d\nu} + \frac{d\phi}{dr_2} \frac{dr_2}{d\nu} = 0 \quad (\text{IV-5})$$

with

$$\frac{dr_2}{d\nu} = -\epsilon \quad (\text{IV-6})$$

$$\frac{dr_1}{d\nu} = -\frac{1}{4} \frac{(1-\nu\epsilon)\epsilon}{r_1}$$

The modulus, $M(\epsilon)$ is given by

$$M = \frac{F}{\epsilon(1-\nu\epsilon)} \quad (\text{IV-7})$$

Fig. 10. Young's modulus M against applied strain. The full circle represents three sample sizes spanning a factor of 4 in area; the moduli were identical within 0.1% independent of size. The straight line is the theoretical behavior of the modulus against strain for a perfect sample. (After ref. 12)

A series of computer calculations was performed over a range of applied strains and sample sizes. The data for M are shown in Fig. 10 together with the theoretical modulus (solid line) calculated by the above equations. The excellent agreement of the theory and the computer calculations, and the observation of no size dependence in the modulus over a factor of four in the sample area, show that the strain dependence of the modulus is understood in a fundamental way for this nonlinear elastic solid. Computer experiments at various applied stresses were also in full agreement with Fig. 10.

In the region of interest in subsequent calculations the modulus-strain dependence is accurately given by the linear relation of Fig. 10, namely

$$M = M_0 - \alpha \epsilon \quad (\text{IV-8})$$

with $M_0 = 83.14$ and $\alpha = 414$.

b. The Two-dimensional Solid Containing a Crack. When a crack is introduced into the sample, with a fixed external strain, the modulus is reduced. This reduction in modulus occurs because the introduction of a crack, at fixed strain, reduces the stored energy. As the effective modulus is related to the stored strain energy, a reduction in modulus results. Again a series of computer calculations of M was carried out at various sample sizes for 38 broken bonds.¹² The data are shown in the bottom half of Fig. 11.

The size dependence of M for a cracked sample may be analyzed by a procedure analogous to that given by Berry²⁰ for a linear elastic continuum. ΔE , the difference in the elastic stored energy of a sample with and without a crack, may be written as

$$\Delta E = (A\epsilon^2/2) [(M'_0 - M_0) - \frac{2}{3}(\alpha' - \alpha)\epsilon] \quad (\text{IV-9})$$

where A is the area and the primes refer to the quantities in the presence of a crack of half-length l . Making the simplifying approximation that the nonlinearity of the modulus is the same with and without a crack, $\alpha = \alpha'$, equation (IV-9) takes on the same form as the linear case. The computer calculations indicate that this is a very good approximation. To evaluate M' , however, a theoretical estimate of ΔE is needed. As the exact form of the strain energy of a crack for a non-linear modulus, for small cracks and large strains, is not known, it was assumed that it is of the usual form with the linear modulus replaced by M' , the effective non-linear modulus: namely $\Delta E = -\pi l^2 \sigma^2 / M'$ where σ is the applied stress. By converting from applied stress to applied strain, equation (IV-9) may be written

$$-\pi l^2 \epsilon^2 M' = (A\epsilon^2/2) (M'_0 - M_0) = (A\epsilon^2/2) (M' - M) \quad (\text{IV-10})$$

Fig. 11. The functional dependence of the modulus and the strain energy difference ΔE on sample size. Data plotted against $1/\text{area}$ as indicated by equations (IV-11) and (IV-12) (all values for full sample). The straight line is the empirical fit to the data. All samples have a crack of 38 broken bonds. (After ref. 12).

and solving for the effective modulus it is found that

$$M' = M / (1 + 2\pi\ell^2/A). \quad (\text{IV-11})$$

This is similar to the form obtained by Berry²⁰ with the linear modulus M_0 replaced by M . According to these results $(M')^{-1}$ should be a linear function of $1/A$, which is indeed the behavior of the computer calculations shown in Fig. 11. The behavior of the modulus as a function of sample size is in excellent agreement with eq. (IV-11).

The size dependence of the strain energy difference is also obtained within the same approximation as

$$\Delta E = -\pi\ell^2\epsilon^2 M'$$

and substitution for M' from eq. (IV-11) gives

$$(\Delta E)^{-1} = -(1 + 2\pi\ell^2/A) / \pi\ell^2\epsilon^2 M. \quad (\text{IV-12})$$

Thus, $(\Delta E)^{-1}$ is also expected to be linear in $1/A$. As indicated in the upper half of Fig. 11, the strain energy response also shows the correct functional dependence, but the slope is larger than calculated from eq. (IV-12). On the basis of this functional dependence the extrapolation to infinite size ($1/A \rightarrow 0$) can be

carried out. Using this procedure, an infinite sample strain energy difference of $21.3 \epsilon_0$ is obtained, which is about 12% larger than that for the largest sample ($19 \epsilon_0$) in the computer simulations.

Thus, the mechanical properties of the triangular 2-D L-J solid are well understood, both in the presence and the absence of a crack. It is to be noted for the subsequent discussion that sample size effects are small for the largest sample used in the computer simulations.

c. Lattice Trapping

Detailed studies were made with a crack consisting of 38 broken bonds (full sample). A series of strains was applied and the simulation continued until either the system came to equilibrium or the crack propagated by further bond breakage, or the crack healed upon restoration of the cut bonds. The results¹² are shown in table 2, where the applied strain, ϵ , the length of the first unbroken bond d_c and the length of the first cut bond d_{c+1} are listed.

Table 2. Data of lattice trapping study.

Applied Strain ϵ	d_c *	d_{c+1} †	Comments
0.0285		<1.60	crack heals
0.02875	1.510	1.614	stable crack
0.0290	1.549	1.646	stable crack
0.0295	>1.60		crack propagates

*Length of first unbroken bond in units of d .

†Length of first cut bond in units of d .

As shown in the table, the crack was found to be stable at two strains 0.9% apart. At these equilibrium positions, the inter-atomic distances of the atoms across the crack surface exceeded $1.6d$, the effective range of the potential, while the unbroken bond was stretched to less than $1.6d$. Restoring the interaction, therefore, did not affect the equilibrium. Upon lowering the strain by 0.9%, d_{c+1} became less than $1.6d$ and the system healed (with and without damping) upon restoration of the interactions across the crack. Conversely, upon increasing the strain by 1.7% the unbroken bond was stretched beyond $1.6d$ and the crack propagated by bond breakage (with and without damping). No attempt was made to obtain closer limits on the strain range of the stable region. It is concluded from these data that the range of lattice trapping is larger than 1% and less than 3%.

As already pointed out, the strain energy difference in the largest sample differs from that in the infinite sample by only about 10%. As the critical strain is approximately proportional to the square root of the energy, the estimate of any critical strain ratio is believed to be correct to better than 10%. Thus, the size effect would shift the critical strains (an increase with decreasing sample size for a given critical energy) but leave the range in critical strains, and hence lattice trapping, essentially unchanged. A study of lattice trapping at half the size confirmed this analysis. Thus, size effects in this study are quite small and it is concluded that lattice trapping is less than 3% for potentials of the form used.

3. Credibility of the Results

There are major advantages to the molecular dynamic simulation of the equilibrium properties of a crack. A realistic semi-empirical interatomic potential, in this case the Lennard-Jones, can be used. The model system can be completely unconstrained except for the correct boundary conditions. With appropriate attention to the required accuracy²¹ in the simulation, the results are exact within the framework of the model.

The major disadvantage of the molecular dynamic technique is the restriction of the system to a finite number of atoms. The basic question is, therefore, how large is large enough to simulate in a relevant way the properties of the corresponding infinite system. In the present case it was shown that the properties of the finite system can be described and understood quantitatively on the basis of simple balance of forces and energies. Thus, extrapolation to infinite size became feasible and the error in using about 10,000 atoms could be estimated quantitatively. As already indicated, the error turned out to be small and did not affect in any significant way the negligible lattice trapping determined for this model.

It should be pointed out that the finite search range of $1.6d$ used in practice renders the L-J potential a snapping potential but with a small snapping range. The importance of the "cut off" may be illustrated in a simple way. In the sketch of Fig. 12 the extensions of the unbroken bond, d_c , and the first broken bond, d_{c+1} , are shown as a function of the applied strain, ϵ . Let r_{c1} and r_{c2} be two cut-off bond distances, i.e. the force goes to zero at $r > r_c$. ϵ_p and ϵ_h are the applied strains for propagation and healing, respectively. At $\epsilon > \epsilon_p$ the bond d_c becomes "broken," while at $\epsilon < \epsilon_h$ the bond d_{c+1} "heals" by coming within the range of the potential. In the simple linear sketch of Fig. 12, $\epsilon_{p1} - \epsilon_{h1} = \epsilon_{p2} - \epsilon_{h2}$. However, the ratio ϵ_p/ϵ_h clearly increases as r_c is decreased, and vice versa. Thus, a continuous potential, for which $r_c \rightarrow \infty$, would be expected to show no lattice trapping.

Fig. 12. Sketch of the influence of the "cut-off" in the potential on the lattice trapping ratio.

Finally one should mention that all molecular dynamic simulations so far have been restricted to two dimensions as even modern computers cannot handle a three-dimensional atomic lattice of any sensible size.

V. MOLECULAR DYNAMICS - DYNAMIC CALCULATIONS

1. Outline of the Method

Weiner and Pear⁸ and Ashurst and Hoover⁹ made the earliest calculations of the dynamic properties of fracture. Weiner and Pear used a quasi one-dimensional geometry and a piecewise linear tensile force law for atoms in the same column. Ashurst and Hoover used a two-dimensional triangular lattice constrained so that Poisson's ratio is zero. They used, for the most part, bond snapping force laws similar to the Thomson et al.¹³ and Esterling¹⁵ lattice static calculations. It is difficult to assess the quantitative aspects of their results both because of the simplifications in the interatomic potential and the constraints against motion transverse to the applied stresses. For example, Weiner and Pear observed supersonic crack velocities at high stress values, whereas the recent molecular dynamic results yield much lower velocities. Ashurst and Hoover obtained energies of crack formation in reasonable agreement with the present molecular dynamic results but also found a lattice trapping ratio of $R=3.7$. Thus, there is no question that molecular dynamic calculations do yield interesting results but always the problem to be resolved is how much of the results arise from simplification in the inter-

atomic potential as well as simplifications in the geometry. The present calculations¹¹⁻¹² may be thought of as an extension of the Ashurst and Hoover calculations, with the bond snapping forces replaced by longer-range forces arising from a Lennard-Jones interatomic potential, no artificial zero Poisson's ratio constraint and the use of larger arrays of atoms (5000 - 10000).

In the present molecular dynamic simulations three methods were used to initiate crack propagation: (a) A crack was introduced into a prestressed sample. A sufficiently large crack would propagate. (b) A crack was introduced in a prestressed sample, and allowed to come to equilibrium and then the applied stress was raised to a greater than critical value in one large increment. (c) A crack was allowed to come to equilibrium and the stress (or strain) increased gradually until crack propagation was obtained.

The method of crack initiation requires some elaboration. A crack was created by cutting the bonds between a given number of atoms between the two rows of atoms at the center of the sample. The interatomic potential between these atoms was set to zero. These conditions correspond to the insertion of a very thin knife to create the crack. There was no damping used in the dynamic simulations subsequent to the creation of a crack. When the boundary condition was that of constant stress a crack would only come to equilibrium as long as the knife condition was retained. When the boundary condition was that of constant strain, a crack would come to equilibrium without the knife condition being retained. Thus, the different boundary conditions in these dynamic simulations produced quite different results.

In the constant applied stress (c-stress) situation, a constant external load was applied to the individual atoms of the uppermost and lowermost rows. All external boundaries were free to move while the load was kept constant. In the constant applied strain (c-strain) case, the strain was applied by specifying and maintaining the vertical displacements of the individual atoms in the uppermost and lowermost rows. All other atomic motions were unconstrained. For the finite samples used, about 5000 atoms, not only do the surfaces look different (see Figs. 8 and 13a) but the shapes of the similar size cracks near critical conditions differ. The c-stress cracks are wider than the c-strain cracks. This shows that the boundary conditions for finite samples can play an important role, and must be understood in some detail if the results are to be credible.

Having established the boundary conditions and the method of introducing the crack and critical stress or strain, the subsequent molecular dynamic calculations are identical to those used to obtain the static results. The atomic positions, velocities, and forces as well as the total energy, work, potential energy,

Fig. 13. A two-dimensional triangular lattice with a crack. Because of mirror symmetry the entire sample can be obtained by reflection about the right-hand side of this figure. Forces are applied to atoms in the 1st and 39th rows (applied σ). Lines are drawn between atoms that are less than $1.6d$ apart. (a) Clean brittle fracture at $\sigma = 0.5$ and $L_0 = 39$ (L_0 is the number of initially broken bonds for the half sample). (b) Incipient dislocation formation at $\sigma = 1.3$ and $L_0 = 19$. The extra lines designate the atoms that have moved into the range of interaction. (c) Dislocation formed at the lower end of the crack tip at $\sigma = 1.3$ and $L_0 = 39$. This dislocation later on propagated to the surface. (After ref. 11)

kinetic energy, and modulus of elasticity were monitored throughout the calculations. The time step in the calculation was chosen to give one part in 10^6 accuracy in the energy. The results were sometimes tested by increasing the accuracy from 2 to 4 times, to confirm that the results were independent of the accuracy of the numerical procedure.

2. Major Results

a. Dynamic Simulations under Constant Load.¹¹ The system for dynamic studies at constant load consisted of 5284 atoms arranged in 39 rows as shown for the half sample in Fig. 13a. The mirror symmetry about the central vertical axis was used to reduce the computation. In these calculations the system was brought to equilibrium under a given constant external force, σ (in units of ϵ/d), before the crack was inserted. A crack was created by cutting the bonds between a given number of atoms in the 19th and 20th rows, i.e. the interatomic potential for these atoms was set at zero. There was no damping subsequent to the creation of the crack. These conditions correspond to the insertion of a very thin knife to create the crack.

As the crack moves under a constant load, applied to both horizontal surfaces, conservation of energy requires that

$$\Delta W = \Delta E_p + \Delta E_k = \Delta E + \Delta E_s + \Delta E_k, \quad (V-1)$$

where ΔW is the work done on the sample, ΔE_p is the change in total potential energy, ΔE_k is the change in total kinetic energy, ΔE is the change in strain energy, and ΔE_s is the change in surface energy of the crack. Conservation of energy was always obeyed in these simulations. ΔE is evaluated as $\Delta E_p - \Delta E_s$, where ΔE_s is taken as two bond energies per pair of interacting atoms, i.e. the depth of the L-J potential, ϵ_0 , per atom. In the Griffith energy treatment ΔE_k is zero. In order to obtain a quantitative criterion for the stress using eq. (V-1) it is necessary to have a relation between ΔW and ΔE . If one assumes macroscopic linear elasticity, $\Delta E = \frac{1}{2} \Delta W$, and therefore, $\Delta E = \Delta E_s$ which is the basic Griffith energy criterion.

In Fig. 14, ΔW , ΔE_s , ΔE , and ΔE_k are plotted versus the relative increase in crack length, $(L-L_0)/L_0$, for two computer simulations at different loads and initial crack lengths. These energy changes were evaluated in the region of early crack motion where ΔE_k is approximately zero and, thus, a direct comparison can be made with the Griffith energy assumption. In these computer simulations $\Delta E/\Delta W$ varies all the way from zero ($\sigma = 0.5$, large crack) to 0.75 ($\sigma = 1.3$, medium crack). While one might say that the Griffith energy criterion ($\Delta E/\Delta W = 0.5$) is approximately true for the latter, clearly the case of zero initial change in strain

Fig. 14. Changes in energy components as a function of fractional increase in crack length during crack propagation. σ is the applied force (0.5 in the upper figure, 1.3 in the lower) and L_0 is the number of initially broken bonds for the half sample (39 in the upper figure, 19 in the lower). The energy components are ΔW , circles; ΔE_e , crosses; ΔE_k , squares; and ΔE_s as defined in eq. (V-1), solid curves. (After ref. 11)

energy would indicate failure of the elastic mode of brittle fracture.

As a matter of fact, the negligible change in strain energy suggests that a rigid tearing mode is a better description of such a fracture. This fracture ($\sigma = 0.5$) exhibited no dislocation formation or bifurcation and was the cleanest example of brittle fracture, with rapid approach to a constant velocity, in these

simulations. One can estimate the critical stress, σ_c , for such a tearing mode of crack propagation by assuming rigid propagation of the changing crack shape to the boundary in calculating ΔW . If all of this work, rather than one half, goes into surface energy, σ_c turns out to be of the same functional form as the Griffith σ_c but is lower by a factor of $\sqrt{2}$. This simple estimate yields, using an effective modulus of $30\epsilon/d^2$, a $\sigma_c = 0.7\epsilon/d^2$ as compared to the simulation value of 0.5. Thus, even though the energy criterion is violated for this fracture mode, the critical stress estimate is approximately valid.

At higher stresses a more complex behavior is observed as shown by the simulations in Fig. 13a to 13c. Figure 13a represents the same simulation whose energetics are shown in Fig. 14 (top), i.e. a large initial crack with an applied σ of 0.5. This crack propagated in a clean brittle manner with very little distortion at the crack tip. Figure 13b, corresponding to Fig. 14 (bottom), shows a crack with large directional distortions near the tip indicated by additional atom-to-atom lines connecting atoms which were originally not in range but have now come into range. Such lines of distortion, which may be considered incipient dislocations, are generated and absorbed as the crack propagates. In Fig. 13c, a large initial crack with $\sigma = 1.3$, the crack propagated to the configuration shown. A dislocation can be seen at the lower end of the crack tip. This dislocation then propagated to the surface and bifurcation occurred. Raising the stress of the crack of Fig. 13b to $\sigma = 3.0$ resulted in the immediate formation of dislocations and the subsequent blunting of the tip, i.e. ductile behavior.

These results can be related to the Rice-Thomson²² treatment of crack-dislocation interaction. They consider a material to be brittle if a dislocation generated in the neighborhood of the crack tip cannot escape from the tip region. The critical distance, r_c , at which a straight dislocation is in unstable equilibrium is obtained from considering the following forces: (1) the repulsive force due to the crack stress field, (2) the attractive image force of the dislocation in the free surface of the crack, and (3) another attractive force arising from the additional surface created by the blunted crack. If r_c is larger than the dislocation core cutoff, r_0 , then the material is brittle. For the present two-dimensional system application of the Rice-Thomson equations yields $r_c = 1.8d$. From Esbjorn and Jensen¹⁹ r_0 for this system is $1.7d$. Consequently, this two-dimensional Lennard-Jones system is barely brittle according to the Rice-Thomson criterion. As indicated above, crack propagation in this system varies from brittle to ductile depending on the applied stress and the detailed dynamics. This suggests that the Rice-Thomson formulation has considerable quantitative validity.

Fig. 15. Healing and propagation of the crack upon various changes in the applied stress.

A more detailed examination of the Rice-Thomson treatment indicates that, as the applied load is increased above critical, the stress at a distance from the crack tip increases. Including this stress dependence in the Rice-Thomson formulation, it is found that r_c is approximately proportional to $(\sigma_c/\sigma)^2$ and thus high applied loads, σ , should reduce r_c and produce a tendency towards dislocation emission. Since the model system is barely brittle at low stresses and low crack velocities, it is not surprising to find dislocation formation and ductility at high applied loads and large crack velocities.

Further information was obtained about the tendency for local deformation by attempting to reach critical stress conditions by very small changes in the applied load for a crack in equilibrium with the bonds cut. By critical damping it was possible to bring the system of Fig. 13a into equilibrium at $\sigma = 0.60$ with the bonds cut (knife present). When the bond interactions across the crack were restored (knife pulled out) the crack healed. When the applied load was raised in small increments the first (r_{01}) and second (r_{12}) unbroken bonds increased slowly as shown in Fig. 15

for the sequence σ_a : $0.60 \rightarrow 0.65 \rightarrow 0.67$ with large local deformation but no propagation and with healing upon restoration of the interactions. The two points worth noting in the constant stress static study are: a stable crack was not possible (with the knife removed the crack always healed) and over a limited range, where crack propagation was expected from linear extrapolation considerations, the crack did not propagate. With a more sudden change of σ : $0.60 \rightarrow 0.67$ propagation occurred with r_{01} rapidly increasing past 1.6 (the search range) (Fig. 15). Thus, at constant load, this system is very sensitive to the rate of change of the applied load.

b. Dynamic Simulations under Constant Strain.²³ As already pointed out, the boundary condition of constant strain is theoretically advantageous because no external work is done leading to a simpler energy analysis. Further, crack propagation can be initiated by a very small change in the applied strain, i.e. from essentially an equilibrium configuration.

In the dynamic simulations, detailed studies were made on a sample 59 rows by 95 columns with initially 38 bonds broken. This system was in equilibrium at an applied strain $\epsilon = 0.0315$. Upon increasing ϵ to 0.0318 the crack propagated and the propagation was followed until the number of broken bonds increased by a factor of 3 (further propagation would get too near the edge of the sample). The crack tip velocity, modulus of elasticity and all energies were monitored during propagation.

The velocity data are shown in Fig. 16b as bonds broken per time step vs. the step number (i.e. time), and crack tip velocity vs. ℓ , Fig. 16a. The most striking feature of the data is the rapid transition to a limiting constant velocity, which turns out to be 11% of the longitudinal sound velocity. The process starts with zero kinetic energy which then increases in a very regular manner. The kinetic energy is discussed later.

The elastic response of the material during propagation is illustrated in Fig. 17 where the changes in the effective nonlinear elastic modulus, M' , and the elastic energy, ΔE , are shown. Both of these quantities behave as expected on the basis of the energy analysis given in section IV for the static simulations. According to equation IV-11, at a constant ϵ , $1/M'$ is linear in ℓ^2 with the slope given by $2\pi/MA$. The area A of this sample is 4772 and M at $\epsilon = 0.0318$ is 70 giving a theoretical slope of 1.88×10^{-5} . The observed slope during dynamical simulation is 1.96×10^{-5} in excellent agreement with the approximate theory for a finite nonlinear elastic material.

According to equation IV-10 ΔE is linear in $\ell^2 M'$ at a constant ϵ with the slope given by $\pi \epsilon^2$. The data of Fig. 17b, where ΔE is the half sample, follow this functional form with a slope of

Fig. 16. (a) Crack tip velocity, v_c , vs. crack length, ℓ , during crack propagation at constant strain. (b) Crack tip velocity (number of broken bands per unit time) vs. time during crack propagation at constant strain.

1.8×10^{-3} . The theoretical slope is 1.59×10^{-3} giving a discrepancy of about 12%. It should be noted that there was a similar discrepancy, 16%, in the static ΔE vs. theoretical ΔE in the static simulation. Overall the agreement with the approximate nonlinear elastic treatment is satisfactory. The important observation to be made from the agreement of equilibrium static formulations with the dynamic results, is that the data demonstrates that the dynamic configurations resemble the equilibrium static configurations. This is the basic assumption made in calculations of dynamic crack propagation and it is reassuring to find that it is valid in the

Fig. 17. (a) The functional dependence of the modulus on crack length during crack propagation at constant strain. (b) Change in elastic energy vs. $l^2 M'$ during crack propagation at constant strain.

constant applied strain simulations.

A theoretical approach to dynamic fracture was made by Mott²⁴ in an extension of the Griffith thermodynamic approach. Mott added a kinetic energy term to the static energy and found the configuration which maintains the total energy content as constant. While this is straightforward, the relationship between the kinetic energy and the crack velocity is based on a number of simplifying assumptions and dimensional analysis arguments. Quantitatively, Mott obtains the relationship for ΔE_k , the kinetic energy, as

$$\Delta E_k = \frac{1}{2} k \rho v_c^2 \ell^2 \sigma_L^2 / E^2 = \frac{1}{2} k \rho v_c^2 \ell^2 \epsilon^2 \quad (V-2)$$

where ρ is the density, v_c the crack tip velocity, σ_L the external stress, E the modulus and k a constant. For constant applied strain, $\epsilon = \sigma_L / E$ and the second form for the kinetic energy is applicable to the present simulations. This is the key Mott result, the rest of the details follow from conservation of energy and must be correct regardless of the form for the kinetic energy. In Fig. 18, the kinetic energy term for the constant external strain case is compared with $v_c^2 \ell^2$; the agreement is striking. It should be noted that initially v_c varies approximately linearly with ℓ and, subsequently, becomes a constant as shown in Fig. 16; nevertheless $v_c^2 \ell^2$ describes the behavior of the kinetic energy throughout.

While the initial behavior of the kinetic energy is somewhat simple to explain, the ℓ^2 dependence, when v_c is a constant, is not so easy to understand nor is the fact that the asymptotic value of v_c is much less than the Mott estimate of ~ 0.4 times the longitudinal sound velocity ($8.49\sqrt{\epsilon/m}$). In the region where v_c varies, $(\ell - \ell_0) / \ell_0 < 1$ and a Taylor expansion can be made of the elastic energy for crack formation as a function of $\ell - \ell_0$. Inserting the conditions that the kinetic energy is zero at $\ell = \ell_0$ and

$$\left. \frac{\partial(\Delta E + \Delta E_s)}{\partial \ell} \right|_{\ell = \ell_0} = 0,$$

one obtains the following expression for the kinetic energy

$$\Delta E_k = -(\Delta E + \Delta E_s) = \frac{(\ell - \ell_0)^2}{2} \partial^2 \Delta E / \partial \ell^2 \quad (V-3)$$

With $\ell_0 = 9.75d$, from $\ell = \ell_0$ to 15.75, $\Delta E_k / (\ell - \ell_0)^2$ only varies by about 15% from the average value, while ΔE_k changes by three orders of magnitude. Thus, the initial behavior of v_c can be well described in terms of the initial constraints on the behavior of $(\Delta E + \Delta E_s)$. The behavior where $v_c = \text{constant}$ is not so easy to describe. Lawn and Wilshaw² use a size dependent relationship for ΔE which would predict that v_c would vary rapidly and vanish much before the crack length had doubled. This does not happen in this simulation. The key difference between the Lawn and Wilshaw analysis and the present one is that they assume (in our notation)

$$\Delta E = -\pi \ell^2 \epsilon^2 (M')^2 / M_0 \quad (V-4)$$

whereas it is found in the simulation that

$$\Delta E = -\pi \ell^2 \epsilon^2 (M'). \quad (V-5)$$

As $M' \propto 1/(1 + \alpha \ell^2)$, the Lawn and Wilshaw crack formation energy decreases with increasing ℓ much more rapidly and this makes the kinetic energy vanish at a small ℓ . If the kinetic energy term is calculated using (V-5) it is found to vanish at $\ell \sim 50d$. While this is much larger than the Lawn and Wilshaw estimate, it is still

Fig. 18. The functional dependence of the kinetic energy on $l^2 v_c^2$ during crack propagation at constant strain.

not in accord with the present results. At first this is quite surprising in that the expression for ΔE is in accord with experiment and thus the calculation for ΔE_k would also be expected to be valid. The reason for the discrepancy is that the agreement of ΔE with experiment is to within several percent, but the ΔE_k is about as large in the region of interest as the error in ΔE . Hence, the calculation of ΔE_k has an error of about 100% and thus, the expression for ΔE is just not described accurately enough to calculate ΔE_k directly from eq. (V-1) with explicit forms for ΔE and ΔE_s .

The constancy of v_c may be approached somewhat differently in terms of the size effect. The main idea of how the size effect limits the velocity is that, because of simple size restraints, the crack height can only grow to some maximum value, δy , limited by the sample size in the y direction. The v_c may be estimated by assuming an average acceleration near the crack tip of $F_{\max}/2m$, and thus

$$v_c \sim 2 \left[\frac{F_{\max}}{2m} \right] \delta y. \quad (V-6)$$

For the Lennard-Jones potential, $F_{\max} = 4.66 \epsilon/d$; for the largest sample $\delta y \sim 0.5d$, and $v_c \sim 1.5\sqrt{\epsilon/m}$ compared to the observed value of $0.9\sqrt{\epsilon/m}$. This is in the right direction to explain both why v_c becomes constant at a relatively small fraction of the sound velocity and also why it is a constant whereas a quantitative examination of $(\Delta E + \Delta E_s)$ suggests a varying value for v_c [i.e. $(\Delta E + \Delta E_s)$ is not simply proportional to l^2 over any wide range of l]. However, if v_c is limited by sample size constraints so that it cannot attain

the limiting value of an infinite sample, simply because the available distance for the crack surface to expand is limited, the observed results seem reasonable. This analysis suggests a sample size effect: the smaller the sample, the smaller the limiting velocity. This prediction is under investigation.

3. Credibility of the Results

The major argument favoring the credibility of the present molecular dynamic results is the close agreement of the size dependence of the modulus (in the static calculations) with theory and the correct functional dependence of the modulus and crack energy of formation on the sample size and on the crack length during propagation. This suggests that the results for crack propagation are quantitatively quite good at the early stages of propagation. Of course, as the crack grows, the size effect becomes more important. This may introduce some systematic size dependence in the crack velocity results but such systematics are outside the scope of the present analysis. The fact that the crack velocities rapidly attain a constant value less than the sound velocity, in accord with experiment, is another argument for the credibility of the dynamic results. As the c-strain results produced a number of results in agreement with our physical understanding of crack propagation and no surprising result inconsistent with this understanding, the c-strain results are regarded as highly credible.

While similar arguments about size effects can be made about the c-stress results and their credibility, the one surprising new result is the crack that propagated with all the applied work (energy) going to create crack surface energy. Can this result be true in nature, or is it some artifact of the simulation? As two out of the three different crack-stress configurations in the c-stress case propagated in the expected manner, this result is certainly not a consequence of some grossly spurious constraint in the simulation. The only feature in the c-stress situation which differs from the usual mode of initiating fracture is the abrupt increase in stress. This rapid stress increase may allow the system to attain a configuration not accessible through the usual equilibrium configurations. Thus, while the unexpected energy sharing in one of the c-stress cases, which is a violation of the assumption of the Griffith model, is not believed to be a size effect it may well be the result of the (artificial) rapid stress increases made in the calculation. Unfortunately, as crack propagation could not be obtained by a slow increase of the stress, a systematic study of the origin of this new effect was not possible and its credibility cannot be established. Otherwise, the results are considered quantitatively reasonably (80 - 90%) correct.

The observation of dislocation formation during crack propagation is quite credible for several reasons. From the static mole-

cular dynamic calculations at c -strain and c -stress it is apparent that the two-dimensional Lennard-Jones solid must be just in the vicinity of brittle-ductile behavior since small variations in boundary conditions and crack shape can drive the behavior either way. Further, the Rice and Thomson model for dislocation formation stresses the importance of the region near the crack tip in determining the brittle-ductile behavior. As the region is quantitatively well described in the molecular dynamic calculations, the formation of dislocations should be realistic and the quantitative results reasonably accurate.

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