# Fracture in one dimension

R. W. Welland
*Department of Mathematics, Northwestern University, Evanston, Illinois 60208*

M. Shin
*Department of Physics, Northwestern University, Evanston, Illinois 60208*

D. Allen
*Department of Physics, Wheaton College, Wheaton, Illinois 60439*

J. B. Ketterson
*Department of Physics, Northwestern University, Evanston, Illinois 60208*
(Received 27 January 1992)

The position- and time-dependent statistical probability for fracture of a one-dimensional string of Lennard-Jones atoms has been evaluated as a function of the temperature, tension, and length. A surprising exponential dependence of the fracture-site probability with distance from a string end is observed.

We will conjecture that a one-dimensional string with a sufficient number of atoms, $N$, linked by any typical intermolecular force, is dynamically unstable when subjected to a tension at finite temperature. It is simply a matter of time until a configuration of the atoms arises (in the $2N$-dimensional phase space in which the system dynamics evolves) that permits "nucleation" and growth of a state involving two separated sections (the broken string segments), which then accelerate in opposite directions (under the action of the force, applied to the end atoms, which was the original source of the string tension).

In spite of a long history, fracture is still a rather poorly understood phenomenon. Admittedly, the most interesting fracture problems involve three-dimensional (3D) solids. Since accurate molecular-dynamics simulations (the technique we use) of 3D materials are costly and the range of structures, environments, and intermolecular-force forms rather vast, we feel it is useful to begin to develop a database of "simple" 1D cases. We are well aware that, if the history of thermodynamic phase transitions (and its dependence on system dimensionality) provides any hint regarding the inherently nonequilibrium character associated with fracture, the one-dimensional case may not generate information which carriers over in a simple way to higher dimensions. The 1D system nonetheless falls in the general class of fracture problems and so we proceed with no further apologies.

In the molecular-dynamics method, one integrates Newton's laws for an ensemble of atoms moving under prescribed intermolecular (and any external) forces. In our work the coupled set of differential equations was integrated using a fourth-order Runge-Kutta algorithm. Once the initial configuration is defined, the time evolution of the system is deterministic. The intermolecular force we chose is the so-called Lennard-Jones form. All interior atoms are subjected to this potential from their neighbors to the left and right (i.e., we include nearest-neighbor forces only). The two end atoms ($j=1$ and $N$), in addition to sensing the adjacent (interior) atoms, are subjected to a force $F$ (to the left and right for atoms 1 and $N$, respectively); this results in a string tension.

For actual calculations we used the potential (written in dimensionless form)

$$V(q)=\frac{1}{12}\left[-\frac{2}{(1+q)^6}+\frac{1}{(1+q)^{12}}\right]; \tag{1}$$

this potential has a minimum for $q=0$. Newton's laws take the form (for a mass of unity)

$$\ddot{q}_j=V'(q_{j+1}-q_j)-V'(q_j-q_{j-1}), \tag{2a}$$

for all interior atoms, and

$$q_N=V'(q_N-q_{N-1})+F \tag{2b}$$

and

$$q_1=V'(q_2-q_1)-F, \tag{2c}$$

for the first and last atoms, respectively.

It is nontrivial to define a sensible set of initial conditions. Since we are assuming our string will ultimately break, it makes no sense to speak of an equilibrium stretched string at finite temperature.[1] In fact, even in the absence of a tension, a finite-temperature string with free ends can "evaporate" atoms (or groups of atoms) off an end. We might think of subjecting an (initially) unstretched, finite-temperature string to a tension at $t=0$ and track its subsequent time evolution. However, the tension causes the string to stretch and the sudden application of the tension generates perturbations which propagate to the interior and damp very slowly; the intersection of traveling perturbations (after single or multiple reflections form the ends of the string) may result in "premature" fracture.[2,3]

We have found that the following start-up procedure

leads to an acceptable time evolution: (i) the atoms were assigned an equilibrium spacing which is obtained from the actual length of strings, which, in earlier runs (at the same temperature and tension), survived for a relative long time without fracture (this is clearly a bootstraplike process); (ii) a set of initial velocities and displacements was generated which corresponds to exponential kinetic- and potential-energy distributions equivalent to some "temperature" $T_s$.[4] If we track the time dependence of the system following such a start-up procedure, we find that any imbalance between the kinetic and potential energies (outside that expected on the basis of fluctuations) decays in an oscillatory fashion (involving an Einstein-like frequency) with a relaxation time constant $\tau_R$, which is generally much less than the characteristics break times $\tau_R$. The equilibrated average kinetic energy is used as a string temperature.

The break time and break point depend (somewhat insensitively as we shall see) on the initial distribution (whose mean alone is fixed). A large number of independent runs were performed to develop an accurate time- and position-dependent breaking probability. New sets of such runs were performed for each tension $F$, temperature $T$, and atom number $N$ studied.

The break time must be defined in some manner. We declared our string to be broken when the spacing between any two pairs of atoms exceeded ten lattice spacings. However, the time at which this occurs involves the time required to accelerate the two string segments to this spacing and is not a reasonable choice for the break time. The actual break was defined as follows. On each Runge-Kutta iteration, the instantaneous separations of all atoms in the lattice were computed and the position of the pair having the largest spacing was stored along with the time. The break *time* was defined as that prior time at which the spacing of the pair that ultimately broke first achieved the largest-spacing status. The average break time is defined as

$$t_B = \frac{1}{R} \sum_{r=1}^{R} t_r \ , \tag{3}$$

where $t_r$ is the break time in any given run and $R$ is the total number of runs (for a given $T$, $F$, and $N$).

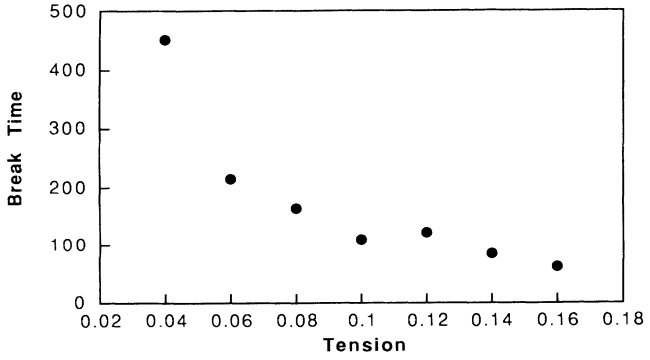


FIG. 1. Plot of the break time $t_B$ as a function of the string tension $F$; here the temperature ($T$) is 0.008 76 and $N=51$.

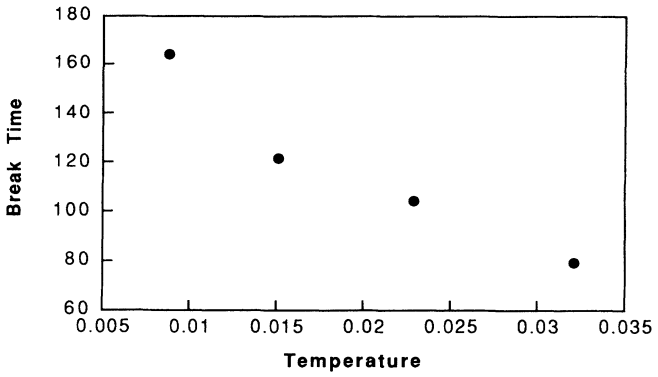


FIG. 2. Plot of the break time $t_B$ as a function of the temperature; here $F=0.08$ and $N=51$.

In the presence of an external string tension, the system is no longer closed; i.e., its energy is no longer constant. An extreme example is the behavior after fracture: The tension is then resolved into two forces, which accelerate the two string segments, and the kinetic energy is then unbounded. We have studied the time dependence of the total energy prior to fracture; we find that it slowly fluctuates both above and below the initial energy, but generally stays within 10% of that value.

We now present some representative results.[5] Figure 1 shows the break time as a function of the string tension, while Fig. 2 shows the break time vs temperature ($T$) (the values of the remaining state parameters are listed in the captions). As would be expected, the break time is longer for smaller tensions and temperatures.

Perhaps the most interesting behavior involves the position at which the string breaks. Rather than averaging the break time irrespective of the break site, we accumulate the number of breaks at a given site irrespective of the fracture time. The fracture-site statistics are shown for three different values of the temperature in Figs. 3(a)–3(c). Clearly, the probability of fracture is strongly site dependent. To analyze these data we introduce a

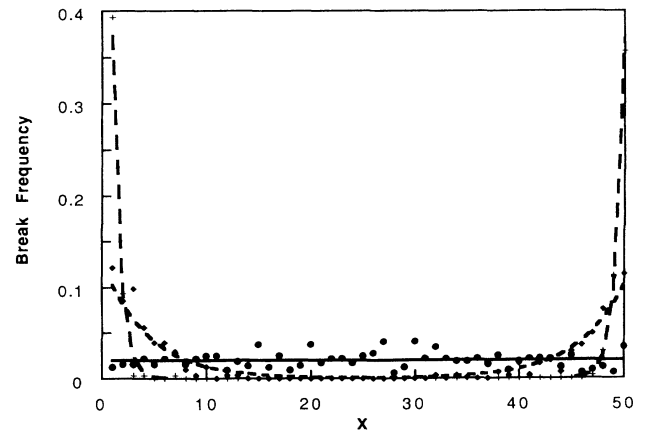


FIG. 3. Fracture-site statistics for temperatures of (a) 0.0038, (b) 0.0088, and (c) 0.050; here $F=0.08$ and $N=51$.

breaking probability function to $P(j,t)$, which depends on the discrete site index $j$ and the continuous time variable $t$. The data shown in Fig. 3 then involve the form[6]

$$p_N(j)=\int_0^\infty P_N(j,t)dt \ . \tag{4}$$

The function $P(j)$ must be symmetrical about the center of the string; i.e.,

$$p_N(j)=p_N(N-j) \ . \tag{5}$$

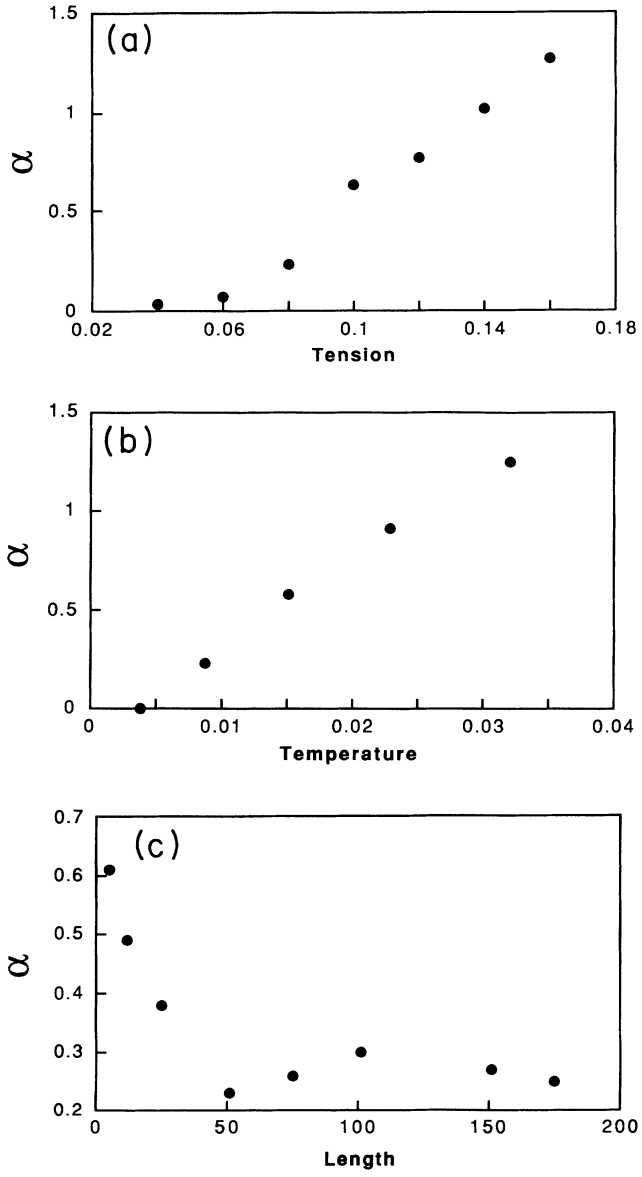


FIG. 4. Plot of the constant $\alpha$ (a measure of the site decay probability) as a function of (a) $F$, (b) $T$, and (c) $N$; the remaining state parameters $F$, $T$, and $N$ have the values 0.08, 0.008 76, and 51, respectively, and where relevant.

The solid lines in Fig. 3 show a least-squares fit to the form

$$p_N(j)=A\cosh[\alpha(j-N/2)] \ , \tag{6a}$$

where

$$A^{-1}=\sum_{j=1}^{N}\cosh[\alpha(j-N/2)] \tag{6b}$$

is a normalization factor. It will be observed that this form provides a rather good representation of the data. This expression says that the probability for fracture decreases exponentially as one proceeds in from either end of the string. We have found that Eq. (6a) provides a good description for a wide range of state parameters. Figures 4(a)–4(c) show the behavior of the decay constant $\alpha$ as function of $F$, $T$, and $N$ (for the values listed of the remaining state parameters).

We performed a number of experiments to test the stability of the fracture site as a function of a change in the initial conditions (velocities only). The initial velocity distribution may be regarded as a point $P$ on the surface of an $N$-dimensional sphere $S$ (with its origin at 0), whose equation is

$$\sum_{j=1}^{N}\dot{q}_j^2=E_{\rm kin} \ , \tag{7}$$

where $E_{\rm kin}$ is the starting kinetic energy.

Our perturbation consisted of choosing a nearby point $P'$ on the same sphere at a distance $d$ $(=d_{P'P})$ from $P$. The fracture experiments were repeated with the initial velocity vector altered from $P$ to $P'$. The $P'$ were chosen at random for various values of $d$. The striking feature was that in a large fraction of the cases, the break site did not change, even for $d/d_{\rm OP}$ as large as 0.1. This relative insensitivity to the initial conditions shows that the phenomenon of one-dimensional fracture is not deterministically chaotic.

In conclusion, we have examined what is perhaps the simplest example of fracture: a stretched 1D lattice. Apart from the rather obvious result that fracture is enhanced by higher temperatures and tensions, an unusual exponential dependence of the probability for fracture at a given site with distance from a string end has been discovered. Clearly, conditions which would lead to fracture when they occur close to an end have an opportunity to mend if they occur further into the lattice. The procedures we have developed for obtaining a set of starting conditions should be useful in studying 2D and 3D fracture.[7]

This work was supported by the Office of Naval Research under Grant No. N00014-88-K-0106 and by the PEW Foundation.

[1]The question of whether all starting configurations having some minimal energy will actually lead to breaking is a subtle one. One can imagine that certain configurations might be stable and not redistribute their energy so as to make a "hot spot" or other nucleation center for fracture. An example of a coherent motion is very-long-lived solitonlike structures, which are relatively easy to generate.

[2]The study of the decay of some initial perturbation in a 1D string has a long history. The early work of E. Fermi, J. Pasta, and S. Ulam, in *Nonlinear Wave Motion,* Vol. 15 of *Lectures in Applied Mathematics,* edited by A. C. Newell (American Mathematical Society, Providence, RI, 1974), p. 143, set the stage for the later identification of the soliton by N. J. Zabusky and M. D. Kruskal, Phys. Rev. Lett. **15**, 240 (1965).

[3]J. Ford and J. Waters, J. Math. Phys. **4**, 1293 (1963).

[4]This is accomplished using the so-called Box Meuller algorithm, which takes pairs of numbers from 0 to 1 at random and converts them into a set of random numbers that have a preassigned standard deviation.

[5]We have been unable to find any systematic studies of 1D fracture in the literature. A study of two cross-linked chains moving in 2D was performed by A. I. Melker and A. V. Ivanov, Phys. Status Solidi A **84**, 417 (1984); the phenomena reported here were not discussed.

[6]In adopting this normalization condition, we are implicitly assuming that any non-fracture-inducing initial conditions are of measure zero.

[7]Several dynamical studies of 2D fracture have been performed. As an example, A. Paskin and O. K. Som, Acta Metall. **31**, 1253 (1983), have studied the propagation of cracks in 2D Leonard-Jones lattices.