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The fracture of perfect crystals under uniaxial tension at high temperatures

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Abstract. The fracture of a perfect crystal at a number of temperatures was investigated using molecular dynamics computer simulations in which a crystal was pulled apart at a constant strain rate. At low temperatures the overall stress increased to a maximum after which a series of distinct structural rearrangements each accompanied by a sharp reduction in stress were observed. The material maintained a high degree of crystallinity. At higher temperatures structural rearrangement was more continuous and the material in the region of fracture was more disordered and somewhat liquid-like. At all temperatures failure occurred through the formation of voids which subsequently fused to leave bridges between the nascent surfaces. These bridges stretched and finally broke. In another series of experiments the failure of a bridge which had formed spontaneously between two nearby surfaces was investigated under similar conditions of steadily increasing strain.

1. Introduction

Although the strength of real materials is determined by the number and the behaviour of dislocations, cracks and other imperfections, the ultimate strength of materials depends on the strength of perfect crystals. Probably the first discussion of the strength of a perfect crystal was given by Zwicky [1] in 1923, when he calculated the change in potential energy of an ionic model of sodium chloride as a function of lattice parameters as it was elongated in the (100) direction. In 1972 Macmillan and Kelly [2] considered the sodium chloride crystal again and also studied a Lennard-Jones model of crystalline argon. They showed that if a uniaxial strain is applied to a face-centred-cubic crystal of Lennard-Jones atoms and the crystal remains homogeneous, the maximum stress which the crystal can sustain (the tensile strength of the material) depends on the direction of the strain and on whether the unit cell dimensions perpendicular to the stress direction are allowed to relax.

Macmillan and Kelly's work treats the crystal as classical and ideal, with no fluctuations in the positions of individual atoms. The strained crystal becomes anisotropic, but remains homogeneous. However, at temperatures above absolute zero there are fluctuations in atomic positions which may provide an alternative mechanism for fracture. Once a crack occurs as a result of a fluctuation it can lead to fracture if it propagates. For this to occur the timescale of the fluctuation forming and closing the crack must not be too short compared to the timescale for its propagation, and Griffith's criterion for propagation must be satisfied. This criterion is derived from a

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continuum model for the material and gives a maximum stress [3], σ_m

$$\sigma_m = \left(\frac{2E\gamma}{\pi l}\right)^{1/2} \tag{1}$$

where E is Young's modulus, γ is the surface energy per unit area of the new surfaces that are formed and $2l$ is the length of the crack.

This treatment assumes that the crystal remains solid. Near the melting point this is not true. Just as a fluid may be solidified by applying pressure (provided the density of the solid is greater than that of the liquid), so a solid may melt under tension. As the temperature is raised a point will be reached when the solid melts under tension before it breaks. Once it has melted its tensile strength is determined by the tensile strength of the liquid rather than that of the solid. In this context it is interesting to note that LaViolette [4] has shown that a Lennard-Jones material at low densities has disordered glassy states that are lower in energy than a uniformly expanded face-centred-cubic lattice. However, in the work described in this paper the expansion is allowed to be non-uniform and it seems unlikely that there are accessible low-energy disordered states with uniform densities at very low temperatures. At non-zero temperatures the question is of how the free energy of the stretched crystal compares with that of a fractured crystal. Even if the bulk of the fractured crystal remains crystalline, the new surface formed may be roughened or disordered, and this affects the statistical mechanics of the fracture process. In a real system with macrosopic dimensions the stretched crystal is less stable than two separated crystals in equilibrium with a gas, as the ratio of the surface energy to the bulk energy can be made arbitrarily small. Provided, however, that the stretched state corresponds to a local minimum in the free energy, it is metastable.

Selinger and co-workers have recently been investigating the statistical thermodynamics of stretched perfect crystals, using a mean-field model and simulations of a two-dimensional Lennard-Jones system to illustrate their ideas [5–7]. They find that as the stress on the crystal is increased a critical value is reached at which the stretched state becomes unstable and fails as a result of the growth of defects caused by thermal fluctuations. They draw an analogy with the approach to a spinodal. If the applied stress is very close to the critical stress, thermal fluctuations can lead to a spontaneous change to the stable state (two separated crystals), but otherwise they find that the metastable lifetime is long. In an investigation of crystals with defects [7] they find that failure occurs when the maximum local stress reaches this critical value although the presence of defect-caused failure at a lower overall stress.

Computer simulation using atomistic models provides a valuable tool for investigating dynamic processes at non-zero temperatures. Although only hundreds or sometimes a few thousand atoms can be simulated for times up to about a nanosecond, careful choice of the model system can be used to gain insight into the microscopic basis of macroscopic phenomena. For example there have been several studies of crack propagation in small regions of metals [8, 9] using such methods. The question of the tensile strength of particular materials was addressed by Parinello and Rahman [10] for a model of nickel and by Soules and Busbey [11] for model silicate glasses. Parinello and Rahman applied uniaxial stresses to an array of 500 atoms arranged on a face-centred-cubic lattice. The system had periodic boundary conditions and the size and shape of the molecular dynamics cell could vary in response to the internal stress. The temperature of the simulation (350 K) was well below the melting point and the results obtained were in good agreement with the predictions of Macmillan and Kelly [2].

In the work described in this paper the behaviour of crystals of methane (modelled by Lennard-Jones spheres) under a steadily increasing strain was investigated using molecular dynamics simulations. In the first series of experiments the starting point is two interacting crystals which are joined by a bridge (formed spontaneously), and in the second series of experiments the initial state is a single perfect crystal. These numerical experiments were performed at a number of temperatures. The lowest temperature used was 50 K, where earlier work [12] showed that the crystal surface remains ordered. The other temperatures used were 80 K, where there is partial disorder in the outermost layer of atoms due to vacancy formation by promotion of atoms into an overlayer, and 100 K which is near the bulk melting point of the model ($\approx$ 105 K). The earlier work also showed that as the surface disorder increased, atomic mobility increased and the surface energy decreased.

Both sets of experiments were dynamic experiments in which the elongation in the z direction was increased uniformly with time at a rate of 4 m s^{-1} (4 Å in 100 ps). No relaxation in the x and y dimensions was allowed. By working under conditions in which the strain rather than the stress is specified it is possible to investigate the microscopic behaviour of the material beyond its maximum stress as it breaks. The most interesting results from these experiments lie in this region. For example, at 50 K, an initially perfect crystal undergoes a series of structural rearrangements, each of which is associated with a sudden change in the stress. At all separations the material remains highly crystalline, and these events correspond to the insertion of additional crystal planes between the original planes with the concomitant formation of voids. At 80 K structural rearrangement events are less well defined, with a much greater degree of disorder in the region of fracture. The formation and fusion of voids are key events in the fracture process at all temperatures.

The work described in this paper follows from earlier work [13] in which two crystals of methane were brought into close proximity and allowed to equilibrate at different fixed separations and a number of temperatures. The observed behaviour depended strongly on whether the temperature was high enough that the isolated crystal surfaces (chosen to be (100) faces of a Lennard-Jones face-centred crystal) were disordered with at least the top layer of atoms being quasi-liquid-like, or sufficiently low that all the layers were ordered and crystalline. When two partially ordered surfaces were placed a few lattice spacings apart atoms were observed to move from the overlayer and the top layer of each surface to form a bridge between the surfaces. At 80 K there was still some crystallinity in the bridge, while at 100 K the bridging atoms appeared to be completely liquid-like. No bridges were formed between the crystalline surfaces at 50 K although at a separation of one lattice spacing the outer layers of the crystal moved towards each other to form a single uniaxially strained crystal. When a crystal is fractured a new surface must be formed, and one anticipates a change in the fracture behaviour of the crystal according to the degree of order of the surfaces that are formed. In the original work [12] it was found that the (100) surface of a multilayer remained crystalline up to 50 K. This same behaviour occurs on the free surface in the present model when parametrized to represent methane.

The nature of the model, in which a slice of moving atoms is sandwiched between bulk material, forces a fracture to occur in this particular part of the crystal and does not allow a uniform homogeneous expansion of a perfect lattice. However, a perfect crystal fractures somewhere and this model is probably more realistic than a model with periodic boundary conditions in the z direction as well as in the x and y directions which would force simultaneous fracture in all the repeated units.

2. Details of the calculation

The model, which represents a pair of fused or partially fused crystals being pulled apart, is the same as that used in earlier work [13]. Each crystal is represented by four layers of moving atoms backed by one layer of fixed atoms and a continuum representing the average interaction of the rest of the crystal. Two crystals are placed with their faces parallel, facing each other, so that there is the equivalent of eight full layers of moving atoms between two fixed layers with a continuum above and below. The distance between the fixed layers is constrained to be constant or to vary in a predetermined way. Thus in these experiments the strain is varied rather than the stress.

The interatomic potential used was the standard Lennard-Jones 12–6 potential

$$V = 4\epsilon\left[\sum_{\text{pairs}}\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right]. \tag{2}$$

All results from simulations using this potential may be scaled by varying the energy factor, ϵ, the distance factor, σ, and the particle mass, m. It is useful to choose a particular material for reference to gain a physical feeling for the time, distance and length scales that are involved in a real system. The Lennard-Jones potential provides a reasonable description of molecular crystals or rare-gas crystals in which the cohesive energy is primarily due to the dispersion interaction. The material chosen here for comparison is molecular deuteromethane with

$$\epsilon/k_B = 149\ \text{K} \qquad \sigma = 3.78\ \text{Å} \qquad m = 20\ \text{amu}$$

where k_B is Boltzmann's constant. The corresponding Lennard-Jones time unit ($\tau_{LJ} = (m\sigma^2/\epsilon)^{1/2}$) is equal to 1.52 ps and the force unit (ϵ/σ) equal to 5.43×10^{-12} N. The results may readily be rescaled to fit argon or krypton. For example for argon

$$\epsilon/k_B = 120\ \text{K} \qquad \sigma = 3.40\ \text{Å} \qquad m = 40\ \text{amu}\,.$$

In all the numerical experiments described here a uniaxial strain is applied along the $\langle 001\rangle$ direction of a face-centred-cubic crystal. The strain direction is designated the z axis. The x and y dimensions of the system are kept constant. In the elastic regime the ratio of the stress to the strain in this direction is equal to the elastic constant C_{11}, and contains no contribution from the shear constant C_{44}. The atoms in the $\{100\}$ planes perpendicular to the strain are not close-packed and, in the ideal crystal, the separation between planes, d_0, is given by

$$d_0 = a_{nn}/\sqrt{2} \tag{3}$$

where a_{nn} is the nearest-neighbour distance, which was set equal to 4.214 Å (1.115σ). This was the internuclear distance found for the bulk crystal at 80 K using the model potential, and was not altered for runs at other temperatures, so that the comparisons are of materials at the same density.

Simulations were carried out using the method of molecular dynamics [14] in which the classical equations of motion are integrated. The leapfrog algorithm [14] was used. It is important to thermostat the system as the application of a varying strain feeds energy into the system. In these calculations this was done by applying a Gaussian thermostat [15] in conjunction with a weak Berendsen thermostat [16] to correct any drift. The time step was 0.005 ps (0.0033 Lennard-Jones units). The potential was cut off at 12 Å (3.175σ).

The computer used was an AMT-DAP with an array of 64 × 64 processors. The highly parallel nature of the architecture was exploited in the way described by Fincham [17]. The 512 moving atoms were divided into eight sets of 64 atoms which were treated together, and the forces between all members of pairs of such sets were calculated simultaneously.

Each run was initiated from a well-equilibrated configuration taken from earlier simulations [13] in which the crystals were held at fixed distances apart [13]. The velocities were reset from a random Boltzmann distribution at the corresponding temperature. The runs were carried out in segments, normally 50 ps (104 time steps) long, during which the layers of fixed atoms were moved apart at a constant rate of 0.04 Å ps^{-1} (4 m s^{-1} or 0.0161 $\sigma\tau_{\mathrm{LJ}}^{-1}$).

The average energy per molecule and the total force due to the rest of the material on each substrate, i.e. on the fixed layers and the continuum backing them, were monitored during the run. Although it is the strain that is specified in these runs rather than the stress, the force per unit area of the substrate is equal to the stress that would have to be applied to maintain the imposed strain.

After each segment of 50 ps the last configuration was stored for later analysis, which included measuring the density profile in the z direction, the distribution function of interatomic distances as a function of r^2 (a quantity closely related to the radial distribution function) and a histogram of the number of nearest neighbours of each atom. A nearest neighbour was defined by an atom within 1.4σ or 5.29 Å and atoms in the layer next to the fixed layers were excluded from the calculation. All the results were obtained from runs on a model system with eight layers of moving atoms. They will be presented as a function of the distortion, d, defined in units of d_0, the ideal interlayer spacing, by

$$d = b/d_0 - 9 \tag{4}$$

where b is the distance between the layers of fixed atoms. In an ideal crystal with eight layers of moving atoms, $d = 0$. The relative distortion is $d/9$.

3. Results

3.1. Bridged crystals

In the first run the initial configuration (figure 1 (top left)) was taken from a simulation at 80 K ($T/\epsilon = 0.53$) in which a bridge had formed spontaneously between two crystal faces held at a constant distance apart $d = 2.75$. This temperature [12] is below the bulk melting point, but high enough that the outer layer of the (100) surface of a free crystal would be somewhat disordered at equilibrium. Figure 1 shows four configurations taken at intervals during a run in which the two crystals are separated at a constant rate, showing how the material in the bridge is pulled out, the bridge gets thinner and finally breaks. Initially the bridge is continuous in the direction perpendicular to these pictures and atoms from the top layer of each crystal (4th from

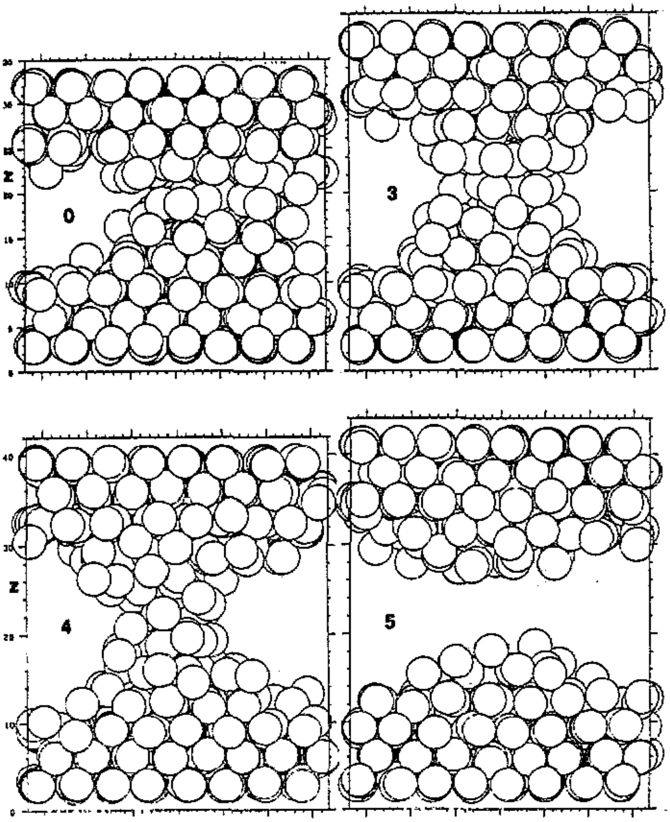

Figure 1. Four configurations showing stretching and breaking of a bridge between two surfaces at 80 K. The numbers correspond to points on the energy and stress graphs in figure 2.

the fixed layer) are pulled into it as it stretches. Eventually it breaks into short lengths in the y direction before finally breaking.

In equilibrium, the stress is the derivative of the free energy rather than the energy, so that the variations of force and energy with extension provide different information. The response of the system to the strain may be studied by comparing these macroscopic quantities (figure 2) with the microscopic information in figure 3 which shows density profiles in the z direction (parallel to the strain) at the points marked on figure 2. Initially there is an attractive (negative) force between the surfaces, which, on a macroscopic view, would be attributed to the surface tension in the bridges. As the crystals are pulled apart the restoring force increases to a maximum near configuration 1. The density profiles for configurations 1 and 2 (figure 3) show that there is a distinct layer structure even in the bridge region, which is stretched. In this range of distortion the bridge is behaving elastically and the structure is unchanged. Between configurations 1 and 2 there is an abrupt decrease in the restoring force and a maximum in the energy. The nature of the structural change that results in the decrease in restoring force is indicated in figure 3. The density profile for configuration 2 shows that an additional layer has been formed in the bridge region. From points 2 to 3 this new structure behaves quasi-elastically, and is followed by another relaxation process between configurations 3 and 4, in which the three-layer structure of the bridge is lost. The quasi-elastic stretching followed by relaxation can be seen most clearly by examining the density maximum of the fourth layer which has been pulled out in configuration 3 and which has relaxed back to near its ideal position in configuration 4. Shortly after this the bridge breaks and the atoms move back into the surface. Notice that some still remain in an overlayer.

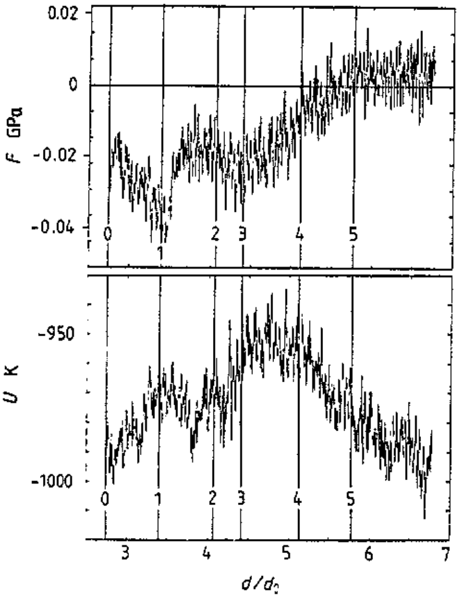

Figure 2. Variation of stress measured as force per unit area between substrates (GPa) and average energy per molecule (K) as a function of elongation, d, for runs in which a bridge between surfaces was broken. The numbers identify the configurations examined. The rate of change of elongation was constant; a time interval of 50 ps elapsed between configurations 1 and 2.

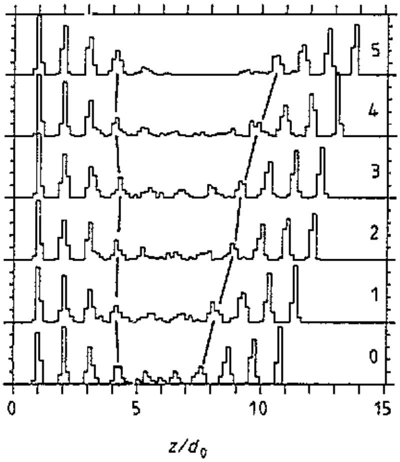

Figure 3. Density profiles along the strain direction for configurations at points marked on figure 2. The lower layer of fixed atoms is at $z = 0$ and the distance scale is in units of the ideal interlayer spacing, d_0. Lines trace the variation in positions of the fourth layers from the substrates.

In another series of runs the simulation was restarted from configuration 3 (which is near an elastic limit) and was allowed to relax at constant separation. The bridge finally broke after 250 ps.

3.2. Runs initiated from single crystals

The general behaviour of single crystals under a constantly increasing extension is somewhat similar to the behaviour in bridged crystals described in the previous section. At first the crystal stretches quasi-elastically, and then a structural change intervenes to give a new structure, which in turn is stretched quasi-elastically until it relaxes to another structure. The kinds of structural changes seen, however, are somewhat different. The first change is the formation of voids in the crystal. These then fuse together leaving bridges between two crystal surfaces and finally the bridges break. In this part of the work the variation of behaviour with temperature was studied. Three temperatures were chosen. The first was 50 K ($T/\epsilon = 0.33$), a temperature at which no surface roughening was found [12] on a flat (100) surface on the timescale of hundreds of picoseconds. The second temperature was the same as that for the first series of experiments (80 K, $T/\epsilon = 0.53$) and the highest temperature was 100 K ($T/\epsilon = 0.67$), which is sufficiently close to the bulk melting point that the disordered outer two layers contain atoms which diffuse at liquid-like rates.

Figure 4 shows the variation of the compressive stress or force per unit area between the crystals (above) and average energy per molecule (below) for runs at these three temperatures as a function of elongation. The variation of both stress and energy is considerably greater than before. Although the breaking stress required for a single crystal ranges from 170 MPa at 50 K to 120 MPa at 80 K and 70 MPa at 100 K, the stress required to break the bridge at 80 K was only 36 MPa. At the lowest temperature a series of very sharp structural changes are apparent in both stress and energy curves, at 80 K the corresponding changes are less sharp, and at 100 K the whole process is fairly smooth. The maximum restoring force, the limit of the initial quasi-elastic regime, occurs at an elongation $d \approx 1$ in all three runs, but the first maximum in the energy-versus-distortion plots, which one can identify as the point at which voids begin to appear, is delayed as the temperature is increased.

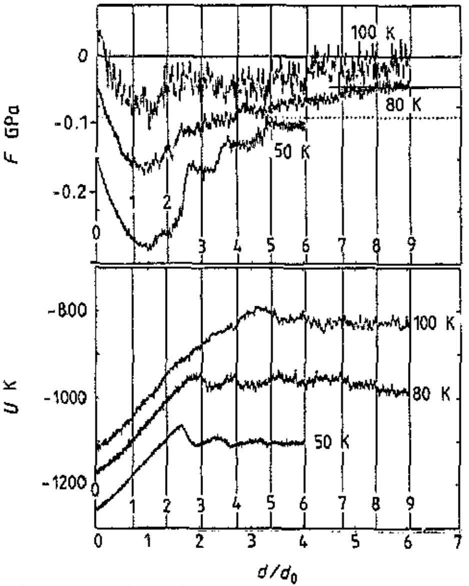

Figure 4. Variation of stress measured as force per unit area between substrates (GPa) and average energy per molecule (K) of a single crystal under a steadily increasing strain. The numbers identify the configurations examined, which are separated by 50 ps intervals. The stress curves for runs at 80 K and 50 K are displaced vertically, but the energy curves are on the same scale.

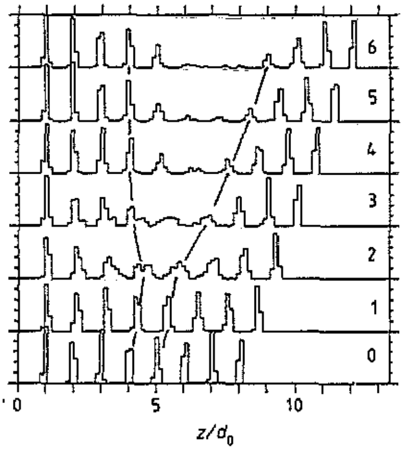

Figure 5. Density profiles along the strain direction for configurations at points marked on figure 4 at 50 K. The lower layer of fixed atoms is at $z = 0$ and the distance scale is in units of the ideal interlayer spacing, d_0. Lines trace the variation in positions of the fourth layers from the substrates. Intervening layers form as the crystal is pulled apart.

One aspect of the structural changes in the low-temperature runs is illustrated in figure 5 which shows a sequence of density profiles in the z direction. The corresponding points are labelled on the energy and stress graphs. Initially the whole crystal stretches elastically, but by point 2 the restoring force has passed its maximum although the energy is still increasing. The density profile shows that the central region is becoming more disordered. This increase of disorder is also shown in the radial distribution functions in figure 6 which are plotted as a function of r^2 so that successive shells of neighbours are equally separated. The disorder is a maximum at configuration 2. Between configurations 2 and 3 both stress and energy plots show a large structural relaxation. The origin of this can be seen in part in the z density distribution, which shows that an additional layer has formed in the central region, so that there are 9 rather than 8 layers. This implies the formation of voids of some kind, as the number of molecules is fixed. The void can be seen in two views of configuration 3 in figure 7. In the upper part of the figure the configuration is viewed from the side, while below is a view of the fifth and sixth layers of the crystal viewed along the strain direction. The shaded atoms are in layer 5 and the others in layer 6. Formation of the void has allowed most atoms to regain ideal lattice postions and the crystal to regain order. This can be seen in the increased sharpness of the third- and fourth-layer peaks in the density plots as well as in the radial distribution plots.

Each of the subsequent steps in the stress curve is associated with the formation of yet another layer intervening between the upper and lower crystals. Between configu-

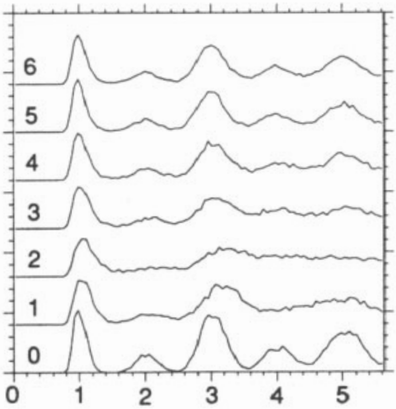

Figure 6. Average number density of atoms as a function of the square of the distance from a given atom for configurations from the run at 50 K. The scale is in units of the ideal nearest-neighbour distance squared. An ideal face-centred-cubic crystal has neighbours at $r^2 = 1, 2, 3$ and 4.

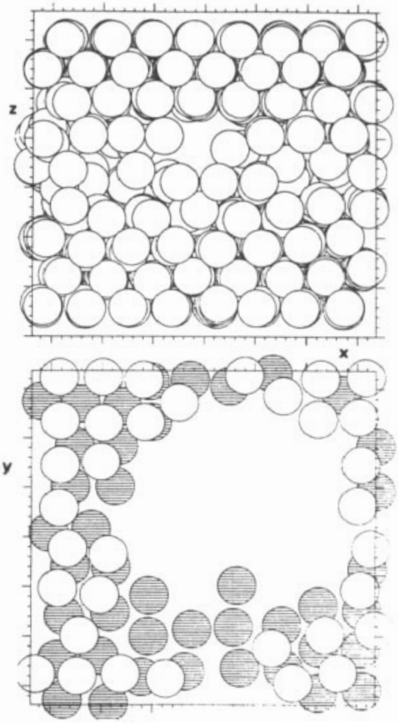

Figure 7. Views of configuration 3 from the run at 50 K. The strain axis is vertical in the top view. The lower view is of a horizontal slice through the configuration between $z = 15$ Å and $z = 22$ Å.

rations 3 and 4 the voids in neighbouring cells fuse so that the separating crystals are joined by bridges. By configuration 6 the bridges are broken and the crystal surfaces begin to flatten.

Three runs were performed at 50 K in order to investigate the reproducibility of the observations. In all the runs these curves were similar and the features associated with successive structural rearrangements were seen. In the initial stage of the stretching the force and the energy curves coincided to within the noise level. After the breaking point was reached at $d \approx 1$ there was some variation between the curves. For example the position of the first vertical step in the force curve fluctuated by about $0.1d_0$ in separation and by about 15 MPa in stress while the second and third steps varied by about $0.3d_0$ in position and 15 MPa in stress.

The general features of the behaviour at 80 K are similar to those at 50 K, but there are some important differences. At this temperature disorder is less unfavourable, and the bridges and surfaces of the crystal are more disordered. As a result the features associated with structural rearrangements in the force and energy curves are much less sharp. Comparing the density profile curves at this temperature (figure 8) with those at 50 K (figure 5) shows that they are indistinguishable up to point 3, that is until voids begin to form. After that point the formation of intervening layers is not seen and the bridge and surface layers appear quite disordered. This is also demonstrated in the radial distribution functions (not shown). The bridge is less easily broken than at 50 K, being still present (although broken into short lengths) in configuration 8 and finally disappearing by point 9.

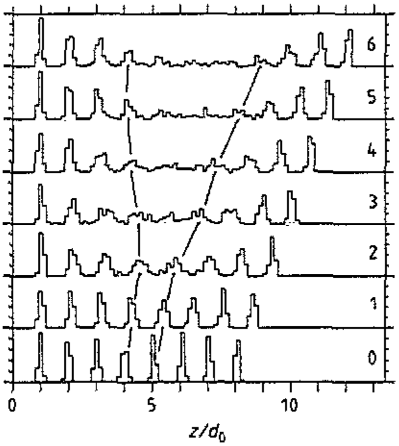

Figure 8. As figure 5 for the run at 80 K.

Compared with the same distortion at lower temperature the voids are smaller, the bridges more persistent and the material in them more liquid-like. This is illustrated in figure 9, which is a view of a slice through the central region at the same distortion as that shown in figure 7. Another comparison between the two temperatures is seen in figure 10 which shows histograms of the numbers of nearest neighbours in the configurations at 80 K and 50 K. At 50 K most molecules have 12 nearest neighbours in all the configurations, and in configuration 3 and higher there is a small peak at 8 nearest neighbours, 8 being the value for an atom in the surface layer. The distribution of nearest neighbours is much less sharp in the runs at 80 K, and behaviour is more liquid-like.

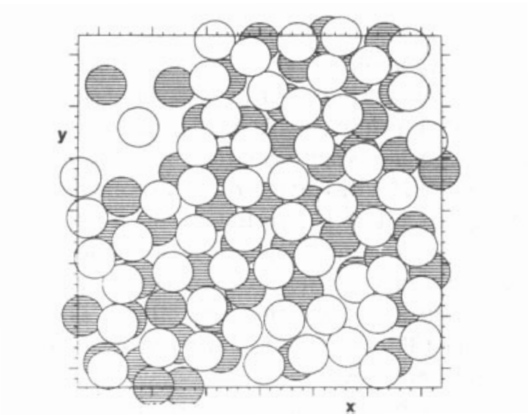

Figure 9. Slice through the central region of configuration 3 from the run at 80 K showing a small void in the top left-hand corner.

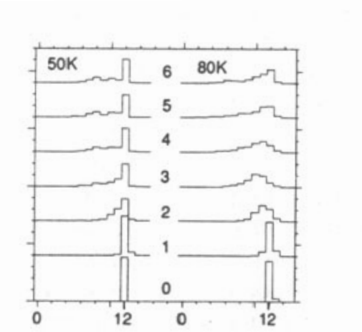

Figure 10. Comparison of numbers of nearest neighbours in configurations from runs at 50 K and 80 K.

4. Conclusions

In most real crystals the behaviour under strain is dominated by defects that are due to the past history of the crystal. In these numerical experiments the initial state is free from defects and all defects are introduced as a result of fluctuations due to the finite temperature of the crystal rather than its past history.

The breaking stress observed in these numerical experiments is significantly lower than those reported by Macmillan and Kelly [2] for homogeneous fracture at 0 K. Rescaling their results for our potential gives a breaking stress of 330 MPa for constrained elongation along (001), while here we find values which range from 90–175 MPa depending on the temperature for the breaking stress due to failure by spontaneous void formation in a crystal at non-zero temperature constrained in a similar way. It should be noted that Macmillan and Kelly found a lower breaking stress for failure accompanied by a shear instability, but all their results apply to zero temperature.

Wang *et al* [6] found that their system behaved reversibly up to the critical stress and that the value of the critical stress varied significantly with temperature. It is likely that the breaking stress measured in the dynamic experiments described in this paper is not much above the critical stress that would be observed in a static experiment. The breaking stress does indeed vary with temperature, but the breaking strain does not. Although the reversibilty of the system in an unloading experiment was not investigated except for one experiment on the bridged system beyond its critical strain, the response of the system at 50 K was reproducible within the noise level for strains less than the breaking strain. The system remains ordered in this range so that it is likely that stretching is fully reversible for strains less than the breaking strain.

There are interesting differences between the behaviour at 80 K and 50 K; the behaviour at 100 K is similar to that at 80 K. This difference can be summarized by saying that at 80 K the structure melts under the strain, but at 50 K it remains a solid. This is in accord with ideas recently put forward by Gelbart [18] who proposes a phase diagram in the temperature–strain plane to describe the fracture behaviour *of defectless crystals.*

The numerical experiments described here are dynamic experiments and are not thermodynamically reversible. Nevertheless it is apparent that the timescale of atomic motion allowed structural changes to occur as the strain changed. At higher distortion rates one expects that the major structural changes such as void formation will happen later. This was confirmed by one run at 80 K at twice the distortion rate. The energy curve was initially similar to that shown in figure 2, but it continued to increase and did not reach a maximum until $d \approx 2.7$. There was no sign of a succession of relaxation events, suggesting that the timescale for structural relaxation is a few tens of picoseconds at 80 K, as the time between configurations in figure 4 is 50 ps. The total length of the runs shown in figure 4 are 450 ps (300 ps at 50 K), and during this time structural relaxation occurs several times even at 50 K.

It must be remembered that in many ways this model is very artificial. Periodic boundaries at 33 Å in the x and y directions undoubtedly affect the system, particularly the process of fusion of voids and the form of the bridges. Modelling of each crystal by four layers of moving atoms on a rigid base, and the imposition of a constant distortion rate are additional simplifications. However, one must, of necessity, make compromises about the number of atoms in a numerical experiment. The model may be artificial, but is simple and well defined, and contains much of the essential physics of a real material.

Acknowledgments

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