COMPUTER SIMULATION OF IMPACT INDUCED FRACTURE AND FRAGMENTATION IN BRITTLE SOLIDS

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A modified molecular dynamics method is used to describe the dynamic fracture of impact loaded brittle solids with realistic microstructural features. This model is based upon the traditional molecular dynamics procedure applied to a spring model, but accounts for the irreversible nature of the fracture process by irreversibly deleting the attractive part of the particle interaction potential when the bond between two particles is stretched beyond a critical length. The model is used to examine dynamic fracture in perfect crystals as well as the influence of pre-existing microcracks on the fracture process. In each case, the majority of impact damage results from tensile waves produced when the initial impact pulse (compressive) reflects from free surfaces. Depending on the magnitude of the impact, the presence of microcracks may either enhance or hinder the material's resistance to impact fracture.

INTRODUCTION

Ceramics and other brittle materials are being employed with increasing frequency in the fabrication of components designed for high energy impact protection. Examples of these applications include monolithic ceramics for armor (1) and coatings for turbine blades (2,3), pistons and cylinders (2,4). The behavior of these materials in impact loading situations depends on many intrinsic properties of the materials such as density, elastic moduli, etc. However, once the composition of matter is determined, the impact performance of these materials may be manipulated by modifying the microstructure of the material. In order to optimize the microstructure of these materials, it is important to have computational tools capable of predicting the effects of microstructural variations on impact performance. In a recent series of papers (5,6), we introduced an extension to the Molecular Dynamics (MD) computer simulation method which is appropriate for examining impact fracture in brittle solids on a microstructural length scale. The model has been applied to the study of impact fracture in perfect material (5) as well as material containing cracks and grain boundaries (6). The purpose of this paper is to describe the effects of microcracks on the fracture behavior of the material and to elucidate a mechanism by which pre-existing microcracks can actually enhance the material's resistance to impact induced fracture.

METHOD

The simulation technique employed in this investigation is described in detail elsewhere (5,6). The method is based upon the molecular dynamics method, but unlike in traditional *atomistic* MD, we do not identify each particle with an individual atom but rather associate each particle with a small, discrete volume of material. The simulation cell is a two dimensional grid in the XY plane spanning 100 particles in the X and 101 particles in the Y directions. The material is discretized such that the initial interparticle spacing is 10 microns and the overall dimensions of the simulation cell are 1 mm in X by 0.86 mm in Y. The edges of the sample are free surfaces.

A finite range pair-potential is used to describe the energy of the system. This potential does not describe individual bonds between atoms, but rather the bonding between the particles, which are large groups of atoms. The parameters of the potential are chosen in order to produce the desired elastic properties of the perfect solid. In the present study, we employ the well known Lennard-Jones potential to describe the interparticle interaction, and adjust

FIGURE 1. Simulation cell and external forces.

the parameters to represent Al$_2$O$_3$ (5).

Since we are interested in brittle materials, the potential must be modified to reflect the fact that "bonds" between particles break if they are stretched beyond a certain cutoff, r_c. Although bond breaking is a reversible process on the atomic scale, in a more macroscopic view (as considered here) breaking "bonds" between the bigger-than-atomic particles is irreversible. Toward this end, when the interparticle distance first exceeds a pre-determined cutoff, the potential is truncated such that the bond's ability to support a load in tension is destroyed, although it retains its strength in compression. In the current work, we have simulated the presence of pre-existing microcracks by breaking selected bonds before the application of the impact load.

As described in Ref. 6, the model may be applied to realistic microstructures by superimposing the microstructure onto the grid of particles. Bonds falling within individual material phases or across interfaces are assigned potential parameters and a cutoff distance appropriate for each phase or interface. In the present work, only perfect homogeneous material and material containing microcracks is considered.

Once the microstructure is discretized into an array of particles, the simulation is started by applying an external impact pulse to pre-selected particles at an external surface of the sample. Forces are applied in the positive Y-direction to the center 10 particles on the Y=0 line of particles. Response to the impact is studied by integrating Newton's equations of motion for each particle forward in time for a total of 5000 time steps of duration 1.0×10^{-10} sec.

RESULTS AND DISCUSSION

Perfect Material

As described in detail in Ref. 5, initially undefected material was impacted with pulse heights ranging from 0.25 to 0.75 N/particle. An example of the final spatial distribution of broken bonds for a simulation conducted with F_{max} = 0.375 N/particle is shown in Fig. 2. The crack begins in a small central region eight lattice spacings ahead of the center of the impact zone and quickly bifurcates into a small X-shaped crack pattern. This crack is driven by the propagation of the initial compressive pulse into the material. Later, two new, independent cracks nucleate on either side of the X-crack and begin to grow parallel to the branches of this original X-crack. These cracks form after the compressive wave is reflected (and inverted) from the vertical free surfaces. At roughly t=2500τ, new cracks begin to from near the top corners of the sample and grow towards the main cracks as the run progresses. These cracks also result from the reflection and inversion of elastic waves from the free surfaces.

The temporal evolution of the number of broken bonds is shown in Fig. 3 for samples subjected to different impact pulse heights. In each case, total damage increases with increasing pulse height. The
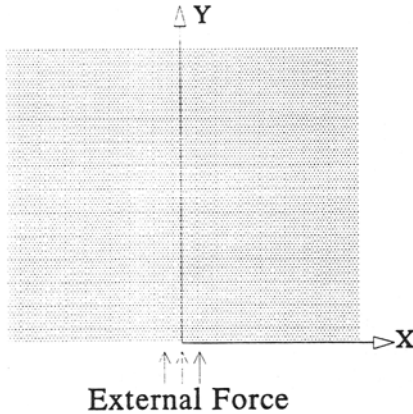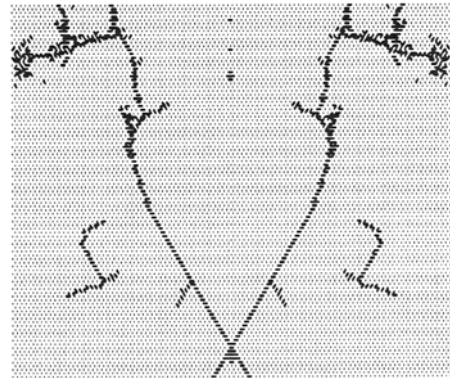

FIGURE 2. Crack pattern following the impact of the initially undefected sample at 0.375N/particle.
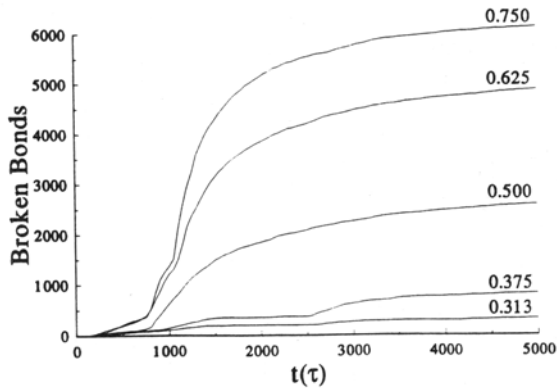
FIGURE 3. Number of broken bonds vs. time for initially undefected samples subjected to various levels of impact.

FIGURE 4. Crack pattern following the impact of the initially 1% microcracked sample at 0.375N/particle.

curves representing the largest impacts show a sudden jump in damage rate near $t=1000\tau$. This time corresponds to the first reflection of the input pulse from the free surface at the top of the sample. This reflection inverts the pulse which travels back into the material as a tensile wave. Since the bonds can support a high load in compression, but fracture if stretched in tension beyond the cutoff, tensile waves produce much more damage in the material and the damage rate accelerates when the tensile wave is formed. When the weaker impact is employed, the tensile wave produced at the first reflection has insufficient energy to fracture a large number of bonds. In these cases, the acceleration in damage rate is delayed until multiple reflections can constructively interfere ($t\approx2500\tau$).

Microcracked Material

Microcracks were introduced into the samples by randomly breaking a pre-determined number of nearest neighbor bonds prior to the start of the simulations (6). A representative distribution of broken bonds at the end of a simulation made with an initial defect concentration of 1% and an impact pulse height of F_{max} = 0.375 N/particle is shown in Fig.4. Comparison with Fig. 2 shows that some additional cracking occurs due to the presence of the initial microcracks, but in other areas (particularly near the top of the sample, where the stress pulse is inverted) the density of damage appears to be reduced in the microcracked case. The main effect of the microcracks is to destroy the coherency of the stress wave.
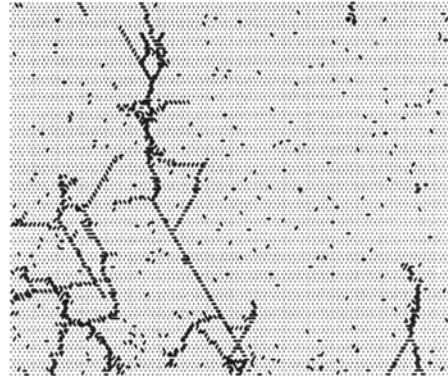
As illustrated in Fig. 5, at low impact pulse heights the presence of microcracks increases the number of bonds broken during the simulations, N_d, but at higher impact strengths the number of broken bonds is reduced when microcracks are initially present. This behavior can be explained by studying the temporal evolution of broken bonds in each case. Figure 6a shows N_d as a function of time for samples subjected to the large impact pulse height, F_{max} = 0.750 N/particle. Near the beginning of the simulations ($t<1000\tau$), the behavior of $N_d(t)$ is similar for each defect concentration. The curves for the pre-cracked samples begin to deviate from that of the initially defect free material only after the pronounced acceleration in damage rate at $t\approx1100\tau$. This is the time which corresponds to the initial reflection and inversion of the incident pulse. These curves indicate that the microcracks retard the
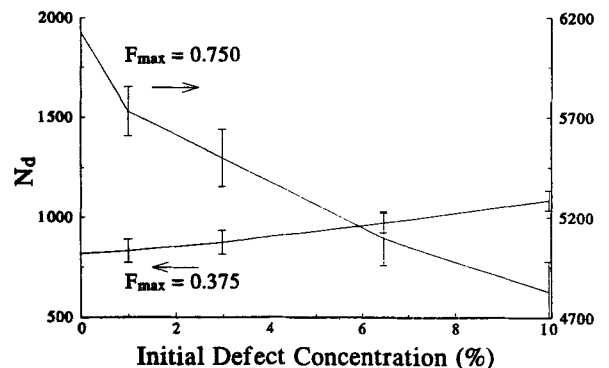

FIGURE 5. Number of bonds broken during simulation vs. initial defect level for impacts of 0.375 and 0.75 N/particle.
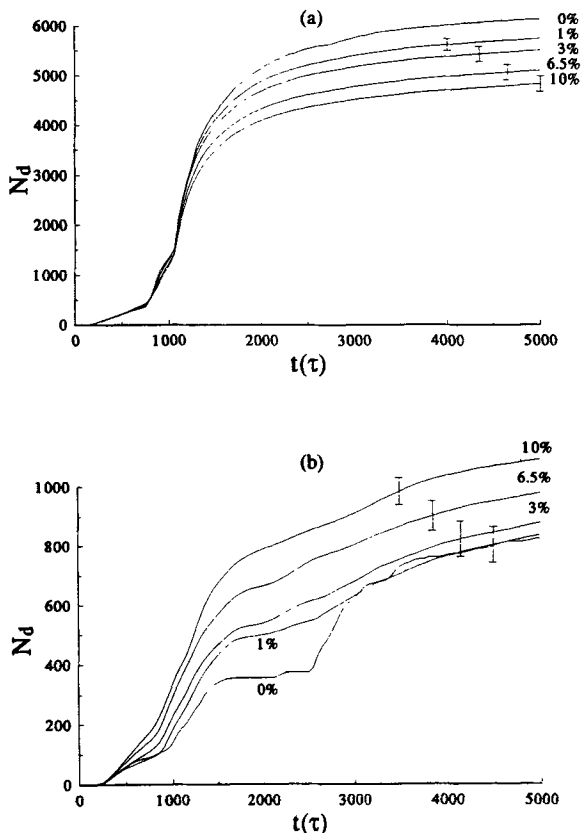
FIGURE 6. Number of bonds broken vs. time for initial defect levels of (a) 0.75 and (b) 0.375 N/particle.

propagation of the reflected tensile wave into the material thereby reducing the damage rate. Since a broken bond will support load in compression, but not tension, the microcracks tend to reflect tensile waves but not compressive waves. For the simulations performed at the lower impact pulse height, F_{max} = 0.375 N/particle, Fig. 6b shows that the behavior of the pre-cracked samples differs from that of the initially defect free material from the very beginning of the simulations. The pre-cracked samples display a higher damage rate prior to $t=1000\tau$ and the damage rate increases with initial defect concentration. In these samples, the pre-existing microcracks accentuate cracking by weakening the material, thereby allowing more damage to develop in the wake of the initial stress wave near the beginning of the simulation. The breaking of additional bonds stems simply from the fact that since a pre-broken bond supports no load in tension then this load must be redistributed amongst

the neighboring bonds. This mechanism is important only at low impact levels where most of the sample is not subjected to stresses strong enough to break bonds in the perfect material.

CONCLUSIONS

It has been demonstrated that the presence of microcracks may either degrade or enhance a material's susceptibility to impact damage (as measured by the number of bonds broken due to impact, N_d) depending on the strength of the impact pulse. The weakening effect results directly from the reduction in load which the material can bear due to the removal of load bearing bonds. The strengthening effect results from the ability of microcracks to destroy the coherency of the destructive tensile stress waves by locally reflecting them. In samples subjected to stronger impacts, the strengthening effect dominates because the majority of broken bonds result from the passage of the reflected tensile waves and the number of bonds broken in this way increases with impact pulse height. When smaller impact pulse heights are employed, the weakening mechanism is more important since the initial pulse is able to break bonds that it does not have sufficient energy to break in the initially perfect material.

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