Breakdown of Heterogeneous Materials

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ABSTRACT

We discuss the threshold activated extremal dynamics that is prevalent in the breakdown processes in heterogeneous materials. We model such systems by an elastic spring network with random breaking thresholds assigned to the springs. Results are obtained from molecular dynamics simulation of the system under constant stress and constant strain conditions. We find that the distribution $P(m)$ of the avalanches of size $m$, caused by the rupturing of the springs till the failure of the network, decays as a power-law: $P(m) \sim m^{-\alpha}$, where $\alpha$ can be closely approximated to $5/2$. The average avalanche size $< m >$ diverges as $< m > \sim (F_c - F)^{-1/2}$ close to the stress $F_c$ at which the total failure of the network occurs. We study the time evolution of the breakdown process: we find that the bonds rupture randomly over the network at initial times but the rupturing becomes highly correlated at late times to give rise to a well-defined macroscopic crack.

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It is known for a long time that defects play a crucial role in the process of nucleation of fracture in a material. A complete theoretical analysis of fracture starting from the elasticity theory and the deformation of elastic field around a defect is, however, viable only in very specific cases: like that of an isolated single defect in the form of a microcrack of suitable geometrical shape [1]. In a heterogeneous medium, consisting of defects of various kinds, shapes and vulnerabilities (from the point of nucleation of fracture) distributed over the medium, fracture phenomena becomes extremely complex due to the cooperative role played by the interacting defects over a wide range of length and time scales. Since fracture, at any stage, develops from the most vulnerable defect (weakest link of a chain), a theory based on a continuous coarse-grained description of fracture is untenable and a realistic computer simulation is almost unfeasible.

Most engineering as well as many natural materials like rocks, wood, glass (cellular), composite materials (fibre-glass, plaster...) are examples of heterogeneous systems. These materials, though widely different in their physical properties and chemical composition, show characteristic features prior to fracture when they are subjected to increasing stress or strain. In these materials, fracture does not develop from a single crack or a microcrack, rather, the macroscopic crack is preceded by myriads of microscopic crack nucleating from the defects and the final breakdown results from the birth, growth and coalescence of these microcracks. The formation of the microcracks are accompanied by release in the stored elastic energy which come out as acoustic signals of varying amplitude (energy). These signals are recorded in experiments and analysed. The experiments show that the probability density \( N(\epsilon) \) of microfractures with energy between \( \epsilon \) and \( \epsilon + d\epsilon \), follows a power-law: \( N(\epsilon) \sim \epsilon^{-\beta} \). Different materials are characterised by different values of \( \beta \): 1.25 in paper [2], 1.3 in synthetic plaster [3], 1.51 in wood [4], 1.9 in fiberglass [5] and 1.5 in cellular glass [6]. On the other hand, the cumulative energy emitted while approaching the fracture also shows power-law in situations where stress is controlled. For instance, in [4, 5], it was found that \( E(P) \sim [(P_c - P)/P_c]^{-\lambda} \), where \( E(P) \) is the cumulative energy released up to pressure \( P \) and \( P_c \) is the critical pressure at which the macroscopic failure occurs. The exponent \( \lambda = 0.27 \) seems to be universal for various substances and loading conditions. Similarly the acoustic emission \( E \) of a material under a constant load (pressure) at time \( t \) measured as a function of time shows \( E \sim (t_c - t)^{-\lambda} \) where \( t_c \) is the time required for the complete failure of the
material [5].

The scale-invariance manifested in the power-law form of the energy density $N(\epsilon)$ and its temporal correlation tells us that the development of fracture in heterogeneous systems does not take place from a single microcrack like what happens in Griffith-like nucleation of fracture [7]. Rather, fracture here is a strongly correlated phenomena where it develops over a large length and time scales from the growth and coalescence of microcracks in a self-similar manner. The crucial points here are that a defect starts to grow only when its stress intensity exceeds the static fatigue limit of the material (like that in a Griffith crack). It is only when a critical tension is exceeded (threshold mechanism) that the self restoration of microdefects is no longer possible leading to the nucleation of fracture. Also at any stress level, only the most vulnerable defect (weakest link of a chain) grows (extremal mechanism). Fracture in heterogeneous systems then corresponds to the dynamical response of a threshold and extremal dynamical system to an external driving (stress or strain). The system under stress has a large number of microscopic metastable states differing in internal stress distribution and crack structure and the dynamics takes the system from one metastable state to another by nucleating a microcrack and emitting energy thereby.

Here, we intend to understand the nucleation and the subsequent propagation of fracture in heterogeneous media from the point of view of statistical physics. We consider a simplified picture of the heterogeneous systems and do not take into account the full details of the defects or their effects on the elastic response of the system as the defects grow. We consider a discrete two-dimensional lattice where the bonds are Hookean springs (of identical spring constant) and mimic the heterogeneity by assigning a random breaking threshold $\tau$ drawn from a distribution $P(\tau)$ to each of the springs. The network is subjected to a tensile stress in both the $x$ and $y$-directions. A spring behaves like a Hookean except that it can be stretched till the threshold value when it ruptures irreversibly. Susequent to a rupture the stress is redistributed over the remaining intact part of the network. A breaking up of a spring mimics the nucleation or onset of fracture. It can lead to further breaking up of the springs and the breaking process continues or the breaking event may stop whereat the stress level on the network is to be increased to induce further breaking. We discuss how the breakdown properties of this random spring network model give rise to power laws in breakdown events.
and compare the results with that of experimental findings.

The study of fracture in random spring network is carried out by molecular dynamics simulation. Our system consists of a $L \times L$ ($L = 50$, 100 and 200) square network with central and rotationally invariant bond-bending forces. The potential energy of the network is

$$V = \frac{a}{2} \sum_{<ij>} (\delta r_{ij})^2 g_{ij} + \frac{b}{2} \sum_{<ijk>} (\delta \theta_{ijk})^2 g_{ij}g_{jk},$$

where $\delta r_{ij}$ is the change in the length of the spring between the nearest neighbor sites $<ij>$ from its equilibrium value (which is the lattice spacing in the starting unstretched condition and is taken to be unity) and $\delta \theta_{ijk}$ is the change in the angle between the adjacent springs $ij$ and $jk$ from its equilibrium value which is taken to be $\pi/2$ to ensure the square lattice structure of the unstretched starting configuration of the network (see Fig. 1). $g_{ij} = 1$ if the spring $ij$ is present and 0 otherwise (when the spring is broken). $a$ and $b$ are the force constants of the central and the bond-bending force terms respectively. The dimensionless equation of motion

$$\frac{d^2 r_i}{dt^2} = \gamma_1 \sum_{<j>} (\delta r_{ij}) g_{ij} + \gamma_2 \sum_{<jk>} (\delta \theta_{ijk}) \frac{\partial \theta_{ijk}}{\partial r_i} g_{ij}g_{jk},$$

involves two parameters $\gamma_1 = at_0^2/m$ and $\gamma_2 = bt_0^2/ml_0^2$ in terms of the mass $m$ associated with the lattice sites, an arbitrary length scale $l_0$ and an arbitrary time scale $t_0$. The ratio $\gamma_1/\gamma_2 = a/l_0b$ is a characteristic of the system under consideration. This suggests that the dynamical features of the network as described by the equation of motion do not depend on the choice of the scale of mass or time. The obvious choice for $l_0$ is unity which is the lattice spacing of the lattice at the unstretched condition. We choose $\gamma_1 = 1.0$ and $\gamma_2 = 0.1$. The small value of $\gamma_2$, much less than the value of $\gamma_1$, allows the fracture to develop without much deformation of the network. We start with all the springs intact so that $g_{ij} = 1$ for all neighboring $ij$’s and with each spring we associate a random breaking threshold $\tau_{ij}$, chosen from a uniform distribution $P(\tau) \in [0, 2]$.

We impose a constant external force $F$ on the sites of the boundary and the system is allowed to evolve dynamically using Verlet’s algorithm [9],

$$\vec{r}_i(t + \Delta t) = 2\vec{r}_i(t) - \vec{r}_i(t - \Delta t) + \vec{F}_i(t)(\Delta t)^2.$$
Here $\vec{F}_i(t)$ is the force (as determined from the potential energy and boundary condition) and $\vec{r}_i(t)$ is the position vector of the site $i$ at time $t$. The simulation involves discrete time $t$ in steps of $\Delta t$. After $n$ iterations the time elapsed is $n\Delta t$ while the real time elapsed is $nt_0\Delta t$. To speed up the computation one would wish to choose a large value of $\Delta t$. However, there is an upper limit to this value given by the convergence time for the fastest developing components of the stress distribution, which is generally very small in disordered systems. We choose $\Delta t = 0.01$. Also, we add a small viscous damping to the evolution to avoid excessive oscillations and to achieve equilibrium for a given applied force faster. For a given applied force, once the system reaches equilibrium, we check if any spring $ij$ is stretched beyond its cutoff value $\tau_{ij}$ and if this happens the spring is snapped irreversibly ($g_{ij}$ for that spring is set to zero). Once the springs are broken, the system is again brought to equilibrium and the springs are checked again to see if the initial set of breaking initiates further rupturing of springs. When no more breaking of springs take place the external force $F$ is increased in small steps. At each step we compute the number of broken bonds, which constitute an avalanche. To average over disorder, the simulation is repeated for 50 different configurations of threshold values $\tau$.

Our simulation shows that the fracture in our spring network develops in a series of bursts of spring rupturing processes. In one such burst, bonds rupture from different parts of the network in a random fashion. Fig. 2 shows the ruptured bonds in a $100 \times 100$ lattice for $F = 0.10, 0.20$ and $0.25$. We find a well defined macroscopic fracture across the network at $F = 0.20$. Below this critical value of $F$ there is no crack that spans the network and the bonds rupture randomly and uniformly over the network. This phenomenon has also been observed in the experiment [4]. Fig. 3 shows the development of fracture in the network with time. At early times, the bonds are broken randomly over the network. At later times the microcracks start coalescing and a large crack develops which wins over the others and engulf nearby microcracks to form a crack which spans the system. We keep track of the clusters formed by the adjacent broken bonds [10]. In this respect, an isolated single broken bond form a cluster of size one. The number $n_c$ of such clusters grows with the stress $F$ following the relation $n_c = L^2g(F)$ (see Fig. 4), where $g(F)$ is a scaling function of $F$. This relation remains valid till the breakdown point indicating that the final crack results from sudden coalescence of few large microcracks without any drastic change in

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the number $n_c$. The final breakdown resembles a first order transition and
the scaling form of $n_c$ further strengthen this point of view. Fig. 5 shows
the variation of the average size $s_c$ of the clusters of ruptured bonds with
the stress $F$. We do not find any evidence of divergence of $s_c$ which is a
strong indication that it is not a a second order phase transition. In fact the
average size $s_c$ remains finite and quite small which suggests that the final
breakdown is a highly correlated phenomenon involving coalescence of very
few microcracks. Next we consider the distribution $P(m)$ of the size $m$ of
burst or avalanche (number of bonds that snaps in a burst) integrated over all
the values of stress $F$ upto the breakdown point $F_c$. We find $P(m) \sim m^{-\alpha}$
with $\alpha = 5/2$ as is shown in Fig. 6. This amplitude distribution can be
transformed into an energy distribution (the energy is proportional to the
square of the amplitude) giving the exponent $\beta = \frac{1+\alpha}{2} = 1.75$. This compares
well with the experimental results. In Fig. 7, $\langle m \rangle$ is plotted against $F$
and we see the linear behavior which suggest $\langle m \rangle \sim (F_c - F)^{-1/2}$ so that
the exponent $\lambda = 0.5$ in our model.

In conclusion, we see that the dynamical response of a simple elastic network
in presence of a threshold and extremal dynamical rules (assigning a random
breaking threshold with each bond and specifying the extremal dynamical
rule in the bond breaking process) produces several features characteristic of
fracture in heterogeneous materials. It gives the power-law behaviors of the
avalanche statistics which are observed in the experiments. The simulation
shows the right trend of development of fracture with time and with stress
as is observed in experiments. It will be interesting to study at what point
the stress concentration factor comes into play so that starting from random
events of bond breaking process over the network one ends up with a well-
deﬁned predominant crack which seems to have the right geometry of a crack
that we generally find in our day-to-day life. The study of the morphology
of the crack structure, for example the roughness of the crack, is in progress.

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Figure 1: Schematic diagram of the elastic network used in the simulation. This is the network prior to the application of the force and with all the bonds intact. The bonds are Hookean springs and there is an angular force between any two adjacent bonds. The deformations are measured from the square configuration of the network.
Figure 2: Ruptured bonds are shown in black in a $100 \times 100$ network for stresses (a) $F = 0.10$, (b) $F = 0.20$ and (c) $F = 0.25$. 
Figure 3: Ruptured bonds are shown in black in a 200×200 network subjected to the stress $F = 0.20$ at molecular dynamics time steps (a) $t = 120000$, (b) $t = 240000$, (c) $t = 360000$ and $t = 480000$. 
Figure 4: The number $n_c$ of clusters of ruptured bonds is plotted against the stress $F$ in a network of size $L = 50 \times 50$.

Figure 5: The average size $s_c$ of the clusters of ruptured bonds is plotted against the stress $F$ in a $L = 50 \times 50$ network.
Figure 6: The size distribution $P(m)$ is plotted against the size $m$ of avalanche of ruptured bonds integrated over all the values of stress up to the breakdown point $F_c$ in a $L = 50 \times 50$ network.

Figure 7: $(<m>/L^2)^{-2}$ is plotted against $F$, where $<m>$ is the average size of the avalanche of ruptured bonds in $L = 50 \times 50$ network integrated up to the stress $F$ and $F_c$ is the stress at which the network fails completely.