From nucleation to percolation: the effect of system size and system disorder

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Abstract

A phase diagram for a one dimensional fiber bundle model is constructed with a continuous variation in two parameters guiding dynamics of the model: strength of disorder and system size. We monitor the successive events of fiber rupture in order to understand the spatial correlation associated with it. We observe three distinct regions with increasing disorder strength. (I) Nucleation – a crack propagates from a particular nucleus with very high spatial correlation and causes global failure; (II) Avalanche – the rupture events show precursors activities with a number of bursts. (III) Percolation – the rupture events are spatially uncorrelated like a percolation process. As the size of the bundle is increased, it favors the nucleating failure. In the thermodynamic limit, we only observe a nucleating failure unless the disorder strength is infinitely high.

Keywords: Disordered systems, Fiber bundle model, Nucleation, Percolation, Spatial correlation

It is nearly a century since Alan Arnold Griffith developed his energy criterion for the fracture propagation of cracks in near-continuous solids [1, 2]. His celebrated work has revolutionized the world of materials science. Griffith considered a single sharp crack in an otherwise homogeneous elastic medium. In Griffith’s theory, the crack propagation is considered as an equilibrium problem where the balance between two energies: reduction of strain energy, and increment in surface energy is measured during the crack propagation. He found that the critical stress \( \sigma_c \) to cause a crack of length \( l \), to extend is \( \sigma_c = (2Y\gamma/\pi l)^{1/2} \) [3], where \( Y \) is Young’s modulus and \( \gamma \) is the surface energy per unit area. However, this is an idealized case that requires a pre-existing crack or notch in a homogeneous medium to concentrate the applied stress. In general, the initiation of a fracture in a solid is a much more complex process. Most engineering materials are far from homogeneous, there will always be a distribution of dislocations, flaws, and other heterogeneity present. The nucleation and propagation of a crack in heterogeneous systems is not understood because of the complexities of the stress singularities at the crack tip [4]. As the applied stress is increased, micro-cracks are likely to occur randomly on the heterogeneity and are uncorrelated. As the density of micro-cracks increases the stress fields of the micro-cracks interact and the micro-cracks become correlated. The micro-cracks eventually may coalesce to form a through-going fracture. This irreversible process is a part of damage mechanics and is an integral part of the nucleation and propagation of fracture in heterogeneous environment.

During the failure process of a disordered system a complex interplay is observed between quenched heterogeneities and local stress concentration. The former one leads to non-localized damage mechanics while the later favors the formation of a localized cracks. As a consequence of this interplay, we observe system size dependence of nominal stress distribution [5–7], scale-free avalanche size statistics [8–11], self-affine crack morphology [12], etc. In the limit of infinitesimal disorder strength, crack grows within a disordered system in a nucleating manner [13–16]. On the other hand, when disorder strength is infinitely high, the effect of local stress concentration becomes irrelevant and the failure process is random in space [17, 18] like percolation. The reason behind the damage mechanics at high disorder is heterogeneities in materials that create energy barriers which act as a resistance on the way of crack propagation and ultimately arrest the crack motion: a phenomenon known as lattice trapping or intrinsic
At intermediate disorder, the situation is more interesting, where the failure process takes place through a number of avalanches showing scale-free distributions of energies emitted during the avalanches [9] and mean-field exponents [25–28]. The order of transition during a failure process is also an important question and has been explored by Zapperi et. al [26].

Here, we study the spatial correlation during fiber crackling in a fiber bundle model (FBM) [29], which is a simple and prototype model of fracture in heterogeneous materials. A transition from a nucleating to percolating failure has been studied recently in the context of FBM with a varying stress release range [30]. At the same time, the fiber bundle model also shows different modes of failure depending on the strength of disorder [31–33]. The spatial correlation is also observed to decrease in extensive amount as the strength of disorder is increased [34]. Apart from this, a high thermal fluctuation as well leads to random failure with the same universality class of site percolation [35]. In this article, through a detailed study of system disorder and system size, we have shown existence and characteristics of three distinct regions: nucleation, avalanche and percolation. These three regions are observed earlier in random fuse network model [36, 37]. The present study is the extension of that in the fiber bundle model.

Fiber bundle model consists of a number of vertical fibers (Hookean springs) in between two parallel bars. The bars are pulled apart with an external stress $\sigma$. Disorder is introduced in the model as strengths of individual fibers which are randomly assigned following a certain distribution. When the applied stress on a fiber crosses its strength threshold, the fiber breaks irreversibly. The stress of the broken fiber is then redistributed within the bundle, either among all surviving fibers in equal amount (equal load sharing scheme) or among the nearest surviving fibers only (local load sharing scheme). After such redistribution, there might be further breaking of fibers due to local enhancement of stress profile. This redistribution might lead to global failure or stops when the stress acting on a fiber could not reach the next threshold limit. At this situation, we increase the applied stress to break the next weakest link and the process goes on until all fibers break. The threshold strength of individual fibers are chosen from the following distribution.

$$\rho(h) \sim \begin{cases} h^{-1}, & (10^{-\beta} \leq h \leq 10^{\beta}) \\ 0, & \text{(otherwise)} \end{cases}$$

Here $\beta$ denotes the width of the distribution or the strength of the disorder. The motivation behind choosing such a distribution is the fact that long-tailed distributions like power-law [39] has already been observed for the distribution of material strength.

A one dimensional fiber bundle model is studied numerically with local load sharing scheme. The strength of disorder (guided by $\beta$) and size of the bundle ($L$) is varied continuously. $\beta$ is varied between 0.4 and 2.0 while $L$ varies from $10^3$ to $10^5$. $10^4$ realizations (bundle replications) are considered for our numerical simulation.

1. Numerical Results

We start our numerical simulation by observing the characteristics of the patches (or cracks) that is generated within the bundle during the evolution of the model. The patch density $\rho$ at time $t$ is defined by number of patches at that time, normalized by the size $L$ of the system. We also note the fraction $B$ of broken fibers at time $t$. $B$ is defined as the number of broken fibers divided by size $L$ of the system. Figure 1 shows the variation of $\rho$ with $B$ for different disorder strength values ranging in between 0.4 and 2.0 for a bundle of size $L = 10^5$.

Figure 1(a) shows a non-monotonic behavior of $\rho$ when $B$ increases from 0 to 1. $B = 0$ stands for the initial configuration where all fibers are intact while we obtain $B = 1$ when all fibers are broken. The patch density $\rho$ is zero for $B = 0$ as no cracks are there in the bundle. On the other hand, when the model is close to the failure point,
Figure 1: (a) Variation of patch density $\rho$ with fraction broken $B$ for $\beta$ values ranging from 0.4 to 2.0. The red dots denotes $\rho_m$, the maximum possible patch density. The dotted line is the locus of $B(1-B)$ and represents random failure events for a 1d bundle. (b) Variation of $\rho_m$ as the disorder strength $\beta$ is varied continuously. We see three different regions. (I) $\rho_m$ is zero here suggesting a single crack propagates through the bundle in a nucleating manner. (II) Here number of cracks originates and the number increases with $\beta$. (III) The failure process here is similar to 1d site percolation. $\rho_m$ has a value close to 0.25 here. The fibers breaks in a spatially uncorrelated manner. The system size is kept constant at $10^5$.

there will be single patch, making $\rho = 1/L$ when $B$ approaches 1. At an intermediate $B$, $\rho$ reaches a maximum value $\rho_m$. Before this maxima, $\rho$ is an increasing function of $B$ as new patches are generated within the bundle. After the maxima, the patches starts to coalesce with each other and we observe lesser and lesser number of cracks with increasing time (hence increasing $B$). Figure 1(a) shows as disorder strength is increased, $\rho_m$ shifts to a higher value. We will discuss the variation of $\rho_m$ with disorder next. The dotted line in the same figure is the locus of $\rho = B(1-B)$. This dotted line represents failure events random in space for a 1d FBM. This can be understood as follows. If $B$ is the fraction of fibers broken, then probability of having a broken and an intact fiber will be $B$ and $(1-B)$ respectively. A patch then will be created by placing an intact fiber beside a broken one, probability of which will be $B(1-B)$ on a 1d lattice. By equating $d\rho/dB$ for this locus to zero we get the maximum $\rho_m = 0.25$ and the $B$ value to be 0.5 at this maxima. The failure pattern becomes more and more random when $\beta$, the disorder strength, is high enough. On the other hand, when the disorder strength is very low ($\beta = 0.4$), we see $\rho = 1/L$ independent of the value of $B$. This suggests a pure nucleating failure starting from the very beginning until the global failure.

Figure 1(b) shows the variation of $\rho_m$ explicitly when $\beta$ is continuously varied. We observe three different regions. (I) Nucleation ($\beta \leq 0.4$): here $\rho_m$ has a value close to $1/L$. This suggests that only a single crack is generated within the bundle in this limit and this crack nucleates to create global failure. Due to low strength of disorder, the failure process here is guided by the local stress concentration at the crack tips. (III) Percolation ($\beta \geq 1.2$): In this limit the behavior of $B$ vs $\rho$ matches closely with $\rho = B(1-B)$. $\rho_m$ has a value close to 0.25. The failure events are random in space here making it reminiscent of percolation in 1d lattice. The failure process is completely guided by the disorder strength and the local stress concentration is almost non-existing. (II) Avalanche ($0.4 < \beta < 1.2$): in the intermediate disorder strength, there is an interplay between the disorder strength and the local stress con-
centration. The failure process here starts in a percolating manner but later the local stress concentration takes over making the rest of the failure events nucleating. We will be discussing this spatial correlation in more details later in this paper.

![Figure 2](image)

**Figure 2**: (a) Effect of system size $L$ on $\rho_m$ for $\beta = 0.3, 0.7$ and $1.2$. $L$ is varied in between $10^3$ and $10^5$. Three regions are observed here. (I) Nucleation: $\rho_m \sim L^{-1}$, (II) Avalanche: $\rho_m \sim L^{-\xi(\beta)}$, (III) Percolation: $\rho_m \sim L^0$. (b) Variation of $\xi$ with $\beta$. $\xi = 1$ and 0 in the region I and III respectively. In the intermediate region II, $\xi$ decreases continuously with $\beta$.

Figure 2(a) shows how the maximum patch density $\rho_m$ responses to the size of the bundle. The results are repeated for three different $\beta$ values 0.3, 0.7 and 1.2, in order to cover all three regions—nucleation, avalanche and percolation, mentioned above. When disorder strength $\beta$ is low (0.3), $\rho_m$ decreases with $L$ in a scale-free manner with exponent $-1$. This suggests that the maximum number of cracks observed in the bundle decreases with increasing size and the model goes towards nucleation more and more as the model approaches the thermodynamic limit. On the other hand, for $\beta = 1.2$, $\rho_m$ is independent of $L$ and saturates at a value close to 0.25. As mentioned above, the failure process is percolating here and remains same irrespective of the size of the bundle. In the intermediate disorder, where the disorder strength and local stress concentration compete with each other, we observe: $\rho_m \sim L^{-\xi}$, where the exponent $\xi$ is a function of $\beta$.

Figure 2(b) shows the variation of exponent $\xi$ with the strength of disorder $\beta$. $\xi$ remains at 1 for low $\beta$ where the failure is nucleating, gradually decreases in region avalanche and becomes constant at 0 in the limit of percolation. The nature of patch density remains the same in the percolation region ($\xi = 0$) only. In both avalanche and nucleation, less and less number of patches grow as the size of the bundle is increased, suggesting that the effect of the local stress concentration becomes more prominent here as the model goes towards the thermodynamic limit.

Here, we will discuss a dynamic parameter that helps us to understand the onset of the nucleation process with time more clearly. As explained earlier, time $t$ here is analogous to total number of redistribution and stress increment prior to global failure. We start by breaking the weakest fiber, say $i$, at time $t = 0$ by the first stress increment. Let us assume further $n_1$ fibers break at the next time step ($t = 1$) upon redistributing the stress...
carried by the weakest fiber. We consider the distance $\Delta r$ between this two consecutive event to be the minimum of distances between fiber $i$ and other $n_1$ fibers that break after redistribution. Here, $\Delta r$ is not the exact lattice distance as only intact fibers are considered while calculating it. Distance across a broken patch is considered to be 1 independent of the size of the patch. This is due to the LLS scheme that we have adopted. Whenever a fiber at a notch breaks and the redistributed stress breaks the fiber at the other notch, the failure is still nucleating, no matter how large this patch is. Next, we square this distance and average it over $10^4$ realizations to get $\langle \Delta r^2 \rangle$ at time $t = 0$. Next we move our reference frame to the fiber among those $n_1$ fibers that had the minimum distance from fiber $i$. Let’s denote this new fiber as $j$. If further $n_2$ fibers break in the next redistribution, $\langle \Delta r^2 \rangle$ at $t = 1$ will be calculated by the same procedure: find $\Delta r$ from the minimum of distances between fiber $j$ and those $n_2$ fibers, square it and average over $10^4$ realizations. Figure 3 shows this variation of $\langle \Delta r^2 \rangle$ with time $t$ for $\beta = 0.3$, 0.7 and 1.2. For all three disorder strength values, $\langle \Delta r^2 \rangle$ starts from a high value at low $t$ and then decreases towards 1 when $t$ is high. A high value of $\langle \Delta r^2 \rangle$ suggests the fibers that break consecutively are far from each other. This is a spatially uncorrelated failure. On the other hand, when $\langle \Delta r^2 \rangle = 1$, the consecutive failures take place from the neighboring fibers only. This behavior stands for pure nucleation. For $\beta = 0.3$, $\langle \Delta r^2 \rangle$ becomes 1 very fast and stays there independent of $t$ until the bundle reaches global failure. For $\beta = 1.2$, we observe the opposite behavior where $\langle \Delta r^2 \rangle$ stays at a high value for a long time and falls to 1 just before global failure. The former behavior is nucleating (I) while the later one is percolating (III). The visualization of the failure process for both (I) and (III) is shown below figure 3. The x-axis of each plot is time and the y-axis is fiber index. The color gradient is over local stress profile. The yellow color stands for the failed fibers. For (I), we see a single crack growing in a nucleating manner from the very beginning. For (III), on the other hand, there is no nucleating yellow-colored fibers and the rupture events are spatially uncorrelated. For the avalanche (II) behavior, there is spatially uncorrelated failure in the beginning as well as nucleation close to global failure. Figure 3 shows the point for $\beta = 0.7$ where $\langle \Delta r^2 \rangle$ becomes 1 indicating onset of localized (nucleating) failure events.
Finally, we have constructed the phase diagram of disorder strength $\beta$ and system size $L$ to show all three failure processes. In figure 4, $1/\beta$ is plotted against $1/L$. This is done in this way so that the origin (0,0) of this plot corresponds to $L \to \infty$ and $\beta \to \infty$, infinite disorder in the thermodynamic limit. As discussed earlier, if the disorder strength is increased, we start with nucleation, goes through avalanche and finally reaches percolation behavior. The spatial rupturing events are shown in the corresponding phases. Now, if the disorder strength is kept constant and the size of the bundle is increased, a percolating behavior moves towards avalanche and a avalanche behavior moves towards nucleation. Due to weak dependence of parameters like $\rho_{m}$ on $L$ (see figure 2), it will not be possible to see (as the system size has to be very high) this change from percolation to avalanche if we are well inside the percolation region. To see this change at relatively lower system sizes, it is required to keep the disorder strength at a value so that the model is closer to percolation-avalanche interface. The opposite happens if the system size is decreased instead of increasing. This suggests we observe only nucleating failure in the thermodynamic limit unless the disorder is infinitely high. This effect of disorder was explored earlier in the context of random fuse network by Shekhawat et al. [36] and Moreira et al. [37]. We observe that fiber bundle model in one dimension follows the same trend.

2. Discussion

In conclusion, we present a detailed study in fiber bundle model, a disordered system acted upon threshold activated dynamics, when the strength of disorder and the size of the model are varied. An increase in disorder strength favors uncorrelated rupture events, random in space while increasing the size of the bundle makes the failure process more and more nucleating. The phase diagram of disorder strength and system size reveals we only have spatially correlated failure like nucleation in the thermodynamic limit unless the disorder strength is infinitely high.

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