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Super-Arrhenius dynamics for sub-critical crack growth in two-dimensional disordered brittle media

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Abstract. – Taking into account stress fluctuations due to thermal noise, we study thermally activated irreversible crack growth in disordered media. The influence of material disorder on sub-critical growth of a single crack in two-dimensional brittle elastic material is described through the introduction of a gaussian rupture threshold distribution. We derive analytical predictions for crack growth velocity and material lifetime in agreement with direct numerical calculations. It is claimed that crack growth process is inhibited by disorder: velocity decreases and lifetime increases with disorder. More precisely, lifetime is shown to follow a super-Arrhenius law, with an effective temperature $\theta - \theta_d$, where θ is related to the thermodynamical temperature and θ_d to the disorder variance.

Introduction. – Sub-critical rupture occurs when a material is submitted to a stress lower than a critical threshold. It is known since the early work of Zhurkov or Brenner [1,2] that sub-critical rupture can be thermally activated. However, prediction of the lifetime, i.e. the time it takes for a sample to break under a given load, has proved difficult when the material is heterogeneous. In addition, although there have been several theoretical attempts to predict the lifetime for homogeneous [3–5] and sometimes disordered [6,7] elastic materials, there have been very few theoretical studies of the actual rupture dynamics in heterogeneous media when thermal activation is the driving mechanism [8–10]. Recently, this dynamics has been modelled for a single macroscopic crack in two-dimensional homogeneous elastic media taking into account stress fluctuations [11]. This model has been successfully faced with experiments of crack growth in fax paper sheets even though this material is actually heterogeneous [12]. In the present Letter, we will take into account heterogeneity by introducing, in the thermal activation rupture model, disorder in the rupture thresholds. We will show that disorder slows down macroscopic crack growth contrary to previous results [8,9] that show the rupture dynamics to be accelerated by disorder in the case of diffuse damage.

Model for sub-critical crack growth in homogeneous brittle media. – In ref. [11], the model that describes sub-critical crack growth in homogeneous brittle media assumes that thermal fluctuations induce local stress fluctuations with time in the elastic material according to a

gaussian distribution, $p(\sigma)$, of mean $\bar{\sigma}$ and variance $\theta = Yk_B T/V$, where Y is the Young modulus, k_B the Boltzmann constant and T the thermodynamical temperature. Here, $\bar{\sigma}$ is the equilibrium value of the stress σ fluctuating in a volume V and θ is the temperature in square stress unit. We assume the volume V to break if the fluctuating local stress σ becomes larger than a critical threshold σ_c . In the two-dimensional case where a single crack is loaded in mode 1 (uniaxial stress perpendicular to the crack direction), stress concentration makes almost certain that breaking occurs at the crack tip. Actually, at the crack tip, linear elasticity predicts a divergence of the stress. However, the average elastic stress σ_m on a volume $V \sim \lambda^3$ at the crack tip does not diverge and can be estimated as:

$$\sigma_m(\ell) = 2 \frac{\sigma_e \sqrt{\ell}}{\sqrt{2\pi\lambda}}, \quad (1)$$

where ℓ is the crack length and σ_e the applied stress. The local stress on the crack tip volume V is submitted to time fluctuations according to $p(\sigma)$ with $\bar{\sigma} = \sigma_m(\ell)$.

The cumulative probability that the instantaneous crack tip stress is larger than the threshold σ_c is $P(\sigma_c) = \int_{\sigma_c}^{+\infty} p(x) dx$. Then, the average time $\langle t_w \rangle$ needed by the crack tip material to break on the mesoscopic scale λ is directly proportional to the inverse of this cumulative probability: $\langle t_w \rangle = t_0/P(\sigma_c)$, where t_0 is a characteristic time for stress fluctuations. The statistically averaged inverse crack velocity, $dt/d\ell$, is constructed as the ratio of the average time $\langle t_w \rangle$ over the growth length due to rupture at each tip of the crack, $dt/d\ell = \langle t_w \rangle / 2\lambda$. Then,

$$\frac{dt(\ell)}{d\ell} = \begin{cases} \left[v_0 \operatorname{erfc} \left(\frac{\sigma_c - \sigma_m(\ell)}{\sqrt{2\theta}} \right) \right]^{-1} & \text{if } \sigma_c - \sigma_m(\ell) \geq 0 \\ v_0^{-1} & \text{if } \sigma_c - \sigma_m(\ell) < 0 \end{cases} = \frac{1}{v_h(\sigma_m(\ell), \sigma_c, \theta)}, \quad (2)$$

with $v_0 = \lambda/t_0$. For critical crack growth, i.e. when $\sigma_m(\ell) > \sigma_c$, the crack simply propagates at its characteristic dynamical velocity: $dt/d\ell = 1/v_0$.

This model was successfully used to describe the growth of a single crack in a fibrous material such as paper [12]. In that case, the scale λ corresponds to the typical paper fiber diameter. However, paper is heterogeneous and distributions in fiber size, position or orientation introduce some disorder which has not been taken into account in this model.

Model extension for disordered media. – Many brittle materials are heterogeneous at a mesoscopic scale. Crack front roughness is one evidence for this heterogeneity. To introduce some disorder in the model, we assume the rupture threshold of the material, σ_c , to be distributed at the scale λ . Our aim is to study the influence of disorder through a varying dispersion of the rupture thresholds keeping the mean properties, and particularly the mean threshold, constant. A commonly used distribution for rupture thresholds that verifies these requirements is a gaussian distribution [7, 10, 13, 14]:

$$p_{th}(\sigma_c) = \frac{1}{\sqrt{2\pi\theta_d}} \exp \left[-\frac{(\sigma_c - \bar{\sigma}_c)^2}{2\theta_d} \right] \text{ for } \sigma_c \geq 0, \quad (3)$$

with a variance verifying $\sqrt{\theta_d} \ll \bar{\sigma}_c$ so that the distribution can be considered normalized. For sake of simplicity, we will consider the crack to grow on a straight line and introduce disorder effects only through the threshold distribution. Then, it is clear that, during its growth, the crack is faced, in statistical average, with the whole intrinsic threshold distribution of the material. The relevance of this simplification will be discussed in the last section.

Using the threshold distribution of eq. (3) at the crack tip, a new expression for the statistical average of the inverse crack velocity can be written:

$$\frac{dt}{d\ell} = \int_0^{+\infty} \frac{p_{th}(\sigma_c) d\sigma_c}{v_h(\sigma_m(\ell), \sigma_c, \theta)}, \quad (4)$$

where v_h is the crack velocity for the homogeneous case. Here, the inverse velocity, $1/v_h$, is weighted by the threshold distribution because the waiting time for the crack to grow by a fixed step λ is the statistical variable. Assuming $\overline{\sigma_c} - \sigma_m \gg \sqrt{\theta} + \sqrt{\theta_d}$, the integrand in eq. (4) takes significative values only for a range of σ_c such that: (i) $\sigma_c - \sigma_m \geq 0$ and the integral can be truncated from σ_m to $+\infty$; (ii) the energy barrier $(\sigma_c - \sigma_m)^2/2\theta$ can be considered far larger than one so that an asymptotic development of the complementary error function can be introduced in eq. (4). After rearrangement, we obtain:

$$\frac{dt}{d\ell} \simeq \frac{e^{\frac{(\overline{\sigma_c} - \sigma_m)^2}{2(\theta - \theta_d)}}}{2v_0 \sqrt{\theta\theta_d}} \int_{\sigma_m}^{+\infty} (\sigma_c - \sigma_m) e^{-\frac{\theta - \theta_d}{2\theta\theta_d} (\sigma_c - \overline{\sigma_c})^2} d\sigma_c, \quad (5)$$

with

$$\overline{\sigma_c} = \frac{\theta \overline{\sigma_c} - \theta_d \sigma_m}{\theta - \theta_d}. \quad (6)$$

Then, we can estimate the integral:

$$\begin{aligned} \int_{\sigma_m}^{+\infty} (\sigma_c - \sigma_m) e^{-\frac{\theta - \theta_d}{2\theta\theta_d} (\sigma_c - \overline{\sigma_c})^2} d\sigma_c &= \int_{\sigma_m}^{+\infty} (\sigma_c - \overline{\sigma_c} + \overline{\sigma_c} - \sigma_m) e^{-\frac{\theta - \theta_d}{2\theta\theta_d} (\sigma_c - \overline{\sigma_c})^2} d\sigma_c \\ &= \left[-\frac{\theta\theta_d}{\theta - \theta_d} e^{-\frac{\theta - \theta_d}{2\theta\theta_d} (\sigma_c - \overline{\sigma_c})^2} \right]_{\sigma_m}^{+\infty} + (\overline{\sigma_c} - \sigma_m) \int_{\sigma_m}^{+\infty} e^{-\frac{\theta - \theta_d}{2\theta\theta_d} (\sigma_c - \overline{\sigma_c})^2} d\sigma_c. \end{aligned} \quad (7)$$

Here, it is important noticing that both terms of eq. (7) are infinite when $\theta < \theta_d$. So, it is clear that, in the case where $\theta < \theta_d$, the inverse crack velocity and the rupture time will become infinite. On the other hand, considering the case where $\theta > \theta_d$, we get:

$$\frac{dt}{d\ell} \simeq \frac{\theta}{\theta - \theta_d} \frac{1}{v_0} \sqrt{\frac{\pi}{2(\theta - \theta_d)}} (\overline{\sigma_c} - \sigma_m) \exp \left[\frac{(\overline{\sigma_c} - \sigma_m)^2}{2(\theta - \theta_d)} \right]. \quad (8)$$

Eq. (8) corresponds, with an additional prefactor $\theta/(\theta - \theta_d)$, to the asymptotic development of eq. (2) for the homogeneous case introducing an effective temperature $\theta_{\text{eff}} = \theta - \theta_d$. Then, eq. (8) can be seen as an approximation of:

$$\frac{dt}{d\ell} \simeq \frac{\theta}{\theta - \theta_d} \frac{1}{v_h(\sigma_m, \overline{\sigma_c}, \theta - \theta_d)}, \quad \text{when } \theta > \theta_d. \quad (9)$$

The conclusion of this part is that crack velocity is lowered by the introduction of disorder in the model material, mainly through the appearance of a lowered effective temperature $\theta_{\text{eff}} = \theta - \theta_d$ in place of the thermodynamical temperature θ . The variance θ_d can then be seen as a temperature of disorder.

Direct numerical analysis of the model. – In order to check the validity of eq. (9), we study numerically the model starting from eq. (4). In fig. 1a), we plot $(\theta - \theta_d)/\theta (dt/d\ell)_{\text{num}}$, obtained by numerical calculation of eq. (4)'s right hand side, as a function of the crack length for a set of particular values for the model parameters. The analytical law, $y = 1/v_h(\sigma_m(\ell), \overline{\sigma_c}, \theta_{\text{eff}})$, fits very well the numerical data using θ_{eff} as a fitting parameter.

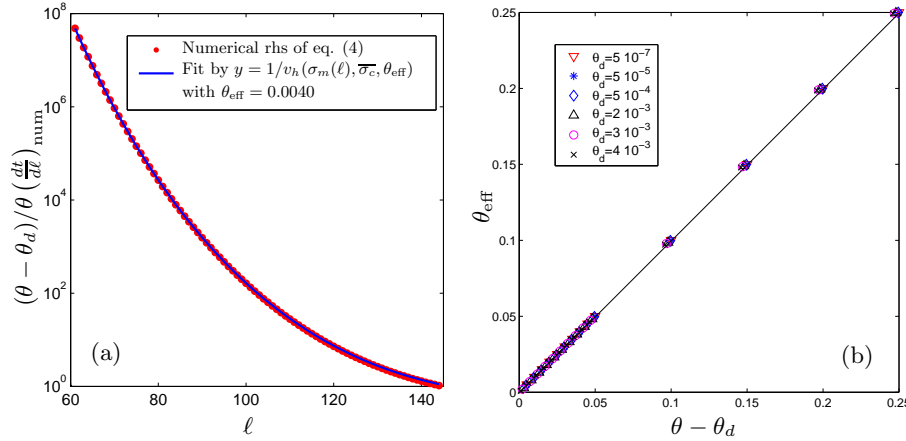


Fig. 1 – On the left: Semi-log plot of numerical $(\theta - \theta_d)/\theta (dt/d\ell)_{\text{num}}$ as a function of ℓ ($v_0 = 1$, $\lambda = 1$, $\bar{\sigma}_c = 1$, $\sigma_e = 0.10$, $\theta = 0.005$, $\theta_d = 0.001$) and its fit by $y = 1/v_h(\sigma_m(\ell), \bar{\sigma}_c, \theta_{\text{eff}})$; on the right: θ_{eff} obtained from the fits as a function of $\theta - \theta_d$, with θ and θ_d both varying ($0.005 \leq \theta \leq 0.25$ and $5 \cdot 10^{-7} \leq \theta_d \leq 0.004$).

It is clear as one can see in fig. 1b) that the effective temperature θ_{eff} obtained from the numerical data fits corresponds very well (within 2%) to the one predicted analytically, $\theta_{\text{eff}} = \theta - \theta_d$, when θ and θ_d are both varying. These numerical results confirm the good quality of eq. (9) even if it is the result of approximate calculations.

Rupture time. – We will now go a step further in the analysis of our model by studying the rupture time dependence with the model parameters. When there is no disorder, rupture time is defined as the time for a crack of initial length ℓ_i to grow until it reaches a critical length ℓ_c such that $\sigma_m(\ell_c) = \sigma_c$. In paper [11], we got an approximate expression of the mean rupture time for homogeneous systems assuming some approximations in eq. (2):

$$\tau \simeq \frac{\sqrt{2\pi}\theta\ell_i}{v_0\sigma_i} e^{\frac{(\sigma_c - \sigma_i)^2}{2\theta}} = \tau_o e^{\frac{(\sigma_c - \sigma_i)^2}{2\theta}}, \text{ where } \sigma_i = \sigma_m(\ell_i). \quad (10)$$

This law has been tested experimentally on the slow growth of a single crack in fax paper sheets [12]. It is shown that statistically averaged crack growth curves are in good agreement with the model predictions as well as the lifetime dependence on applied stress, initial crack length and Young modulus.

Backing on the calculations of paper [11], we easily get an analytical expression for the mean lifetime in the heterogeneous case from eq. (9):

$$\tau \simeq \frac{\theta}{\sqrt{\theta - \theta_d}} \frac{\sqrt{2\pi}\ell_i}{v_0\sigma_i} e^{\frac{(\bar{\sigma}_c - \sigma_i)^2}{2(\theta - \theta_d)}} = \tau_o^{\text{des}} e^{\frac{(\bar{\sigma}_c - \sigma_i)^2}{2(\theta - \theta_d)}}, \text{ when } \theta > \theta_d. \quad (11)$$

We note that the lifetime is super-Arrhenius. Fig. 2 shows the logarithm of the lifetime, obtained by numerical integration of eq. (4) and rescaled respectively by τ_o (on the left) and by τ_o^{des} (on the right) as a function of the energy barriers $(\bar{\sigma}_c - \sigma_i)^2/2\theta$ (on the left) and $(\bar{\sigma}_c - \sigma_i)^2/2(\theta - \theta_d)$ (on the right). Eq. (10) does not rescale the data when θ_d is varied. But, it is clear that the rescaling by eq. (11) makes all the data for different θ and θ_d fall very well on the $y = x$ straight line. This confirms the relevance of eq. (11) which predicts

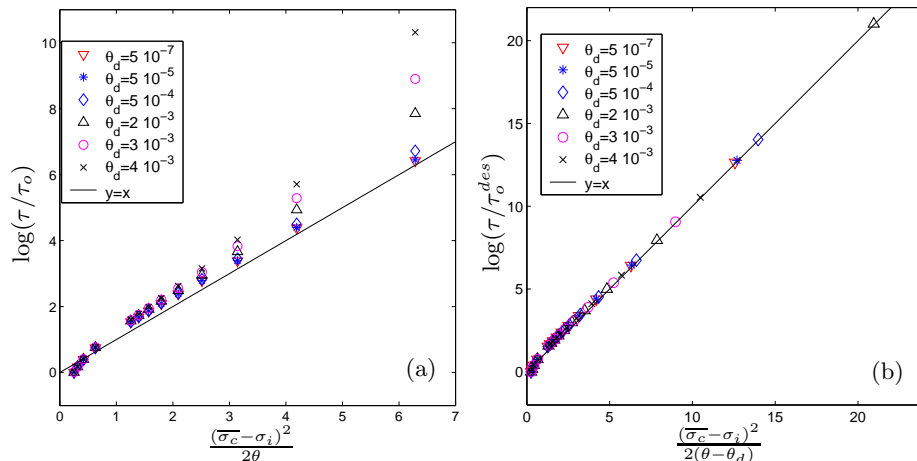


Fig. 2 – On the left: logarithm of the rupture time as a function of the energy barrier $(\bar{\sigma}_c - \sigma_i)^2/2\theta$ for many different growth conditions ($0.005 \leq \theta \leq 0.25$ and $5 \cdot 10^{-7} \leq \theta_d \leq 0.004$); on the right: logarithm of the rupture time as a function of $(\bar{\sigma}_c - \sigma_i)^2/2(\theta - \theta_d)$ for the same numerical data.

an increase of the lifetime with θ_d . Once again, analytical and numerical calculations confirm the deceleration of the crack growth due to disorder.

At this point, we may question the generality of the results presented in this Letter with respect to the shape of the threshold distribution. The quadratic exponent of the gaussian distribution used here appears to be a critical value since the same exponent appears in the distribution of stress fluctuations. For a threshold distribution with a tail decreasing slower than the gaussian tail (e.g. for centered Weibull distribution with $m < 2$ [14]), crack velocity will be zero and mean rupture time infinite whatever the variance of the distribution. For a distribution tail decreasing faster than the gaussian one ($m > 2$ for the centered Weibull distribution), the slowing down of the crack growth dynamics with an increasing disorder remains completely valid. However, in the latter case, there will be no more transition temperature like θ_d under which rupture time is infinite.

Facing the results with previous theoretical works. – The results presented in this Letter differ from previous theoretical works on one-dimensional Disordered Fiber Bundle Model (1d-DFBM) describing the influence of disorder on the fracturing process [7–10]. In the 1d-DFBM, as long as the critical fraction of broken fibers is less than 50% [10], the introduction of a threshold distribution actually accelerates rupture with an effective temperature larger than the thermodynamical temperature. The rupture process starts from the weaker fibers and progressively affects the stronger ones. As a result, the distribution of breaking thresholds is truncated from below by a front moving with time towards higher thresholds. Because rupture can occur everywhere in the system, this dynamics is non-local and the damage rate is given by how many fibers break at each time step. Consequently, the effect of disorder is obtained by averaging the damage rate over the threshold distribution. This is not at all the process which occurs when a large crack propagates in a 2d disordered system. Here, the probability of breaking at the crack tip is greatly enhanced by stress concentration effects even for a large disorder. Then, the rupture dynamics becomes local, and one needs to average over disorder the time to break the fiber at the crack tip, i.e. the inverse of the damage rate. Finally, it is worth noticing that there are similarities between our model for crack growth predicting a

super-Arrhenius rupture time and the trap model introduced by Bouchaud [15] to describe dynamics in glassy systems.

Discussion on the straight line growth hypothesis. – In our analysis, we assume the crack to grow on a straight line even if roughness is experimentally observed for sub-critical cracks in heterogeneous materials. Is this hypothesis relevant for crack growth in heterogeneous materials? Two viewpoints can be raised.

One could think that roughness is due to the fact a crack, at each moment, grows in the direction where the material is the weakest. In this case, the crack, during its growth, will not experience the intrinsic threshold distribution of the material, but only a part of this distribution that corresponds mainly to the lowest thresholds. Then, the distribution to be used in eq. (3) is not the intrinsic threshold distribution of the material.

But, one could also think that crack growth occurs in the direction where the stress intensification is the largest. Statistically, the larger the stress, the higher the probability to grow in the corresponding direction. This idea is supported by recent theoretical and experimental works [16, 17]. In this framework where the crack tip stress distribution rules the roughness, it is fair to consider the intrinsic threshold distribution of the material to rule the crack growth so that our model is not restricted to straight cracks.

Experimental reality is probably a compromise between the two competing mechanisms: growth governed by stress intensification and growth following the path through the weakest regions. In the case of a material with a mesoscopic structure, such as paper, the crack tip is surrounded by a finite number of fibers so that the crack can grow only in a finite number of directions. The determination of the growth direction is clearly due the competition between stress intensification on each fiber compared to its toughness. It is worth noticing that crack tip structure complexity can create a complex stress distribution. Consequently, the largest stress is not necessarily in the crack main direction so that roughness can appear even if the crack always grows in the maximum stress direction.

Some numerical work has been performed to illustrate a situation where the crack is allowed to "choose" between a finite number of growth directions. We model a two-dimensional elastic system as a network of springs forming a lattice. More details about the simulations are given in [11]. The only differences with the simulations presented there are the use of a hexagonal lattice instead of the previously used square lattice and the introduction of a rupture threshold distribution. We can see in fig. 3a), that the crack can actually "choose" between three directions (so called upper, straight and lower directions) at each step. In fig. 3b), a typical crack pattern after a thermally activated growth is presented. We can notice that the crack grows almost straight. Actually, the stress intensification on the upper and lower springs is only about 80% of the one of the straight spring. So, the crack will grow through the springs on the sides only if the rupture threshold of the straight spring is very large. This is only a rare event and we can say that the crack experiences essentially the intrinsic threshold distribution truncated of the very large thresholds only. In this simulation, the crack path is mainly ruled by stress intensification. Experimentally, the number of fibers joining at the crack tip can be larger than three so that variations in stress intensification between fibers are probably smoother than in the simulation.

No definitive conclusion on the growth process can be given because, depending on the considered material, one of the two competing mechanisms (growth controlled by stress intensification and weakest fibers) will dominate. The results presented in this letter hold essentially for media where the crack path is ruled by stress intensification.

Conclusion. – Assuming the existence of thermal stress fluctuations in the material, we modelled sub-critical crack growth in disordered materials. The influence of material disorder

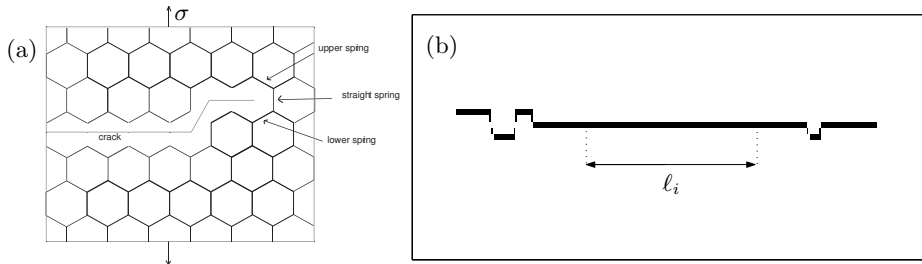


Fig. 3 – On the left: Geometry of the hexagonal spring lattice of the numerical simulation with a non-straight crack; on the right: image of a crack created from an initial crack of length ℓ_i by simulating thermal activation in the hexagonal spring lattice.

on the growth of a single crack in two-dimensional brittle elastic material is described through the introduction of a gaussian rupture threshold distribution. Analytical predictions of the crack velocity and material lifetime have been derived in agreement with direct numerical calculations. The conclusion is that the crack growth process is inhibited by disorder: velocity decreases and lifetime increases with the temperature of disorder θ_d . This inhibition is not restricted to the case of a gaussian threshold distribution. In the case of a gaussian distribution, the influence of disorder is simply accounted for by introducing an effective temperature $\theta_{\text{eff}} = \theta - \theta_d$ for $\theta > \theta_d$. Hence, lifetime follows a super-Arrhenius law. If the existence of this super-Arrhenius regime were to be confirmed experimentally, it would give an important clue about the actual shape of the experimental rupture threshold distribution. In that case, the analogy with glassy systems suggests that the growth of a crack in a disordered material could possibly occur in a "glassy" regime, i.e. when $\theta < \theta_d$.

* * *

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