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Abstract. – Slow crack growth in a model of homogenous brittle elastic material is described as a thermal activation process where stress fluctuations allow to overcome a breaking threshold through a series of irreversible steps. We study the case of a single crack in a flat sheet for which analytical predictions can be made, and compare them with results from the equivalent problem of a 2D spring network. Good statistical agreement is obtained for the crack growth profile and final rupture time. The specific scaling of the energy barrier with stress intensity factor appears as a consequence of irreversibility. In addition, the model brings out a characteristic growth length whose physical meaning could be tested experimentally.

Introduction. – Although tensile rupture of atomic bonds requires a stress comparable to the Young's modulus, brittle solids commonly rupture at a much lower applied stress (typically 3 orders of magnitude lower). Griffith's pioneering work [1] has clarified the origin of this apparent weakening, postulating that small cracks usually preexist in real solids, with stress concentration at the crack tip strongly enhancing rupture. A somewhat similar and quite striking effect is the occurrence of failure even though the solid is stressed below its experimental breaking threshold (i.e., even if stress concentration due to flaws is taken into account). The physical process, sometimes referred to as subcritical rupture, leads to a delay in the time for complete macroscopic failure of the solid, with a strong dependence on the amplitude of the applied stress.

A possible driving mechanism for subcritical damaging processes is thermal activation as supported by the early experimental work of Brenner and Zhurkov [2,3]. Zhurkov introduced a kinetic concept of strength of solids, where time to rupture follows an Arrhenius law with an energy barrier decreasing with increasing stress [3]. Interestingly, there is still debate about whether temperature fluctuations might be sufficient or not to nucleate microcracks and trigger crack growth. Recent theoretical works [4–7] have emphasized the effect of disorder in decreasing the effective energy barrier (conversely increasing the "effective temperature"). Other authors [8, 9] have used equilibrium statistical thermodynamics to study how cracks might naturally appear from thermal fluctuations in an otherwise homogenous material which

goes into a metastable state when stretched. However, another fundamental ingredient not usually taken into account is the irreversibility of the rupture mechanism, leading to dynamics out of equilibrium.

Temperature fluctuations in real materials are usually considered too weak to be able to overcome a potential energy barrier estimated as the free energy cost to reach Griffith's critical crack length. But, the energy cost would be much smaller if rupture was considered as an irreversible process, where thermal fluctuations need only to be able to break atomic bonds one after another. Irreversibility has already been taken into account by Golubovic *et al.* [10], with the introduction of a minimum crack opening beyond which the crack can not heal back. However, Golubovic introduces a complex behaviour of stepwise growth involving several bonds at a time, and eventually find that lifetime is dominated by a critical crack length in the same fashion as predicted directly from Griffith's criteria, albeit with a smaller critical length and a different power law dependence on applied stress. In this paper, we present a different approach by choosing ab initio a distribution of stress fluctuations directly linked to thermal fluctuations. Since our goal is to describe irreversible crack growth, we are considering the general case of a preexisting initial crack in a flat sheet of material. In order to clarify our approach, we derive first the energy barrier corresponding to our geometry in the framework of Griffith's energy concept. Then, we give analytical solutions of our model which yield the complete growth dynamics for the case of a single crack. Finally, we compare the predictions of our model to the results obtained with a numerical simulation of a bidimensional elastic system in antiplane deformation.

Energy barrier from Griffith's energy concept. – Griffith's prediction of a critical crack size beyond which there is rupture, i.e. irreversible and fast crack growth, is derived from a potential energy taking into account elastic energy due to applied stress σ and surface energy γ needed to open a crack as a function of a unique order parameter, the crack length ℓ. For a bidimensional geometry consisting of a flat sheet with a crack perpendicular to the direction of stress, the potential energy per unit thickness of the sheet reads:

$$U = -\frac{\pi \ell^2 \sigma^2}{4Y} + 2\gamma\ell + U_0 \tag{1}$$

where Y is the Young modulus and U_0 is the elastic energy in the absence of crack. This energy reaches a maximum for a critical crack length ℓ_c beyond which no stable state exist except the separation of the solid in two broken pieces. From this expression of the energy, it is clear that a stressed solid without crack is in a metastable state with a lifetime depending on the possibility to nucleate a crack with critical length.

Many authors [9–11] have used models essentially inspired by Griffith's energy concept to show that the lifetime should follow an Arrhenius law with an energy barrier scaling as $\Delta U \sim \sigma^{-2}$ in a bidimensional geometry and $\Delta U \sim \sigma^{-4}$ in a three-dimensional one. Following these authors, but taking into account the preexistence of a stable initial crack of length ℓ_i and introducing stress intensity factors $K_i = \sigma\sqrt{\frac{\pi}{2}\ell_i}$ and $K_c = \sigma\sqrt{\frac{\pi}{2}\ell_c}$, the energy barrier becomes :

$$\Delta U = U(\ell_c) - U(\ell_i) = \gamma\ell_i \left(\frac{K_i}{K_c} - \frac{K_c}{K_i}\right)^2 = \gamma\ell_i f\left(K_i, K_c\right) \tag{2}$$

Note that the energy barrier is a linear function of the initial crack length multiplied by a function depending only on stress intensity factors. This choice for the energy barrier implicitly assumes that there is a possibility for the crack to explore reversible states of crack length

between initial and critical crack length, and cannot be a good description if irreversibility of crack growth is to be taken into account.

Energy barrier for an irreversible crack growth. – Let us reflect on the fact that thermal fluctuations induce stress fluctuations in the material. The uniaxial loading state of an homogeneous solid at fixed temperature is described by its free energy density: $\varphi(\sigma) = \sigma^2/2Y$. Treating stress as a fluctuating internal variable in a fixed volume V, the probability to find a given stress is proportional to a Boltzmann factor $\exp(-\varphi V/kT)$. Expanding free energy about an equilibrium position σ, the distribution of stress σ_f is :

$$p(\sigma_f) \simeq \frac{1}{\sqrt{2\pi\langle\Delta\sigma\rangle^2}} \exp\left[-\frac{(\sigma_f-\sigma)^2}{2\langle\Delta\sigma\rangle^2}\right] \tag{3}$$

where k is Boltzmann constant, T temperature and $\langle\Delta\sigma\rangle^2 = kT/(V\partial^2\varphi/\partial\sigma^2) = kTY/V$ [12]. When a crack is present, stress concentration increases the probability that breaking occurs at the crack tip rather than anywhere else. We assume that stress distribution at the crack tip remains the same as eq. (3) despite the strong divergence of stress and the breakdown of linear elasticity. Since the stress intensity factor $K \approx \sigma\sqrt{\ell}$ gives a measure of stress intensity close to the crack tip for a crack with length measurement ℓ when external load is σ, we choose to work directly with this quantity. The threshold for rupture at the crack tip will be given by a critical value of stress intensity factor K_c as is usual laboratory practice. The cumulative probability that stress intensity is larger than a given value η is then : $P(\eta) = \int_\eta^\infty p\,(x)\,\mathrm{d}x$. Since breaking is assumed to be an irreversible process, the typical velocity of crack should be directly proportional to the probability to have fluctuations giving stress intensity larger than $\eta = K_c$:

$$\frac{\mathrm{d}\ell}{\mathrm{d}t} = V_0 P(\eta = K_c) \simeq V_0\sqrt{\frac{EkT}{2\pi}}\frac{1}{K_c - K}\exp\left[-\frac{(K_c-K)^2}{2EkT}\right] \tag{4}$$

where E is a dimensional constant proportional to the Young modulus. In eq. (4), the last equality is valid as long as $kT \ll \eta^2/2E$. We also introduced a typical velocity V_0 which represents the crack velocity when the condition for crack advance is verified at all times ($P = 1$). This quantity is typically the ratio of a microsopic scale (interatomic distance) and a characteristic time (inverse vibrational frequency). Since K is a function of crack length ℓ , eq. (4) is a differential equation for crack evolution. To solve this equation requires additional approximations since the dependence of stress intensity factor on crack length is non-linear. First, we introduce a reduced crack length $\phi \equiv (\ell - \ell_i)/(\ell_c - \ell_i)$ to measure crack evolution as it grows from its initial value ($\phi = 0$) to its ultimate stable value ($\phi = 1$). Then, stress intensity factor can be written:

$$K \approx \sigma\sqrt{\ell} = \sigma\sqrt{\ell_i + (\ell_c - \ell_i)\phi} \simeq K_i\left[1 + \frac{1}{2}\left(\frac{\ell_c}{\ell_i} - 1\right)\phi\right] \tag{5}$$

where the last equality is a reasonable approximation giving less than a 2% error on stress intensity factor as long as $\phi < 1/2$ and $\ell_c < 2\ell_i$. Another approximation will be to take $K = K_i$ in the pre-factor of the exponential, because neglecting the variation in stress intensity factor leads only to a logarithmic correction of the crack velocity. As a consequence of the last approximation, the crack velocity will tend to be underestimated. Solution of the differential equation (4) is then :

$$t = \tau\left[1 - \exp\left(-\frac{\phi}{\phi_c}\right)\right] \tag{6}$$

where τ gives the lifetime of the sample before fast rupture:

$$\tau = \tau_0 \exp\left[\frac{(K_c - K_i)^2}{2EkT}\right] \tag{7}$$

with

$$\tau_0 = \frac{2\sqrt{2\pi EkT}}{K_i}\frac{\ell_i}{V_0} \tag{8}$$

and ϕ_c is related to a characteristic growth length λ:

$$\phi_c = \frac{\lambda}{\ell_c - \ell_i} = \frac{2EkT}{K_i(K_c - K_i)}\frac{\ell_i}{\ell_c - \ell_i} \tag{9}$$

Note that the crack velocity : $\frac{\mathrm{d}\ell}{\mathrm{d}t} = \lambda/(\tau - t)$, diverges as time comes closer to lifetime τ, which simply means that when time τ is reached slow crack growth due to thermal activation is no longer the driving mechanism, and a crossover towards fast dynamic crack propagation will occur. The lifetime τ appearing in eq. (7) follows an Arrhenius law with an energy barrier function of initial and critical stress intensity factors similar to eq. (2), but instead, there is no additional proportionality to initial crack length. A similar scaling for the energy barrier was found by Marder [13].

Results from the simulation of a 2D elastic spring network. – In order to check predictions from the previous analysis, we model a bidimensional elastic system as a network of springs forming a square lattice whose nodes can move only along an axis perpendicular to the undeformed plane of springs. The elastic restoring force of the spring is proportional to the variation in displacement along the moving axis. This is a simplified model of an antiplane deformation. A constant force is applied at two opposite sides of the lattice, the direction of the force being parallel to the moving axis, but reversed from one side to the other. Starting from an equilibrium configuration, an external force obtained from a normal distribution is applied in parallel to each spring. A new static equilibrium configuration is determined to find the fluctuations of spring forces. In this procedure, fluctuations are quasi-statically coupled to a temperature bath. Making the elastic constant between force and displacement equal to unity, the temperature coefficient kT is numerically identical to the variance of spring force fluctuations. Whenever the force on a spring exceeds a breaking threshold f_c, the spring is cut and, since it is never repaired, the process is irreversible. The crack itself is modelled as a series of broken parallel springs, with the crack direction parallel to the sides where the constant force is applied. The size of the square lattice (100×100 springs) is determined to reduce finite size effects and obtain the correct scaling of stress intensity factor with applied stress and crack length. Time scale in the simulation is given as the constant time between two configurations of force fluctuations in the system, and length scale as the distance between two nodes of the lattice.

The distribution of lifetimes τ obtained in the simulations is a decreasing exponential with a typical width $\sqrt{\langle \Delta\tau^2 \rangle}/\tau \approx 0.5$. In fig. 1 and 2, we plot the lifetimes averaged over an ensemble of 10 to 50 simulations for samples with different initial crack lengths and different temperatures. In fig. 1, the logarithm of the lifetime is plotted as a function of the energy barrier given by eq. (2) and scaled by temperature coefficient kT. For a given initial crack length, a good scaling is obtained at various temperatures. However, when the initial crack length is changed, the scaling with the energy barrier does not work at all. In fig. 2, the logarithm of the lifetime scaled by τ_0 is plotted as a function of the energy barrier given by eq. (7). This energy barrier scaling appears to be correct whatever is the initial crack length or

temperature. It seems that the lack of dependence on initial crack length in the energy barrier given by eq. (7) is a signature of irreversibility. Indeed, if one considers the potential energy landscape obtained from eq. (1), we can describe a growth process where small irreversible steps δ occur, with the energy barrier to overcome each of these steps proportional to the derivative of the potential energy. It can be seen from eq. (1) that this energy barrier would be expressed only as a function of stress intensity factor as in eq. (7). For each step, the energy barrier can be written $\Delta U = \frac{\mathrm{d}U}{\mathrm{d}\ell}\delta = \left(K_c^2 - K^2\right)\delta/Y$, and the waiting time for the crack to advance with step δ is given by an Arrhenius law. Integrating the time it takes to go from ℓ_i to ℓ_c gives in the limit $\delta \ll \ell_i$ the following scaling relation:

$$\tau \approx \exp\left(\frac{K_c^2 - K_i^2}{YkT}\delta\right) \tag{10}$$

Although this approach does correct the problem of scaling with ℓ_i, it completely fails to give the correct scaling of the energy barrier with stress intensity factors; furthermore, for a given initial crack length, temperature scaling is lost as can be seen from the insert in fig. 2.

To determine the characteristic growth length λ which appears in our model, it is necessary to look at the complete growth dynamic. As for lifetimes, there is a strong dispersion in growth curves obtained for different simulations with the same temperature and initial crack length. In order to get statistical information about crack growth, we determine the average time it takes for the crack to reach a certain length. In fig. 3, which shows flowing time as a function of crack length, the exponential behaviour obtained in eq. (6) is recovered and yields a value of λ. In fig. 4, we plot λ scaled by the coefficient $\alpha = 2E\ell_i/[K_i(K_c - K_i)]$ as a function of kT. The linear dependence of λ on temperature predicted by eq. (9) appears clearly for various initial crack lengths and applied forces. In addition, the correct rescaling of data with initial crack lengths is mainly related to the linear dependence of λ on ℓ_i. Dispersion of data for a given temperature and initial crack length occurs systematically above prediction of the model (see solid curve in fig. 4). This can be understood as a consequence of the approximations in our model underestimating crack velocity. This interpretation is consistent with the increase in dispersion of the data as ℓ_c increases.

Conclusion. – We have shown that by taking into account distribution of stress fluctuations, we can describe thermally activated and irreversible crack growth and obtain the correct scaling of lifetime with applied stress and initial crack length. Previous predictions based on Griffith's potential energy [9–11] fail to take into account irreversibility of the rupture process, thus do not apply to our configuration. Our challenge is to find a way to include irreversibility in a problem of total potential energy minimization, since simple arguments fail to give the correct behaviour. More work should be done to check that stress divergence at the crack tip does not preclude the derivation of stress distribution presented in this paper. Direct comparisons with experiments can be performed to test the relevance of the characteristic length scale for crack growth introduced in our model, as well as scaling of both lifetimes and characteristic growth length on initial crack length.

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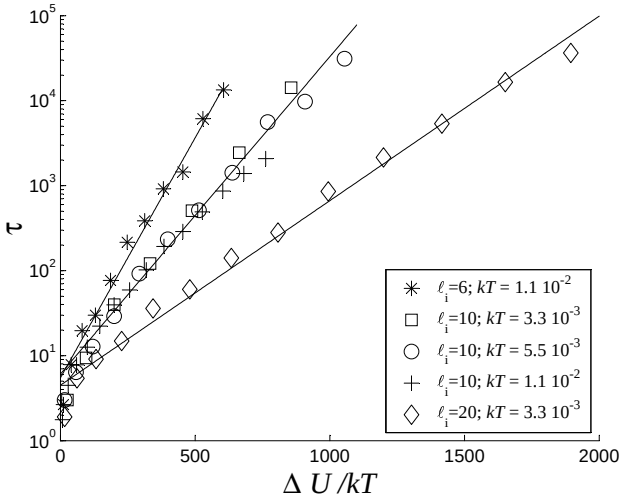

Fig. 1 – Logarithm of lifetime as a function of the energy barrier as predicted by eq. (2). Failure of data to scale with initial crack length is the main observation. Straight lines are a guide for the eye.

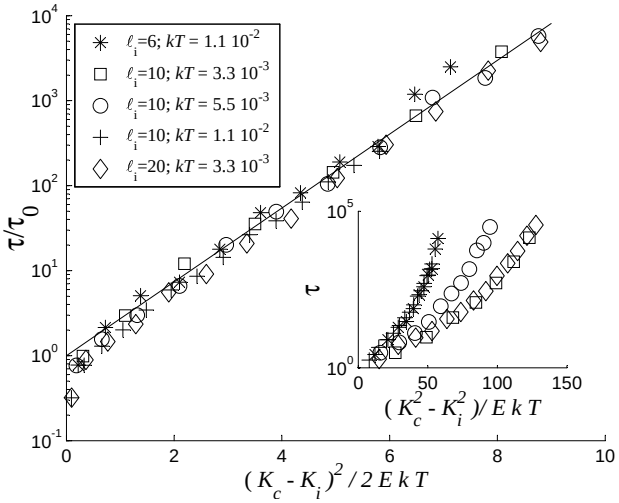

Fig. 2 – Logarithm of lifetime as a function of the energy barrier as predicted by eq. (7). Scaling works for various temperature and initial crack length. The straight line, slope 1, is prediction from eq. (7). The inset shows failure of scaling with energy barrier as predicted by eq. (10).

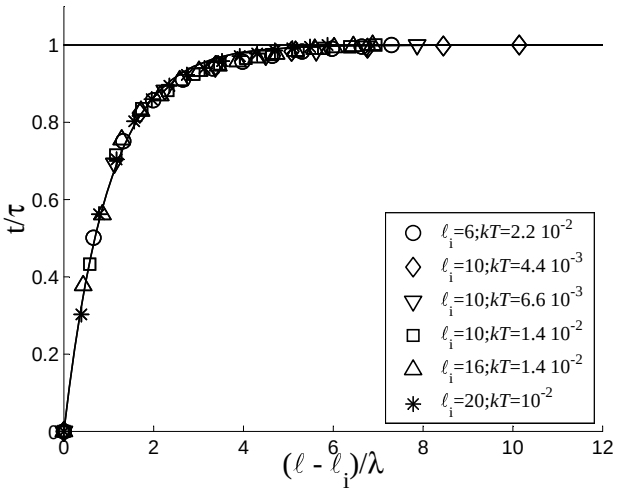

Fig. 3 – Rescaled time as a function of rescaled crack length for various initial crack lengths and temperatures. For each set of data, λ is extracted as the only fit parameter since lifetime is known. Solid line corresponds to eq. (6).

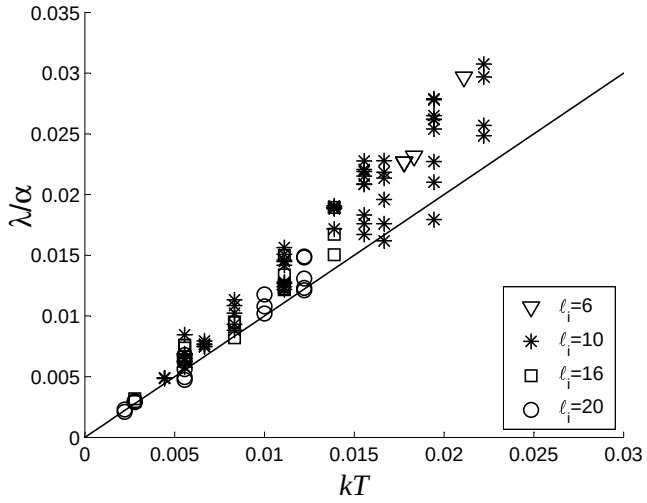

Fig. 4 – Linear dependence of λ/α with temperature coefficient kT for various initial crack lengths and applied forces. The solid line shows the behaviour expected from the model (slope = 1).