Failure time in heterogeneous materials—Non-homogeneous nucleation

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Failure time in heterogeneous materials —Non-homogeneous nucleation

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Abstract. – The changes in the time to failure in creep problems, brought about by the inherent existence of flaws in materials, are calculated. Results agree with experimental ones and predict the time distribution dependence on temperature.

Introduction. – In a recent series of papers, Ciliberto and his collaborators [1–5] have succeeded in accurately measuring times to failure of heterogeneous materials (wood, fiberglass, etc.) under different subcritical stresses. They have shown that these times follow an exponential behavior predicted by Pomeau [6] on the basis of the Arrhenius-type homogeneous-nucleation process. A similar model was proposed by Golubovic and Feng [7] and was extended to fractal dimensions [8].

Although the agreement with the Arrhenius plot was excellent, the authors of refs. [1–5] found two somewhat annoying results: The distribution of times for the same stress did not follow a Poissonian curve as was expected, and the temperature dependence of breaking times under loads with constant increasing rates was deemed strange in that it apparently showed an ambient temperature of $\sim 3000\,\mathrm{K}$ instead of $\sim 300\,\mathrm{K}$ in which they were working.

A heterogeneous nucleation approach will be presented here and shown to a) render fracture nucleation easier, b) reproduce the Arrehenius plot, c) relate to the temperature problem and d) predict a time distribution form which depends on temperature.

Homogeneous vs. non-homogeneous nucleation. – For the sake of completeness, we repeat and present here the homogeneous-nucleation approach of Pomeau [6]. The calculations are performed schematically only for the two-dimensional (2D) case and the results for the 3D case are then presented directly. We consider nucleation under stress of a Griffith flaw, *i.e.* the appearance of a flaw large enough to fulfill the Griffith criterion for rapid fracture. Nucleation is accomplished by thermal fluctuations, via an Arrhenius-type process. Assuming homogeneous nucleation, the rate of appearance of a critical flaw is given by [6] as

$$\nu = \nu_0 \exp[-W/(kT)], \tag{1}$$

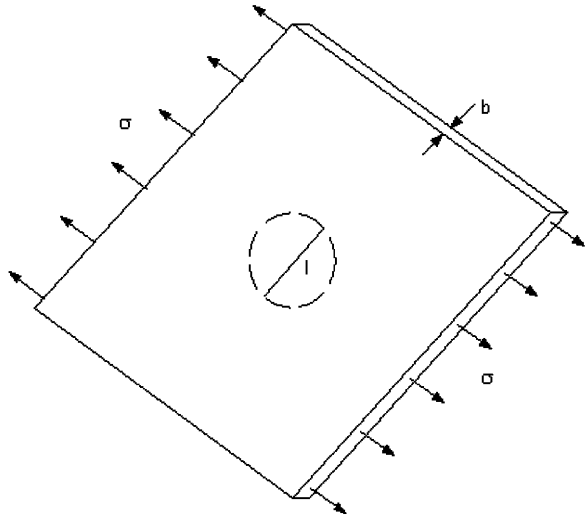

Fig. 1 – A schematic "2D" homogeneous nucleation of a crack of length l in an infinite plate under remote tensional stress σ.

where ν_0 is a normalizing rate, k is the Bolzmann constant, T is the absolute temperature and W is the needed enthalpy. Here we assume that volume and pressure are unchanged in the process and therefore W becomes the energy barrier needed to be overcome by the process. This energy is schematically calculated as follows (fig. 1): A fracture of length l in a 2D solid causes the release of elastic energy, the density of which is $\frac{\sigma^2}{2E}$ per unit volume, from the volume, shown in fig. 1, surrounding l:

$$W_1 \cong -\frac{\sigma^2}{2E}\pi l^2 b, \tag{2}$$

where σ is the stress field in the medium, E is the Young modulus and b is the thickness (assumed small with respect to the other dimensions) of the sample. The energy needed to create the two new surfaces is

$$W_2 = 2\Gamma l b, \tag{3}$$

where Γ is the surface energy. The total energy is therefore

$$W = -\frac{\sigma^2}{2E}\pi l^2 b + 2\Gamma l b. \tag{4}$$

Figure 2a depicts W as a function of l. The maximum W_{m} of W occurs for $l_{\mathrm{m}} = \frac{2\Gamma E}{\pi\sigma^2}$ and is

$$W_{\mathrm{m}} = \frac{2\Gamma^2 E b}{\pi\sigma^2}\,. \tag{5}$$

If no flaws exist in the material (homogeneous nucleation), the energy for the creation of a Griffith flaw equals W_{m}, and hence the rate of nucleation of such flaws should be

$$\nu = \nu_0 \exp\big[-\sigma_0^2/\sigma^2\big], \tag{6}$$

where $\sigma_0^2 \cong \frac{2\Gamma^2 E b}{\pi k T}$.

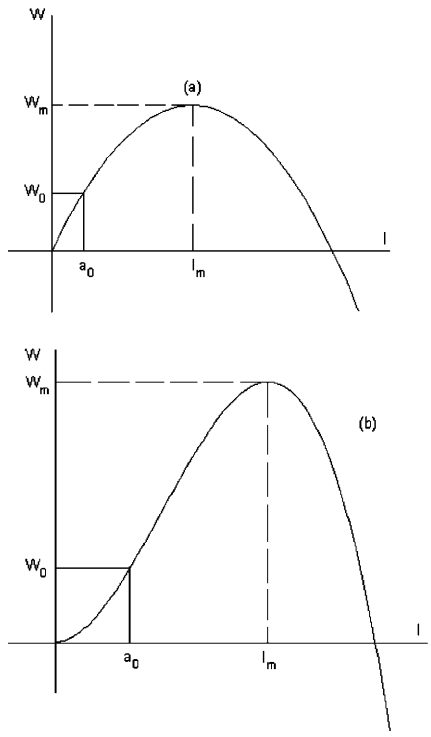

Fig. 2 – Total energy (relieved elastic and surface energies) as a function of l. (a) 2D case, (b) 3D case.

In three dimensions (3D) a similar calculation leads to a total energy given (fig. 2b) by

$$W = -\frac{\sigma^2}{2E}\left(\frac{4}{3}\pi l^3\right) + 2\Gamma\pi l^2. \tag{7}$$

Its maximal value occurs for $l_{\mathrm{m}} = 2\Gamma E/\sigma^2$ and is

$$W_{\mathrm{m}} = \frac{8}{3}\pi\frac{\Gamma^3 E^2}{\sigma^4}\,. \tag{8}$$

The nucleation rate becomes

$$\nu = \nu_0 \exp\left[-\sigma_0^4/\sigma^4\right], \qquad \sigma_0^4 = \frac{8\pi\Gamma^3 E^2}{3kT}\,. \tag{9}$$

Under a constant load which is below the critical stress, the times to failure for 2D and 3D materials are given by the reciprocals of the rates, namely,

$$\tau_2 = \tau_{02} \exp\left[\sigma_0^2/\sigma^2\right] \tag{10}$$

and

$$\tau_3 = \tau_{03} \exp\left[\sigma_0^4/\sigma^4\right], \tag{11}$$

respectively. Here τ_{02} and τ_{03} are characteristic times, equal to the $(1/\nu_0)$'s for 2D and 3D, respectively. Note that the dependence on σ, especially for the 3D case, is very strong: a small change in σ can lead to a large change in τ. Therefore, the measurements must be done very

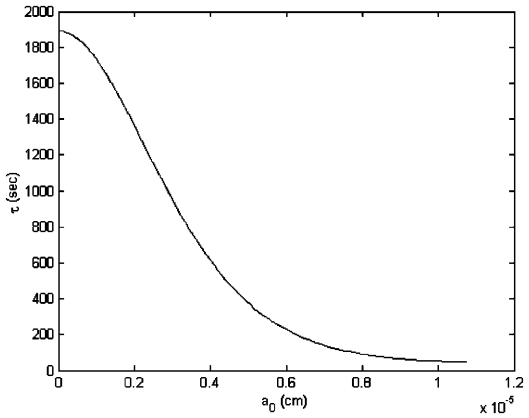

Fig. 3

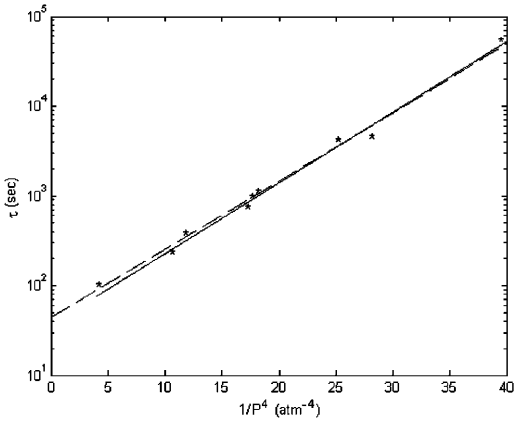

Fig. 4

Fig. 3 – The lowering of the time to failure for an existing crack of length a_0 in a 3D sample due to the decrease of the energy barrier. The value $a_0 = 0$ is for homogeneous nucleation. Here $l_{\rm m} = 1.3{\cdot}10^{-5}$ cm above which $\tau = \tau_0$.

Fig. 4 – Time to failure (for wood, $\tau_0 = 50.5\,{\rm s}$), τ, *vs.* $1/P^4$: our results (solid line), experimental results (*) (ref. [4]) and a best-fit line (dashed) for the experimental results (ref. [4]).

delicately to avoid a situation where the material either breaks immediately or does not break at all (the time to failure is above that of the experiment). Ciliberto's group [1–5] succeeded in obtaining very accurate measurements and verify the $\tau(\sigma)$ behavior for 3D fractures (see, *e.g.*, their results in fig. 4).

These are the results [6] of homogeneous nucleation, namely, the thermal fluctuations were supposed to overcome an energy barrier which started from zero —thus completely disregarding the existing flaw distribution in the material. Next, the non-homogeneous thermal nucleation of fracture is treated, *i.e.* nucleation where the stressed sample contains internal (or surface) flaws, which reduce the energy barrier.

The calculation is carried out for the three-dimensional case. Results can easily be extended to solids of other dimensions. The assumption is, therefore, that at the moment of loading the sample already possesses a flaw distribution. The length component of any flaw, perpendicular to the highest principal stress direction, is denoted by a. According to fig. 2b the barrier becomes smaller since thermal fluctuations need only to augment an existing flaw from a_0, say, to $l_{\rm m}$, rather than create a crack of length $l_{\rm m}$ from the start. The energy barrier is now given by (fig. 2b) $W = W_{\rm m} - W_0$, where

$$W_0 = -\frac{2}{3}\pi\frac{\sigma^2}{E}a_0^3 + 2\pi\Gamma a_0^2\,. \tag{12}$$

The value of W_0 is larger than zero for $a_0 < l_{\rm m}$. The time to fracture under such conditions is therefore

$$\tau = \tau_0 \exp\left[\frac{1}{kT}\left[\gamma/\sigma^4 + \alpha\sigma^2 a_0^3 - \beta a_0^2\right]\right], \tag{13}$$

where

$$\alpha = \frac{2}{3}\pi/E, \qquad \beta = 2\pi\Gamma, \qquad \gamma = \frac{8}{3}\pi\Gamma^3 E. \tag{14}$$

Clearly, eq. (13) shows that flaws facilitate failure. Thus, denoting by $\tau_1 = \tau_0 \exp[\gamma/(\sigma^4 kT)]$ the Pomeau result (eq. (9)), fig. 3 depicts the decrease in τ with a_0 ($0 \le a_0 \le l_{\rm m}$) from τ_1 to τ_0.

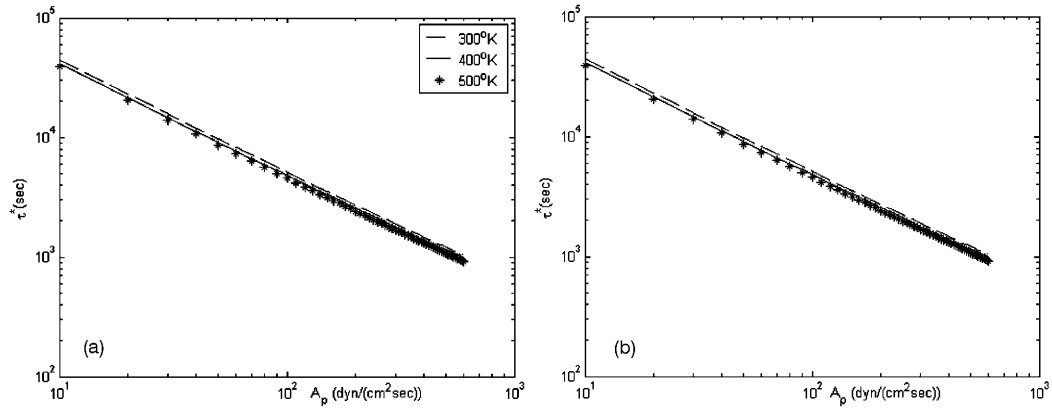

Fig. 5 – Time to failure (for wood) for a linearly increasing stress as a function of stress rate A_p. (a) $a_0 = 0$, simulating Guarino *et al.* [4] results. (b) Averaged times for a_0 chosen according to eq. (15).

Now, the most "important" flaw in a sample, the one for which the barrier is the smallest and hence leads to the shortest time to fracture if augmented, is the flaw with the longest a_0. Denoting the length of this flaw by a_l, eqs. (12) and (13) (with a_l replacing a_0) provide the lowest-energy barrier and the shortest (hence the measured) time to fracture, respectively.

According to the statistics of extreme values [9, 10], the longest cracks can have only one of three distributions, Gumbel, Frechet or Weibull. Since the "basin of attraction" of the Gumbel distribution includes the exponential and the Gaussian ones, both of which serve as possible distributions of flaws [11], it is conceivable that longest flaws here assume the Gumbel distribution. The probability density function of a_l is therefore [10] assumed to be

$$p(a_l) = \frac{1}{q} \exp[-(a_l - \mu)/q] \exp[-\exp[-(a_l - \mu)/q]], \tag{15}$$

where μ, q are parameters to be determined.

The following procedure was adopted. For specific chosen values of μ and q, an a_l value is chosen randomly from the $p(a_l)$ distribution. The τ for this a_l is calculated by eq. (13) for a definite stress σ and temperature T. Note that the choice mechanism can generate a_l values which are already above the Griffith criterion. For these cases τ is chosen to be τ_0 (see eq. (13)). In this way a histogram of τ's for these values of σ and T is obtained, from which the average $\bar{\tau}$ of τ under these conditions is calculated. Changing σ for the same T, these averages are drawn as a function of σ, $\bar{\tau}(\sigma)$. This procedure is repeated for different μ and q values, until the $\bar{\tau}(\sigma)$ agrees with the experimental results, at which point the values of μ and q are considered to be the correct ones for the flaw distribution. Results for wood are shown in fig. 4. Here (Guarino *et al.*, 2002), $E = 1.8 \cdot 10^8\,\mathrm{New/m^2}$, $T = 300\,\mathrm{K}$, hence $kT = 4 \cdot 10^{-21}\,\mathrm{J}$, $\Gamma = 5.9 \cdot 10^{-6}\,\mathrm{J/m^2}$ yielding $\alpha = 1.16 \cdot 10^{-10}\,\mathrm{m^2/New}$, $\beta = 3.76 \cdot 10^{-5}\,\mathrm{J/m^2}$ and $\gamma = 5.8 \cdot 10^5\,(\mathrm{mks})$. It is seen that, although $\ln(\tau)$ of eq. (13) is no longer directly proportional to $1/\sigma^4$, the changes are minimal and the agreement with experiment is good.

A straightforward understanding of the situation can be obtained by considering $\ln\tau$ as function of $x = 1/\sigma^4$. By eq. (13) we obtain

$$\ln\tau = c + \frac{1}{kT}\left(\gamma x + \frac{\alpha a_0^3}{\sqrt{x}}\right), \tag{16}$$

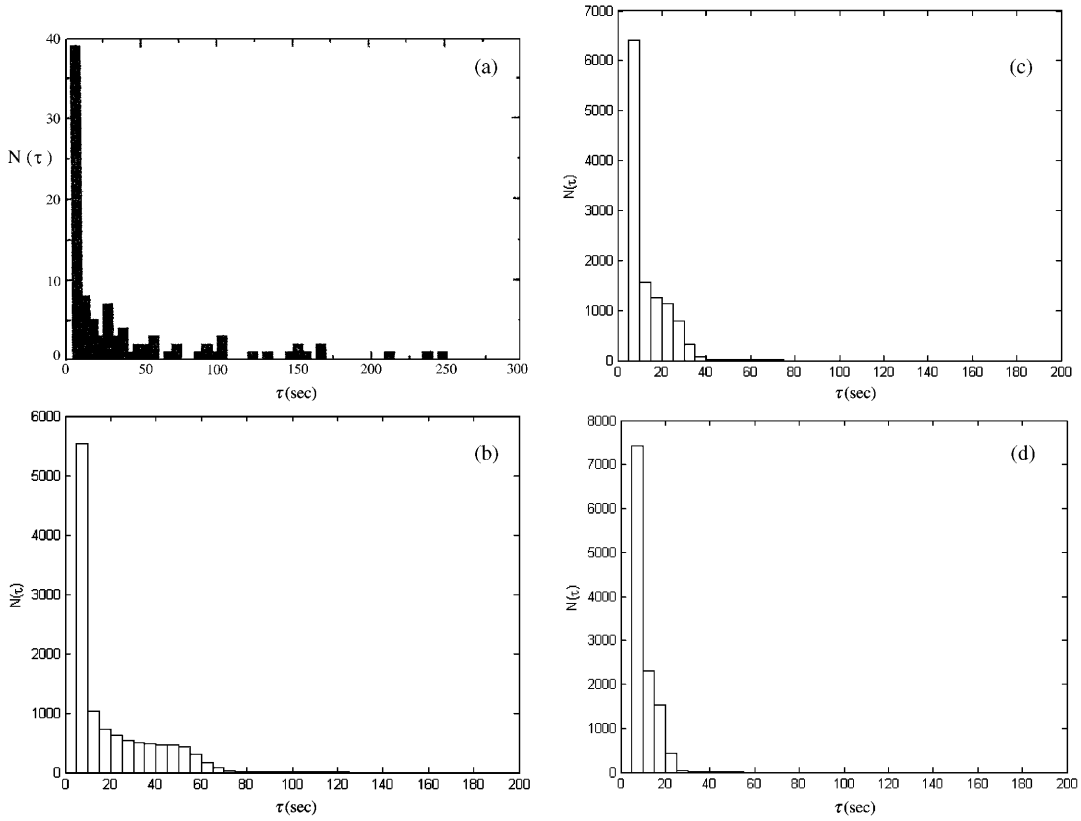

Fig. 6 – Time-to-failure distributions for various temperatures (for fiberglass, $\tau_0 = 2.7\,\mathrm{s}$). (a) Experimental results (ref. [4]), $T \cong 300\,\mathrm{K}$ (b), (c), (d): results of our calculations (eqs. (13) and (15)) for $T = 300\,\mathrm{K}$, $400\,\mathrm{K}$, $500\,\mathrm{K}$, respectively.

where $c = \tau_0 \exp[-\beta a_0^2/kT]$. Hence $\ln\tau$ has a minimum at

$$x_1 = \frac{1}{\sigma_1^4} = \left(\frac{\alpha}{2\gamma}\right)^{2/3} a_0^2 \tag{17}$$

below which it diverges. Therefore, if the stress values used in the experiment are much larger than σ_1, then $\ln\tau$ would still follow a straight line. For fig. 4, the largest experimental σ or (P) is $\sim 0.7\,\mathrm{atm}$ while for our simulations $a_0 = 1.2 \cdot 10^{-6}\,\mathrm{cm}$ and therefore $\sigma_1 \approx 3.5\,\mathrm{atm}$.

A second experiment, analyzed, *e.g.*, in ref. [4], is where a load, which is linearly increasing with time ($\sigma = A_p t$ for a constant A_p), is applied to different samples until they fail. The breaking times are drawn as a function of A_p in a log-log plot yielding a straight line. In the experiment [4] two temperatures were used, $300\,\mathrm{K}$ and $380\,\mathrm{K}$, with almost no difference in the obtained straight lines. On the basis of this invariance, the investigators concluded that there was something amiss, and invoked [5] fiber bundle theory to explain this apparent difficulty.

The difficulty is, however, only a sham difficulty as can be seen from the following "numerical experiment". First, we follow the method used in [4] to treat breaking time problems where the stress changes with time. Regard [4] the variable $1/\tau$ (either of eq. (11) for homogeneous or eq. (13) for non-homogeneous nucleation) as the "density of damage" per unit

time. Breaking is certain to occur after a time τ^*, if

$$\int_0^{\tau^*} \frac{1}{\tau(t)} \mathrm{d}t = 1. \tag{18}$$

We now apply eq. (18) to find τ^* numerically by integrating eq. (11) with $\sigma = A_p t$, or perform a similar calculation using eq. (13) with an appropriate choice process (of a_l) as described before. We obtain (fig. 5) the "surprising" result that, in both cases, *results are almost independent of temperature*. The results of Guarino *et al.* (ref. [4], fig. 8) are therefore completely natural and in line with both the homogeneous– and non-homogeneous–nucleation theories.

We now turn to the time distribution function. Experimental results for fiberglass (ref. [4], fig. 6) show a distribution which is definitely neither Poissonian nor Gaussian. Using eq. (13) and choosing a_l values randomly according to eq. (15), a series of τ values is thereby generated. In this way we calculated τ-distribution functions of fiberglass for several temperatures. Here $E = 10^{10}\,\mathrm{New/m^2}$, $\Gamma = 3.17 \cdot 10^{-7}\,\mathrm{J/m^2}$, $\tau = 2.7\,\mathrm{s}$ yielding $\alpha = 2.09 \cdot 10^{-12}\,\mathrm{New/m^2}$, $\beta = 1.99 \cdot 10^{-6}\,\mathrm{J/m^2}$, $\gamma = 2.66 \cdot 10^5\,(\mathrm{mks})$ and $kT = 4 \cdot 10^{-21}\,\mathrm{J}$, $5.33 \cdot 10^{-21}\,\mathrm{J}$, $6.67 \cdot 10^{-21}\,\mathrm{J}$ for $T = 300$, 400, 500 K, respectively. Distribution results are shown in fig. 6 for different values of temperature. It is seen that a) the distribution function for 300 K is very similar to the experimental results (compare figs. 6a and b). b) The change of distribution function with temperature is interesting. Thus, a relatively small temperature increase causes the "balance" of the distribution to move somewhat towards shorter times, while a large increase (in fig. 6 from 300 K, say to 500 K) causes the distribution to become quite concentrated near τ_0.

It is therefore seen that thermal nucleation [6, 7] is indeed the process behind failure of heterogeneous samples under creep conditions. An improvement of the theory by the use of non-homogeneous nucleation, where account is taken of the existing flaw distribution inside the sample, leads to easier fracture and to a prediction of the change of lifetime distribution with temperature.

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