Atomistic Fracture and Nano-Macro Transition for Strength and Lifetime Statistics of Quasibrittle Structures

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Abstract

This paper presents a physically based theory to model the strength and lifetime distributions of quasibrittle structures. The theory is derived from the fracture mechanics of atomic lattice cracks propagating through the lattice by tiny jumps over numerous activation energy barriers on the surface of the free energy potential of the lattice, caused by crack length jumps by one atomic spacing. The theory indicates that the strength threshold is zero, and that the strength distribution for a quasibrittle structure depends on its size, as well as geometry, varying from Gaussian distribution (modified by far-left power law tail) for small-size structures, to Weibull distribution for large-size structures. The theory is further extended to model the lifetime distribution of quasibrittle structures under constant loads (creep rupture). It is shown that, for quasibrittle materials, there exists a marked size effect on not only the structural strength but also the lifetime, and that the latter is stronger. For various quasibrittle materials, such as industrial ceramics and fibrous composites, it is demonstrated that the proposed theory correctly predicts the experimentally observed deviations of strength and lifetime histograms from the classical Weibull theory, as well as the deviations of the mean size effect curves from a power law.

1. Introduction

Engineering structures must generally be designed for tolerable failure probability $P_f \leq 10^{-6}$ per lifetime. Experimental verification by histogram testing for such a low failure probability is impossible. Obviously, a physically based theory is needed. For the limiting special cases of plastic or brittle failure, the type of probability distribution of structural strength is known and the distribution function can be calibrated by calculating its mean and variance. For plastic failure, the failure load is essentially a weighted sum of the strength contributions from all the RVEs, which are random. Therefore, according to the central limit theorem, the failure load must follow the Gaussian (normal) distribution. For brittle failure, in which the failure of one RVE causes the failure of the whole structure, the weakest-link model applies. If the number of RVEs that could trigger the failure is very large ($>10^4$), then the failure load must follow the Weibull distribution.

Quasibrittle materials, which include concrete, fiber composites, rocks, stiff cohesive soils, tough ceramics, rigid foams, sea ice, wood, bone, various bio- and high-tech materials, and most materials on approach to nano-scale, are brittle heterogeneous materials where the fracture process zone (FPZ) is not negligible compared to the structure size. It has been demonstrated that the behavior of quasibrittle materials transits from quasi-plastic to brittle with increasing structure size. Such a transition has a significant consequence for structural reliability and lifetime prediction of quasibrittle structures. Extensive histogram testing shows that the cumulative distribution function (cdf) of strength of many quasibrittle materials deviates from the two-parameter Weibull distribution. This deviation was thought to imply the three-parameter Weibull distribution with non-zero threshold. However, for a broad-range strength histogram with many thousands of data, a systematic deviation from the experimental histograms still remains [1, 2, 3].

This paper reviews a recently developed theory that explains the deviations of strength histograms of quasibrittle materials from the Weibull distribution, and then focuses on extending the theory to model the lifetime distribution of these materials. The new theory is validated by optimum fitting of the strength and lifetime histograms of various quasibrittle materials such as industrial ceramics and fibrous composites.

2. Strength Distribution at Nanoscale via Atomistic Fracture Mechanics

Consider a nano-scale size atomic lattice block undergoing fracture as shown in Fig. 1 [4]. At the fracture front, the interaction force (the cohesive force along the interatomic crack) and the corresponding separation between the atoms are characterized by a local bond potential Π_1 (Fig. 1) which is a part of the overall potential function Π (or more generally, free energy) of the atomic lattice (crudely, Π_1 could be described as the Morse or Lennard-Jones potential, but a specific form is not needed here).

The interatomic crack propagates by jumps from one crack length to another (Fig. 2b, c). During each jump, one barrier on the potential Π as a function of u must be overcome (see the wavy potential profile in Fig. 2c). Due to thermal activation, the state of the atomic lattice block fluctuates and can jump over the activation energy barrier in both forward and backward directions (Fig. 2b, c, d), though not with the same frequency due to the presence of the remote stress. Let Q_0 be the activation energy barrier at the current crack length. When the cohesive crack length (defined by the location of state 3 in Fig. 1c) jumps by one atomic spacing, h_a (i.e, from a_i to a_{i+1}, i = 1, 2, 3,...), the activation energy barrier is changed by a small amount ΔQ corresponding to the energy release by fracture (Fig. 2c,d) associated with the equilibrium load drop ΔP (Fig. 2a).

Within the framework of fracture mechanics, the energy release rate of the atomic lattice can be expressed as : $G = D_a\, g(\alpha)\sigma^2/E$ where E = elastic Young's modulus for the continuum approximation of the lattice, D_a = total length (or dimension) of the cross section of the lattice (Fig. 1a), σ = remote average stress (Fig. 1a) applied on the lattice (which is proportional to P/bD_a, b = length of crack front in the third dimenstion), $g(\alpha) = k^2(\alpha)$ = dimensionless energy release rate function of linear elastic fracture mechanics of continuous bodies, characterizing the fracture and block geometry, $k(\alpha)$ = dimensionless stress intensity factor [12, 13], and $\alpha = a/D_a$. Accordingly,

$$\Delta Q = h_a\left[\frac{\partial \Pi(P,a)}{\partial a}\right]_P = h_a b\mathcal{G} = h_a b D_a g(\alpha)\sigma^2/E = \sigma^2 V_a/E \qquad (1)$$

where $V_a = V_a(\alpha) = h_a b D_a g(\alpha)$ = activation volume of the lattice crack (if the applied stress tensor is written as $\sigma \boldsymbol{s}$ where σ = stress parameter, one could more specifically write $V_a = \boldsymbol{s} : \boldsymbol{v_a}$ where $\boldsymbol{v_a}$ = activation volume tensor, as in atomistic theories of phase transformations in crystals [4]).

Since the crack jump by one atomic spacing h_a is very small, the activation energy barrier for a forward jump, $Q_0 - \Delta Q/2$, differs very little from the activation energy barrier for a backward jump, $Q_0 + \Delta Q/2$. So the jumps of the state of the atomic lattice block, characterized by its free energy potential Π, must be happening in both directions. According to the transition-rate theory [6, 7], in the limit of a large free-energy barrier, $Q_0 >> kT$, the first-passage time for each transition is given by Kramers' formula [8], and the difference in the frequencies of the forward and backward jumps, or the net frequency of crack length jumps, is

$$f_b \sim \nu\left(e^{-[Q_0-\sigma^2 V_a/2E]/kT} - e^{-[Q_0+\sigma^2 V_a/2E]/kT}\right) = 2\nu e^{-Q_0/kT}\sinh\frac{\sigma^2 V_a}{2EkT} \qquad (2)$$

where $C_f = \dfrac{\nu\sigma^2 V_a}{EkT}e^{-Q_0/kT}$, T = absolute temperature, k = Boltzmann constant, V_a corresponds to some effective crack length α, and ν is a characteristic attempt frequency for the reversible transition (e.g. kT/h, where h = Planck's constant, which can be set by a shift of the activation free energy).

The failure of the atomic lattice occurs when the nano-crack propagates from its original length a_0 to a critical length a_c. In other words, the crack experienced many length jumps, i.e. n jumps, where the frequency of each jump is given by Eq. 2. At the atomic level, it is generally assumed that the each jump is independent (the frequency of the jump is independent of the particular frequency of breaks and restorations that brought the nanocrack to the current size). Since the probability is proportional to the frequency of quasi-stationary process, the failure probability of the atomic lattice block can be written as:

$$P_f(\sigma) = \sum_{i=1}^{n} f_{bi} \sim \int_{\alpha_0}^{\alpha_c} 2\nu e^{-Q_0/kT}\sinh\frac{\sigma^2 V_a(\alpha)}{2EkT}\,\mathrm{d}\alpha \approx \left(\frac{\nu e^{-Q_0/kT}}{EkT}\int_{\alpha_0}^{\alpha_v} V_a(\alpha)\mathrm{d}\alpha\right)\sigma^2 \qquad (3)$$

The last expression is an approximation for small stress σ, which is justified by the fact that only the left far-out tail of cdf of strength matters [1, 2, 4]. More

specifically, we require $\Delta Q << kT << Q_0$ or $\sigma << \sqrt{EkT/V_a}$. It is essential that the tail of strength distribution at nanoscale follows a power law and that the stress threshold is zero.

3. Strength and Lifetime Distribution at Structural Scale

The transition from the atomic scale to the RVE scale may be statistically described by a model consisting of a hierarchy of elements coupled in parallel and in series [1, 2]. The parallel couplings reflect the fact that a passage from one scale to the next higher scale involves strain compatibility conditions, and the series couplings reflect the equilibrium conditions, in the sense of the weakest-link chain model, reflect damage localization into microcracks. It has been shown that the parallel coupling raises the tail exponent in an additive manner and drastically shortens the reach of power-law tail, and series coupling preserves the tail exponent while extending the reach of power-law tail. It has been demonstrated [2] that the RVE must be statistically modeled by a hierarchical model consisting of bundles (or parallel couplings) of only 2 long sub-chains, each of them consisting of sub-bundles of 2 or 3 long sub-sub-chains of sub-sub-bundles, etc., until the nano-scale of atomic lattice is reached. The power-law cdf tail is transmitted through all the scales from nano to macro while its exponent is gradually raised from 2 on the atomistic scale to a value equal, on the RVE scale, to the Weibull modulus of strength distribution (typically between 10 and 50).

The consequence of the hierarchical model is that the strength cdf for one RVE must have a very broad Gaussian core, onto which a power-law tail of an exponent equal to the Weibull modulus is grafted at the failure probability about 10^{-3} to 10^{-4}. Numerical simulations reveal that the transition from Weibull cdf to Gaussian cdf occurs smoothly but over a relatively short segment of cdf. Therefore, for the sake of simplicity, we may consider a Weibull cdf to be grafted from the left onto a Gaussian cdf, with only the cdf value and its slope being continuous at the grafting point [1, 2]:

$$P_1(\sigma_N) = 1 - \exp[-(\sigma_N / s_0)^m] \qquad (\sigma_N \le \sigma_{gr}) \qquad (4)$$

$$P_1(\sigma_N) = P_{gr} + \frac{r_f}{\delta_G \sqrt{2\pi}} \int_{\sigma_{gr}}^{\sigma'} e^{-(\sigma' - \mu_G)^2 / 2\delta_G^2} \, \mathrm{d}\sigma' \qquad (\sigma_N > \sigma_{gr}) \qquad (5)$$

where P_{gr} = grafting probability, m, s_0 = Weibull modulus and scale parameter for the Weibull tail, r_f = normalizing parameter such that $\int_0^\infty p_f(\sigma)\,\mathrm{d}\sigma = 1$ (p_f is the corresponding probability density function (pdf)). μ_G, δ_G = mean and standard deviation of the Gaussian distribution. Hence, in total, there are 6 statistical parameters in the model, with two constraints (the normalizing condition and the continuity of pdf at the grafting point). Four parameters are needed to define the cdf uniquely.

It is postulated that, when an RVE is subjected to a certain load history, the randomness in its lifetime is related to the randomness in its strength. In this study, we focus on the simplest loading history, which is the case of creep- rupture. Consider two loading cases: 1) the load rapidly increases at a constant rate until the failure, which defines the strength of RVE, 2) the load rapidly increases till a certain level which then sustained until the failure, which defines the lifetime. The relationship between the strength and lifetime can be obtained through the concept of the growth of subcritical crack on the RVE level.

Consider an RVE with some dominant subcritical crack a_0. Under certain loading history, the crack grows to its critical length a_c and then the RVE fails. It is assumed that this process can be described by Evans' law [9, 10, 11, 12]:

$$\frac{\mathrm{d}a}{\mathrm{d}t} = Ce^{-Q_0/kT}K_I^n \tag{6}$$

where n = constant, K_I = stress intensity factor, which can be written as $K_I = \sigma\sqrt{D}k(a/D)$. By separation of variables, one can integrate the foregoing equation for the two cases mentioned above and obtain the relationship between the strength and lifetime of the RVE:

$$\sigma_N = [\lambda(n+1)]^{n/(n+1)}\sigma_0^{n/(n+1)}\tau^{1/(n+1)} \tag{7}$$

Note that the RVE strength σ_N is random in nature. Its distribution is described by Eqs. 4 and 5. With Eq. 7, one obtains the lifetime distribution for one RVE:

$$P_1(\tau) = 1 - \exp[-(\tau/s_\tau)^{m/n}] \qquad (\tau \le \tau_{gr}) \tag{8}$$

$$P_1(\tau) = P_{gr} + \frac{r_f}{\delta_G\sqrt{2\pi}}\int_{\gamma\tau_{gr}^{1/(n+1)}}^{\gamma\tau^{1/(n+1)}} e^{-(\tau'-\mu_G)^2/2\delta_G^2}\mathrm{d}\tau' \qquad (\tau_N > \tau_{gr}) \tag{9}$$

where $s_\tau = s_0^{n+1}\beta^{-(n+1)}\sigma_0^{-n}$, $\tau_{gr} = \beta^{-1}\sigma_0^{-n}\sigma_{N,gr}^{n+1}$, and $\gamma = \beta\sigma_0^{n/(n+1)}$. Note that the Weibull modulus for lifetime distribution for the creep rupture case is much lower than it is for the strength distribution. Compared to the strength distribution, the core of lifetime distribution does not follow Gaussian distribution, but it can be analytically derived from the Gaussian core of strength distribution by using Eq. 9.

In the context of softening damage and failure of a structure, RVE must be defined as the smallest material volume whose failure causes the failure of the structure [2]. Therefore, by the virtual of the joint probability theorem, the failure probability of the structure can be written as:

$$P_f(\sigma_N, \tau) = 1 - \prod_{i=1}^{N}[1 - P_1(\alpha_i\sigma_N, \tau)] \tag{10}$$

where α_i = dimensionless stress distribution parameter describing the stress at the center of the i^{th} RVE. Here, it is useful to introduce the concept of equivalent number of RVEs, N_{eq}, for which a chain of N_{eq} elements subjected to a uniform stress σ_N gives the same cdf:

$$P_f(\sigma_N, \tau) = 1 - [1 - P_1(\sigma_N, \tau)]^{N_{eq}} \tag{11}$$

Note that N_{eq} is independent of strength σ_N for the Weibull portion of $P_1(\sigma_N)$, while it is a function of σ_N for the Gaussian portion of $P_1(\sigma_N)$. Consider now a

large size structure ($N_{eq}\to\infty$); the structure fails at very small stress, or for a short lifetime, so what matters is the tails of the strength and lifetime cdfs of one RVE, which are power laws. Obviously, for large-size structures, both the strength and lifetime cdfs approach Weibull distribution.

4. Optimum Fitting of Strength and Lifetime Histograms

Extensive efforts have been devoted to investigate by histogram testing the strength and lifetime distributions of various quasibrittle materials, such as concrete, ceramics and fiber composites. The two-parameter Weibull model has been widely used to fit these histograms, however, often the fit has not been close.

Fig. 3 shows the optimum fits of the strength histograms of various engineering ceramics by the present theory and by the two-parameter Weibull distribution [4]. It is clear that, in the Weibull scale, the strength histograms exhibit a kink which separates the entire distribution into two segments, and the two-parameter Weibull distribution is not able to fit both segments simultaneously. In contrast, the present theory can fit the both segments with the location of the kink very well. Within the framework of the present theory, the existence of the kink indeed reflects the quasibrittleness of the structure.

Fig. 4 presents the optimum fits of the lifetime histograms of Kevlar 49 fiber composite [13]. The specimens were tested in high temperature environment (100°C to 110°C) to accelerate the failure. Similar to the strength histograms, in the Weibull scale, there exists a kink separating the histogram into two segments. The present theory gives perfect fits of the histograms. From the fitting, the Weibull modulus of lifetime distribution is estimated to be around 2.3 to 3, which is significantly lower than the typical value of Weibull modulus of strength distribution of Kevlar 49, which is around 40.

5. Size Effect on Mean Structural Strength and Lifetime

Knowing the size effects on the strength and lifetime cdfs, one can compute the size effects on the mean strength and lifetime. For small structure sizes, both size effect curves deviate from the power-law size effect of Weibull theory, due to quasibrittleness of the structures. It has been shown that the calculated mean size effect on structural strength agrees well with the experimental observations of the size effect on the structural strength of concrete [14], as well as the predictions of several models such as nonlocal Weibull theory [15, 16], non-local damage model [17], crack-band model [18], and cohesive crack model [18, 19]. Though the analytical expression for the mean size effect on strength is impossible, it can be approximated via asymptotic matching [19]:

$$\bar{\sigma}_N = \left[N_a / N + \left(N_b / N\right)^{s/m}\right]^{1/s} \tag{12}$$

where N is the equivalent number of RVEs represented by the number of elements in the weakest-link model of the structure, and N_a, N_b, m, s are constants to be found from four asymptotic matching conditions. It is shown that the m-value must be the same as the Weibull modulus of the material. To obtain the remaining three parameters, one may solve three simultaneous equations expressing three asymptotic matching conditions: $\left[\overline{\sigma}_N\right]_{N\to 1}$, $\left[\mathrm{d}\overline{\sigma}_N/\mathrm{d}N\right]_{N\to 1}$, and $\left[\overline{\sigma}_N N^{1/m}\right]_{N\to\infty}$.

The size effect on structural lifetime can be derived from Eq. 7 since the lifetime is related to strength via Eq. 7. Hence, one has:

$$\overline{\tau} = \left[C_a / N + \left(C_b / N\right)^{s/m}\right]^{(n+1)/s} \tag{13}$$

where m = Weibull modulus of strength cdf, n = exponent of Evans' crack growth law. Parameters C_a, C_b, and s can be obtained by three asymptotic matching conditions similar to those for Eq. 12. It is clear that the size effect on structural lifetime under constant loads is much stronger than the size effect on structural strength.

6. Conclusion

The present theory improves the previous explanation [1, 2] of the derivations of strength histograms of quasibrittle materials, and extends this explanation to similar deviations in the histograms of lifetime. Both the types of strength and lifetime distributions are size- and geometry- dependent, and there exists strong size effects on both the mean structural strength and the lifetime. Furthermore, it is shown that the Weibull moduli of the strength and lifetime distributions are related through the exponent of Evans' crack growth law.

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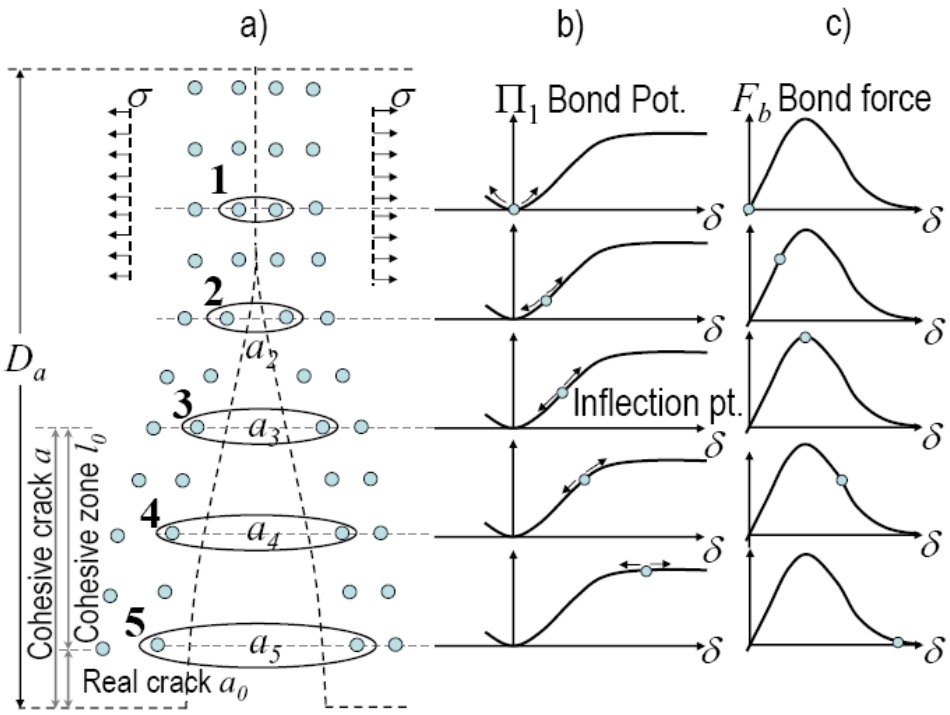

Fig. 1 Fracture of atomic lattice

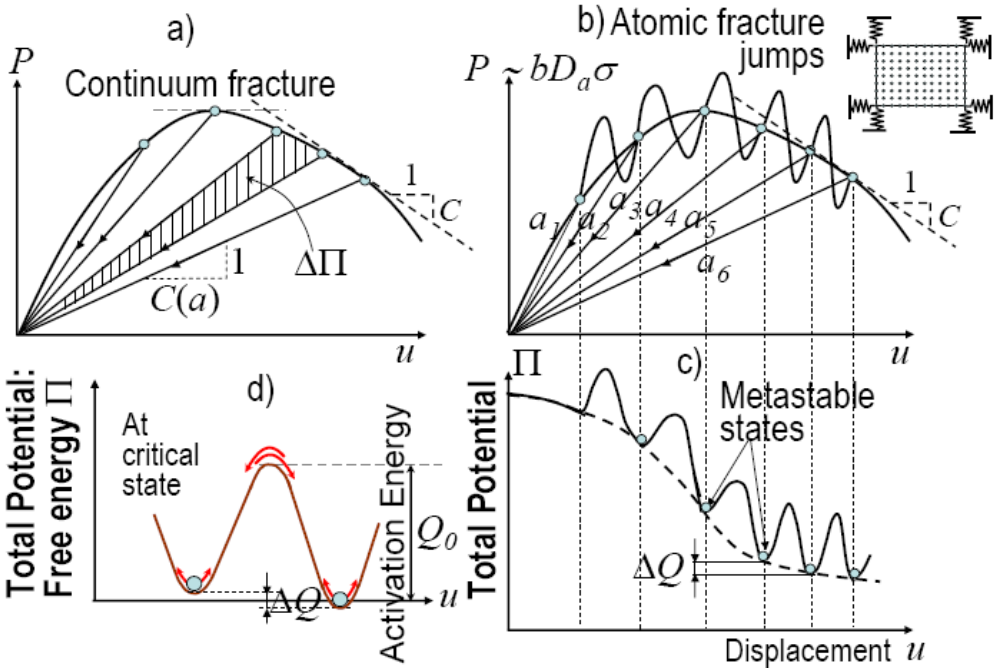

Fig. 2 Load displacement curve of atomic lattice block

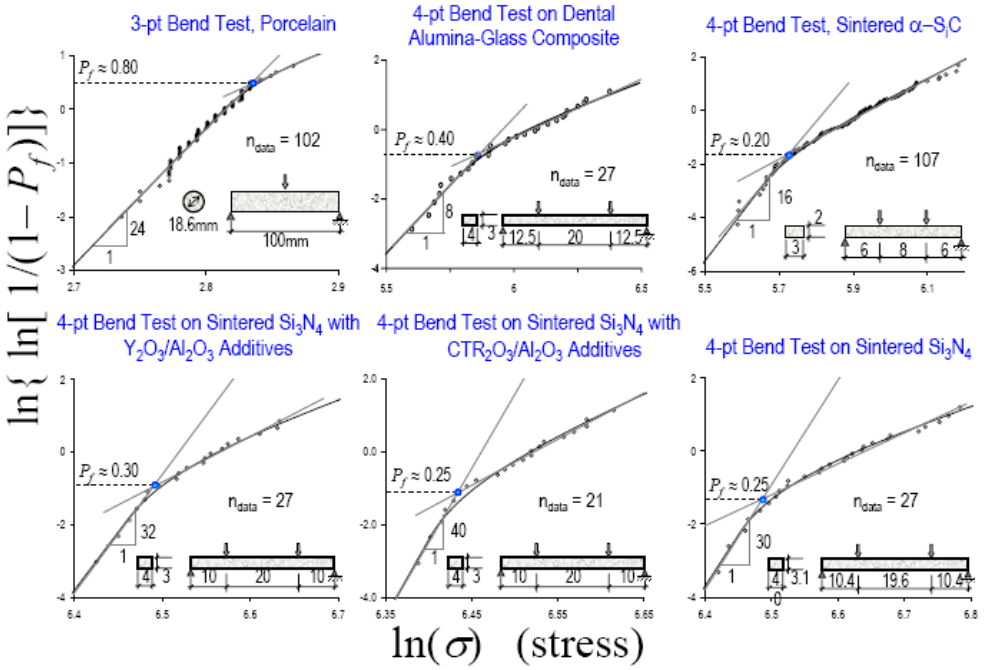

Fig. 3 Optimum fits of strength histograms for industrial ceramics

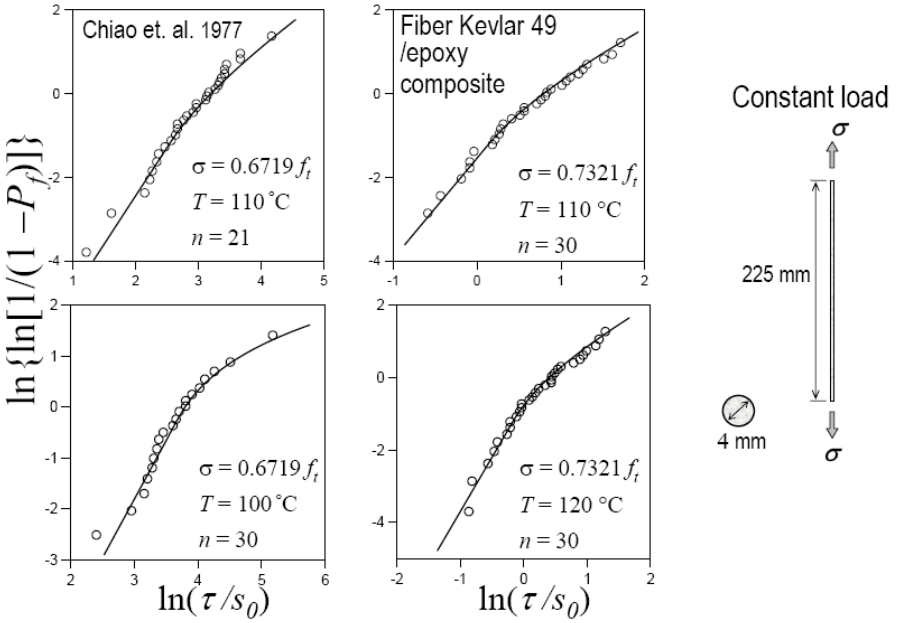

Fig. 4 Optimum fits of lifetime histograms for organic fibrous composites