

# Reliability Theory of Stochastic Fracture Processes in Sustained Loading: Part I

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It is shown that the physical mechanism of thermally activated subcritical crack growth is always a stochastic process and leads, therefore, to probabilistic crack propagation. This process is the result of the random breaking of atomic bonds and has to be clearly distinguished from the well known Weibull distribution. A Markov chain analysis leads to the normal distribution of crack sizes. The results demonstrate that conventional deterministic finite life-time designs are unsatisfactory and can lead to early failure of machine or structure elements as the consequence of the probabilistic process of crack propagation. The conclusions lead to the reliability analysis of Part II.

## 1. Introduction

Structures and machinery components always contain defects and microcracks, which may lead to fracture by slow, time dependent, stable crack propagation. Because both the size and the distribution of the imperfections are random, fracture life is probabilistic [1], and is usually described with the Weibull distribution function. In the following, it will be shown that the physical process of crack propagation itself is also stochastic, so that the fracture life-time is probabilistic even in homogeneous, defect-free materials [2]. The resulting probability distribution is superposed on the Weibull distribution. The effect of this physical process is analyzed from the reliability point of view in Part I and the corresponding reliability theory will be developed in Part II.

## 2. The Physical Process of Crack Propagation

Crack propagation is a consecutive process; the atomic bonds break one-by-one at the moving crack tip. In temperature dependent slow crack propagation thermal activation, together with the mechanical work, provides the energy needed for bond breaking. Since thermal activation is always a stochastic physical phenomenon, temperature dependent crack propagation is always probabilistic.

All major studies of thermally activated fracture employ a rate theory [3–9] (usually called transition state theory, or activated complex theory, or absolute rate theory [10, 11]), which considers that these processes occur by passing through an energy state associated with an activated complex of atoms that take part in the bond breaking or healing step [12–17].

The physical reason for the full validity of the theory that is presented here rests in the stochastic character of thermally activated processes: Any change in atomic interaction, and therefore in crack propagation, is stochastic and leads to the same type of mathematical treatment. Thus the macroscopically observed crack propagation is the net result of bond breaking and healing steps, both of which, as it has been well established, can take place in brittle fracture [4–7, 12–17]. Because the process is thermally activated, the time between two bond breaking (or healing) steps is a stochastic quantity. The reciprocals of these waiting times are the rates of bond breaking and of bond healing. The average rate of bond breaking, that is, the average number of bonds broken per unit time is expressed by the breaking rate constant  $k_b$  as [6, 11, 18]

$$k_b = \frac{kT}{h} \exp\left(-\frac{\Delta G_b}{kT}\right) = \frac{kT}{h} \exp\left[-\frac{\Delta G_b^* - W}{kT}\right], \quad (1)$$

and the average rate of bond healing as

$$k_h = \frac{kT}{h} \exp\left(-\frac{\Delta G_h}{kT}\right) = \frac{kT}{h} \exp\left[-\frac{\Delta G_h^* + W}{kT}\right]. \quad (2)$$

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In (1) and (2),  $\Delta G_b^\ddagger$  is the free energy needed to break the atomic bond as the crack propagates by one atomic distance, and  $W$  is the mechanical work contributed to the crack propagation by the stress through the stress intensity factor so that  $W = f(K)$ . It is important to note that (1) and (2) are physically rigorous expressions, in which  $k$  and  $h$  are precise universal constants, and the other quantities are defined exactly by the appropriate physical, chemical, or fracture mechanics theories. In other words, the rate constants do not contain "loose" parameters, empirical quantities, or "fudge factors".

The movement of cracks is identical to a step-wise process in which the crack tip waits for an average time of  $1/k$  before transition over the energy barrier into the next (or previous) valley [6, 11, 18]. As it was pointed out, the rate constants, expressing the frequency of transitions from one location into the other, are stochastic quantities. Furthermore, it is usually accepted in linear elastic fracture mechanics that the crack tip movement is controlled by the condition that exists at time  $t$  only and is independent from any previous history. Because the present study will be restricted to the investigation of crack propagation when the rate constants are independent of time, the process is Markovian. The Markov chain that corresponds to the physical process of crack propagation is shown in Figure 1. Position 0 represents the tip of the initial crack, the development of which is outside the scope of crack propagation study: It is generally considered that a distribution of small cracks is always present in engineering materials, and the ones that are under favourable conditions for propagation, will do so. The fact that healing does not proceed below the initial crack size is indicated in the figure. Crack propagation will terminate when the last thermal activation occurs and the specimen parts. This is also indicated in the figure by noting the movement of the crack tip from position  $n-1$  to  $n$ , where the specimen reaches the fractured state and, obviously, healing cannot take place.

To determine the crack-size distribution, the usual Markovian system of first order linear differential equations has to be assembled. Each equation expresses the fact that at each position of the crack tip (at each station of the Markov chain) the change per unit time in the number of specimens with cracks of this size is equal to the number of cracks moving *into* this position (forward by bond breaking and backward by bond healing) minus the number of cracks moving *out* of this position (by bond breaking due to forward activation, and by bond healing due to backward activation) per unit time. Exceptions are the 0-th and the  $n$ -th stations where some of the breaking and healing components are not presented, as indicated by Figure 1. In their physical meaning, the equations express the conservation of the number of specimens with cracks: The crack size can change during the fracture process from 0 to  $n$ , but new cracks are not initiated, nor can a specimen disappear.

The conservation equation system is written as:

$$\begin{aligned}\frac{dQ_0}{dt} &= -k_b Q_0 + k_h Q_1, \\ \frac{dQ_1}{dt} &= k_b Q_0 - (k_b + k_h) Q_1 + k_h Q_2, \\ &\vdots \\ \frac{dQ_i}{dt} &= k_b Q_{i-1} - (k_b + k_h) Q_i + k_h Q_{i+1}, \\ &\vdots \\ \frac{dQ_{n-1}}{dt} &= k_b Q_{n-2} - (k_b + k_h) Q_{n-1}, \\ \frac{dQ_n}{dt} &= k_b Q_{n-1},\end{aligned}$$

where  $Q_i$  is the number of specimens with cracks of size  $X_i$ .

The solution of this type of differential equation system is well known in reliability theory. Subject to the initial condition, at the moment of loading all

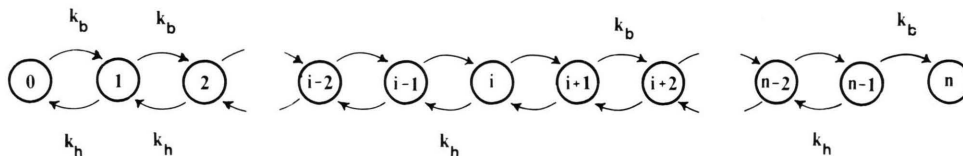


Fig. 1. The Markov chain model of a crack propagation process.

specimens have only initial sized cracks, that is, at  $t = 0$ ,  $q_i = 0$ , except  $q_0 = q_t$ , where  $q_t$  is the total number of specimens.

After a sufficiently large number of steps, the crack size distribution will be well approximated by the normal distribution. This statement is also valid when  $\mathbf{k}_h = 0$ . Because the length of each individual step is equal to the atomic distance (approximately  $1$  to  $4 \times 10^{-10}$  m), even a large number of steps (say, hundreds) will not change essentially the initial crack size. For reliability purposes, therefore, the crack-size distribution is expressed by

$$P(X, t) = \left[ \frac{1}{2\pi a^2 (\mathbf{k}_b + \mathbf{k}_h) t} \right]^{1/2} \cdot \exp \left\{ -\frac{[X - a(\mathbf{k}_b - \mathbf{k}_h) t]^2}{2a^2 (\mathbf{k}_b + \mathbf{k}_h) t} \right\} \quad (3)$$

This is a powerful result.

The expectation value

$$E(a, t) = a(\mathbf{k}_b - \mathbf{k}_h) t \quad (4)$$

identifies the average crack size, and  $v = a(\mathbf{k}_b - \mathbf{k}_h)$  describes the average crack propagation velocity rigorously and in terms of physical quantities: the atomic distance  $a$ ; the time  $t$ ; the atomic bond energy  $\Delta G^\ddagger$  expressing the chemical composition and the structure of the material; the temperature; the mechanical (loading) and geometrical (specimen shape and size) conditions  $W$  through the stress intensity factor of the crack driving force [4]. The changes in the composition and in the structure, caused by environmental effects as in stress corrosion cracking, are expressed through  $\Delta G^\ddagger$ , the bond energy. Indeed, all factors affecting the crack propagation velocity are represented in (3), and so in (4), and therefore, can be used in reliability analyses.

Similarly, the relation, expressing the spread in crack propagation

$$2\sigma^2 = 2a^2 (\mathbf{k}_b + \mathbf{k}_h) t,$$

(where  $\sigma$  is the standard deviation) is described fully and rigorously by the same physical quantities as the velocity.

Designs for long service life require an average of nearly zero crack velocity, or a very slow crack propagation. The corresponding condition is  $W_b \cong W_h \cong \frac{1}{2} \Delta G_b^\ddagger$ . Materials science considerations

have shown that in crystalline materials (metals, many ceramics and polymers)  $\Delta G_h^\ddagger = 0$  [19–21]. Therefore, when  $W_b = W_h = \frac{1}{2} \Delta G_b^\ddagger$ , it follows from (1) and (2) that

$$\begin{aligned} \mathbf{k}_b &= \frac{kT}{h} \exp \left\{ -\frac{\Delta G_b^\ddagger - \frac{1}{2} \Delta G_b^\ddagger}{kT} \right\} \\ &= \frac{kT}{h} \exp \left\{ -\frac{\Delta G_b^\ddagger}{2kT} \right\} \end{aligned}$$

and

$$\mathbf{k}_h = \frac{kT}{h} \exp \left\{ -\frac{\Delta G_h^\ddagger}{2kT} \right\}.$$

Therefore,

$$\mathbf{k}_b = \mathbf{k}_h = \mathbf{k},$$

and the expectation value is

$$E(a, t) = a(\mathbf{k}_b - \mathbf{k}_h) t = 0,$$

and so is the average crack propagation velocity, as required by safety restrictions. But, because the process is stochastic and a time-dependent crack size distribution exists, a number of cracks will propagate with a finite velocity: In other words, there is a finite probability that a fraction of the components will fail at time  $t$ , before the designed service life. As a convenient mathematical device, it can be considered that a slight occasional overload has shifted the crack size distribution sufficiently far from the zero-th position. Therefore, the crack size distribution can be considered by the normal distribution function, expressed as

$$P(X, t) = \frac{1}{2(\pi a^2 \mathbf{k} t)^{1/2}} \exp \left\{ -\frac{X^2}{4a^2 \mathbf{k} t} \right\}. \quad (5)$$

Equation (5) defines the probability of failure at time  $t$  for specimens with cracks of size  $X$  in the direction of crack propagation.

These conclusions are important, for they contradict the usual, classical, design and fracture mechanics concepts that are based on deterministic theories. The theory presented here considers the actual stochastic character of the real physical process and thus leads to a probabilistic life time prediction: It is more realistic, safer, economical, and well in line with the actual high technology requirements of reliability engineering.

### 3. Application to a Simple Reliability Problem

The severe consequence of the stochastic character of the physical process can be illustrated with a simple example.

A component has to be designed that is subjected to a stress level at which no crack propagation will take place according to conventional, deterministic, non-stochastic crack propagation concepts. To increase the clarity of the presentation, the model will be an ideally homogeneous material (that is: a single initial-sized crack is in the component, or, what is the same for the present purpose, a number of identical cracks, but each with the same probability for growth), subjected to constant  $W$ .

It was shown in the foregoing, that according to conventional concepts, cracks would not propagate when  $W \leq \Delta G^*/2$ . To achieve optimum performance, it is desirable to design for a service load that will produce a driving force at which  $W = \Delta G^*/2$ . In this case,  $\mathbf{k}_b = \mathbf{k}_h = \mathbf{k}$ , and the average propagation velocity is zero because the expectation value is

$$a(\mathbf{k}_b - \mathbf{k}_h) t = 0,$$

and consequently, no crack propagation is expected in the conventional sense. This concept is dangerous. It is clear from the results of this study that because crack propagation is a stochastic process, some cracks *will* propagate: a distribution of crack propagation will be observed. Under service conditions when crack propagation can be approximated by the normal distribution function, the standard deviation about the zero average crack velocity (for which the component was designed) is expressed as

$$\sigma = a(\mathbf{k}_b + \mathbf{k}_h)^{1/2} t^{1/2} = a(2\mathbf{k} t)^{1/2}.$$

For metallic or ceramic materials at room temperature and when

$$\Delta G^* \cong 0.8 \text{ eV}; \quad W = 0.4 \text{ eV},$$

at thirty years of service life the standard deviation is

$$\sigma = a(2\mathbf{k} t)^{1/2} = 5.35 \times 10^{-3} \text{ m},$$

and after a service time of 6 months it is

$$\sigma = 6.86 \times 10^{-4} \text{ m}.$$

For a material with a slightly lower bond strength of 0.74 eV the 30-year standard deviation is nearly

$1 \times 10^{-2} \text{ m}$ , and  $\sigma = 7.5 \times 10^{-4} \text{ m}$  after only two months of service time: Safety inspections conducted a few months after the start of operation will already show the development of macroscopic cracks in more than one third of the components! The replacement of these parts may be required, because under certain circumstances fast crack propagation can take place even when the cracks are smaller than the critical size; the production and installation of the components and the loss of operating time would increase the service cost unduly. It can be concluded that components, such as pipes, pressure vessels, containers with a wall thickness of 1 cm may fail in actual service under the condition discussed above, although considered safe in conventional design. The purpose of this example was to illustrate in a qualitative, rather than a quantitative manner the very strong effect of the stochastic character of the thermally activated, time dependent crack propagation process.

### 4. Closing Comments

The major studies [4–6] of subcritical brittle fracture are deterministic; they predict a one-to-one relation between the load and crack velocity for a given geometrical, material, and environmental condition. The present study follows a different approach by emphasizing that under identical conditions, the essentially stochastic physical character of crack propagation leads to a distribution of crack velocities, rather than to a single defined value for the velocity. It follows from the properties of Markov chains [22] that in the limit the two approaches merge, both giving the same description: the expectation value is identical to the value obtained in the deterministic theory and, simultaneously, the standard deviation is small. It is only then that the deterministic models give sufficiently good approximations of the true physical processes. Generally, the difference between the two approaches becomes important when the backward activation is significant (e.g. near the threshold). Although the elements of the probabilistic character of the physical process are of basic importance and are, indeed, implicit in the major models [4–7], the stochastic approach is not developed in any of them.

It is of interest to note that by discussing the detailed chemical and physical processes of stress corrosion cracking (SCC), [4–7] provide valuable



information for the further application and expansion of the kinetics discussed in the present report: these and the related studies can be employed well to enlarge and refine the details of the theory for specific applications. These references present models that are essentially based on the transition state theory of rate processes introduced and established in the 1930's by Becker, Polanyi, Eyring, Wigner and further employed by Vineyard: it was reviewed in the context of plastic flow and fracture by Krausz and Eyring [18]. In all of these approaches to subcritical crack propagation the foundation is common with the present work. The difference lies in our development of nonsteady state condition and in the introduction of the probabilistic nature of failure in place of the usual treatment. The model of Fuller and Thomson [6] extends the deterministic analysis and the go-no go type classical Griffith model to environmentally assisted crack propagation having a realistic discrete energy barrier system. Thomson's works on the modified Griffith condition is a very significant development. In the present study however, the environmental effects and the Griffith condition are not treated explicitly. Instead, a more general condition is established by not stating in detail the relation between the applied stress (stress intensity factor, or crack driving force) and the mechanical work, and by allowing a general treatment through the introduction of the Markov chain system. An application to simple models of SCC was presented before [23–25]. These models were in agreement with the typical condition of thermally activated fracture in static SCC as described in the excellent reviews by Pollet and Burns [4] and by Wiederhorn [5]. These reviews show that in glass, Regions I and II are controlled by chemical and transport processes, respectively. Subcritical, slow, crack propagation can, however, occur in brittle materials without corrosion as well. A typical example is the Region III process of consecutive bond breaking – possessing clearly all attributes of the Markov chain behaviour. The theory presented here applies to these conditions and we want to underline the statement [5] that “improved reliability in structural design requires a thorough understanding of the physical conditions that control subcritical crack growth so that this type of failure can be avoided”. The abovementioned authors [4, 5] also point out that crack velocity expressions are either of the type in which the stress dependence

appears in the exponent (as in the present study in  $\mathbf{k}$ ), or as a pre-exponential power function relation. It was shown ([18], also see Acknowledgement) that no preference can be assigned to any of the various power function models: The exponent can be determined only within  $\pm 50\%$  (The heavy scatter of the values is mainly caused by the inhomogeneity of the ceramic samples); these models are in part empirical; the functional dependence on stress differs from the physical form of reaction rate processes; the exponent itself is a function of the stress and temperature. A further difficulty arises when the model consists of many parameters, and consequently, almost any behaviour can be represented. The rate constant used in the present study, however, consists of universal constants ( $k$  and  $h$ ) and there are only the three parameters  $T$ ,  $\Delta G^*$  and  $W$ , all well defined quantities. When analysing any thermally activated process, the specific consideration of the temperature, the atomic bond strength and the work that drives the process is, of course, indispensable. Less than these three leaves the physical state indeterminate: under no condition can the problem be reduced to fewer parameters. It is a particular value of the approach taken that meaningful conclusions can be obtained with the strictest economy of terms.

The force varies along the crack tip and an exact description of the crack tip movement can not be obtained, only that of an average effect. The rate constant  $\mathbf{k}$  is such a quantity: it is the average number of bond breaking events. The mechanism of the process can be studied by the investigation of the stress and temperature dependence of this average rate constant  $\mathbf{k}$  and its relation to the velocity. Attention is drawn in this respect to the thoughts of Schoeck [3] and to the excellent review of Wielke [8] on the analysis of thermally activated processes in solids. Because in the threshold zone the stochastic approach differs significantly from the deterministic theories, it is in this zone where experimental comparisons and verification can be sought, using the principles and techniques discussed by Schoeck [3], Wielke [8], and Krausz and Eyring [18]. While the critical tests will be both difficult and time consuming to perform, the results could be valuable in comparing the various models for the understanding of slow crack propagation in brittle solids and in engineering applications where the commonly employed high safety factors [5] may then be reduced. It

has been noted, however, that empirical models (and even theoretical ones) are notoriously elusive to experimental verifications. The good curve fittings that are often obtained cannot be taken as proof, because various models may provide equally good fits as shown by Krausz et al. [26, 27] and noted by Wiederhorn [5].

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