The Probabilistic Theory of Crack Initiation

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ABSTRACT

Dislocation movement is a randomly changing event and therefore a probabilistic approach is essential for the study of crack nucleation. A model of edge dislocation pile-up is used, and two conditions are investigated: (1) the absorption of new dislocations is independent from the size of the existing pile-up, and (2) the absorption is the function of the size. In both cases the results show that the probabilistic approach should be favored over the conventional deterministic approach. The latter is shown to underestimate the critical crack nucleus size by about 20 percent, a difference that in many instances may create dangerous engineering design and operating conditions.

KEYWORDS

Crack nucleation; random motion; thermal activation; rate constant; dislocation pile-up; probabilistic approach; activation energy; forward-backward activation; Fokker-Planck relation; Markov chain.

INTRODUCTION

Conventional structural design is deterministic: a given load will be carried by a material of well-defined strength at a definite cross section. The increased demands from designers for improved service performance and also for cost efficiency requires the application of probabilistic concepts (Krausz and Krausz, 1982). The consideration of strength and stress as statistical quantities satisfies both those demands. In addition, the probabilistic approach improves the safety of service failure predictions.

This report addresses the conditions that govern crack initiation; it will be shown that the very start of fracture failure is probabilistic in consequence of the stochastic character of the physical process itself.

Crack Initiation Model

Failure by fracture occurs in two stages, each controlled by different physical mechanisms. The first stage is the initiation, nucleation, of cracks; the second is the growth of these microscopic, or submicroscopic cracks. The two stages are distinctive, but, as always in this type of physical consideration, no definite boundary can be drawn between the two and no specific size can be attached to either stage. A pronounced overlap exists between nucleation and crack growth even at the earliest stage of the nucleation. Accordingly, the probabilistic behavior of the second stage will also be discussed to some extent: the presentation thus serves as a substantial guide to probabilistic single-component damage-tolerant design.

It is now generally accepted that crack nucleation develops by the process of atomic bond breaking at sites where inherent structural weakness exists, or where a weakness develops during mechanical loadings. Depending on the composition and properties of the material, the weakened regions and the bond breaking processes may be developed by different conditions and mechanisms. From the point of view of this report, these can be well illustrated by one of the well-known models, the dislocation pile-up mechanism of crack nucleation, shown in Fig. 1(a) (Nabarro, 1967; Hirth and Lothe, 1968). Other, more-or-less closely related mechanisms, such as shown in Fig. 1(b) can be accommodated within the framework of the present study.

The model chosen to represent the crack nucleation process for the analytical development produces a microcrack when edge dislocations are pushed into a conglomeration, a pile-up, by the shear stress. By its very existence, each edge dislocation is already an elementary crack, a unit-cell of a crack, as shown in Fig. 2. The pile-up, consisting of n dislocations, is then a submicroscopic crack of about n-times the size of a single dislocation unit-cell.

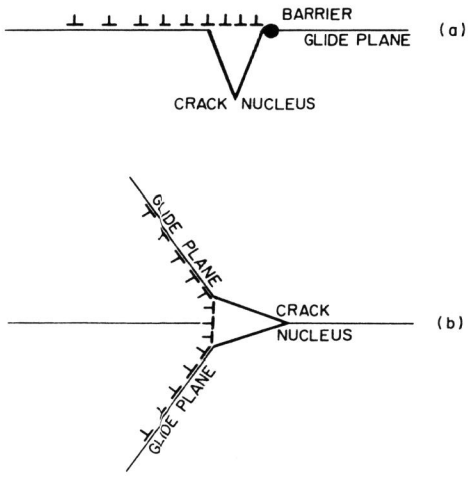

Fig. 1. (a) The Zener model of crack nucleation: the dislocation pile-up at a barrier. (b) The Cottrell model: the dislocation coalescence on intersecting glide planes provides the barrier.

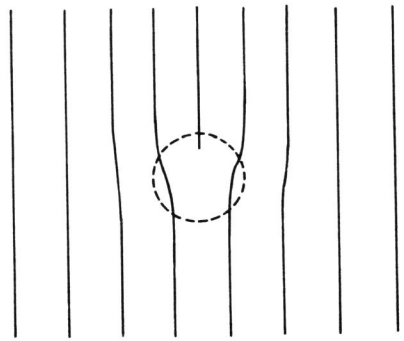

Fig. 2. The unit cell of a crack associated with a single edge dislocation. The figure shows the usual schematic representation of an edge dislocation, the dashed circle encloses the wedge-shaped region of the unit crack-cell.

A crack nucleus then develops, grows, as more and more dislocations are pushed into the pile-up. Each time a new one arrives, the nucleus grows by one unit. This unit growth may be a crack-size increase of one atomic distance, or a length not very different from that. The unit growth may even be changing as the nucleation proceeds. Within the context of this study, this aspect, the exact growth of the nucleus at the absorption of each dislocation, is of no immediate significance and will be identified only by the instantaneous size of the crack nucleus a.

The Probabilistic Aspect of Nucleation

Dislocation movement is a random process: the velocity of a dislocation changes at any instant, and the individual dislocations move at a randomly distributed velocity. Consequently, the arrival of dislocations to the pile-up is also a random process.

In any real material of engineering significance an extremely large number of potential crack nucleation sites are present. Some will grow faster than the others because the arrival of dislocations to the sites is random; in fact, there is a distribution of nuclei sizes at any instant during loading. To apply successfully the probabilistic concept of nucleation to design purposes, this distribution has to be determined. The following description provides the machinery for the analysis (Krausz and Krausz, 1984, 1985; Feller, 1970; Kanninen and Popelar, 1985).

Two conditions will be examined:

(1) the absorption of dislocations in the pile-up is independent of the pile-up size;
(2) the absorption is the function of the pile-up size.

The first condition is a convenient approximation; it is also a good illustration of the physical concepts and mathematical processing.

Condition 1: arrival rate independent of pile-up size.

Consider that the range of nuclei sizes can have discrete values only. This

is so because at the atomic level, where nucleation occurs, i number of dislocations at a site produces a nucleus of a definite a_i size. Fig. 3 illustrates that as a new dislocation arrives to the nucleus, the crack grows by Δa. There will be then a large number of nuclei of size a_{i-2}, a_{i-1}, a_i, a_{i+1}, etc., as shown in Fig. 4 for an a_i sized nucleus.

As a dislocation arrives to a nucleus of size a_{i-1}, the tip moves from X_{i-1} to X_i: it grows from a_{i-1} to a_i size. Similarly, the arrival of a dislocation at X_i moves the tip to X_{i+1}: the size grows from a_i to a_{i+1}. Consider that at time t the number of a_i sized nuclei is ρ_i. During unit time k dislocations reach each nucleus: k is the rate of arrivals. Each dislocation arrival causes a nucleus to grow one size larger. Consequently, there will be $k\rho_i$ nuclei that grow from size a_i into size a_{i+1} per unit time; also $k\rho_{i-1}$ nuclei will grow from a_{i-1} into a_i, because at the instant t there are ρ_{i-1} nuclei of size a_{i-1}. The net change, from say a_i sized nuclei (in the forward direction only), is net change = growth into a_i-growth out of a_i and the rate of change is

$$\frac{d\rho_i}{dt} = k\rho_{i-1} - k\rho_i . \qquad (1)$$

(Eq. (1) and the corresponding system of differential equations can be recognized as the birth-process Markov chain).

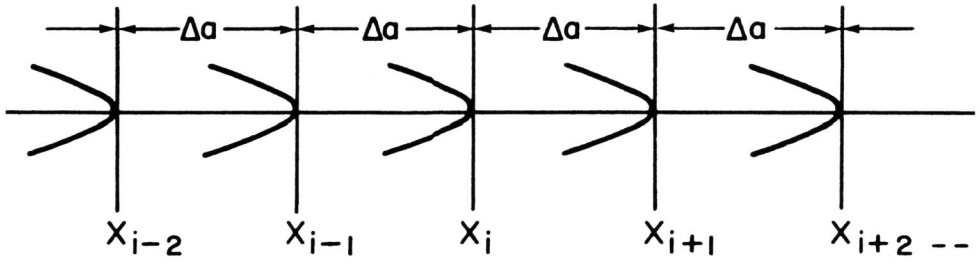

Fig. 3. The schematic representation of the growth of a nucleus. The nucleus grows by Δa as each new dislocation arrives and moves from position X_{i-2} to X_{i-1} to X_i to X_{i+1}, etc.

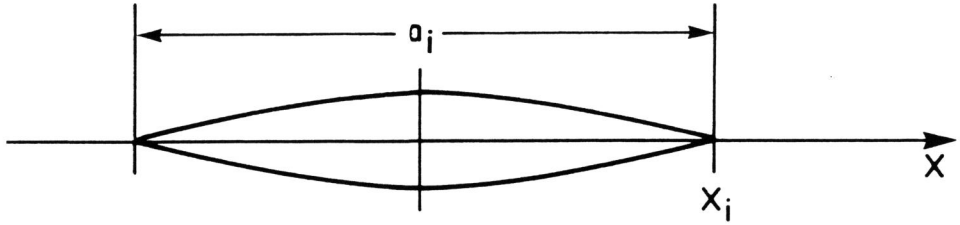

Fig. 4. The relation between crack-nucleus tip location along the X-axis and the crack size.

This equation contains two unknowns, ρ_{i-1} and ρ_i. However, for each group of nuclei of the same size one equation of the same type can be written. There is then n equations for the zero to n sizes and, of course, n nuclei groups each of the same size: the system of differential equation is then defined. This system is recognized to represent the Poisson distribution with the solution

$$\rho_i(t) = \frac{(k\,t)^i}{i} \exp(-k\,t) , \qquad (2)$$

where i goes from 1 to n. When i is very small Eq. (2) can be easily evaluated with standard Poisson tables. For larger values of i (that is, for larger nuclei), it is shown in probability theory that the Poisson distribution can be well approximated by the binomial distribution (Krausz et al., 1983; Chandrasekhar, 1943; Krausz and Krausz, 1988; Krausz, 1979):

$$\rho_i(t) = \frac{1}{|2\pi(\Delta a)^2 kt|^{\frac{1}{2}}} \exp\left|-\frac{(X-\Delta akt)^2}{2\Delta a^2 kt}\right| . \qquad (3)$$

In Eq. (3) Δakt is the expectation value μ, that is, the average crack nucleus size at time t; and $\Delta a(kt)^{\frac{1}{2}}$ is the variance of nucleus size, that is, the standard deviation σ. Fig. 5 illustrates the nucleus distribution size in fractional terms ρ_i/ρ_t, where ρ_t is the total number of nuclei.

A simple example will illustrate the considerable scatter, randomness, of the nucleus size distribution. When 25 dislocations form a nucleus, the average size given by the expectation value is $\mu = \Delta akt = 25\,\Delta a$ (because over a unit time k dislocations move to the nucleus, and over time t there are 25). The standard deviation is $\sigma = \Delta a(kt)^{\frac{1}{2}} = 5\Delta a$. The ratio of the two expresses the fractional difference from the average for one standard deviation,

$$\frac{\sigma}{\mu} = \frac{\Delta a(kt)^{\frac{1}{2}}}{\Delta akt} = \frac{1}{(kt)^{\frac{1}{2}}} = 0.2 . \qquad (4)$$

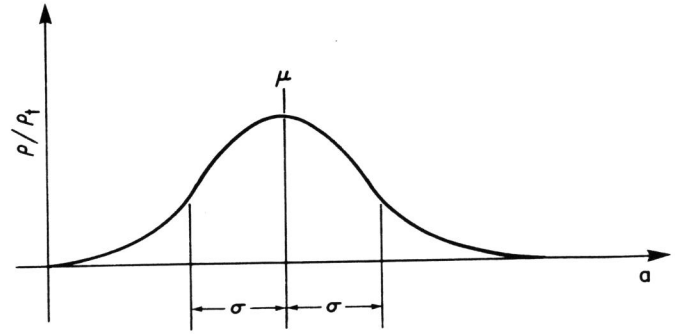

Fig. 5. The crack size distribution, described by Eq. (3). For ease of representation a continuous distribution density is considered. In the Figure, ρ_i/ρ_t = fraction of nucleus size; a = nucleus size; μ = expectation value (average nucleus size); σ = variance.

Because about 33% of the nuclei are larger than one standard deviation size, about 1/3 of the nuclei will be longer than the average by at least 20%, a very significant probabilistic deviation from the average, that is, from the deterministic nucleus size μ.

Condition 2: nucleus-size dependent arrival rate.

We may now consider the distribution of crack nuclei when the dislocations in the pile-up interact; as, of course, realistically they do so. The rate constant of the i-th dislocation moving in the direction of the front of the pile-up is

$$k_{if} = \frac{kT}{h} \exp\left|- \frac{\Delta G^{\dagger}_{if}(W_{if})}{kT}\right| , \tag{5}$$

where $\Delta G^{\dagger}_{if}(W_{if}) = \Delta G^{\dagger} - W_{if}$, and $W_{if} = W - W_{ipu}$.

In these equations $\Delta G^{\dagger}_{if}(W_{if})$ is the thermal energy needed to activate the dislocation movement into the pile-up of the i-th sized nucleus. The mechanical energy W_{if} is the function of the work contributed by the applied force, W, as expressed by the appropriate fracture mechanics form. Because the scale of the model is small compared to the grain size, a strictly applied concept of linear elastic fracture mechanics is not valid. On the scale of the nucleus the proper quantities are interatomic forces and displacements that result from the surrounding large-scale continuum which lends itself to stress-strain field description. The consideration of the mechanical energy supplied to the pile-up is further complicated by the constraint exercised on the grain by the continuous environment in which it is embedded. The force-displacement state is also affected by the anisotropy of the grain and by the local microstructure. The probabilistic approach provides the means to overcome some of these complexities. For instance, in the probabilistic analysis of large number of samples the different orientation and different defect structure of each grain with a nucleus will appear as averages. It is to be expected that these microstructural components will form a normal distribution pattern, as shown by probability theory. At the present time, the mechanical work, W, has to be related to the stress intensity factor, or other fracture mechanics quantity: similitude is of obvious importance and help. It is also to be noted that energy-based fracture mechanics quantities lend themselves best to the consideration of the thermal energy need — these are more immediately related to the scalar character of interatomic energy change which is, so to say, the final arbiter.

The second term, W_{ipu}, expresses the effect of the pile-up on moving in the forward direction by one atomic distance. It considers not only immediate-neighbor interactions, but of those farther away as well. It is, therefore, a function of the number of dislocations, n: in general, an increasing function of n. The exact functional relation, while important in quantitative analysis, is not a necessary element for the present purpose. It is sufficient to regard this as a back stress, or internal stress effect.

Dislocations do move out of the pile-up at the rate determined by the backward activation rate constant, k_{ib}, away from the front. It is defined as

$$k_{ib} = \frac{kT}{h} \exp\left|- \frac{\Delta G^{\dagger}_{ib}(W_{ib})}{kT}\right| , \tag{6}$$

where $\Delta G^{\dagger}_{ib}(W_{ib}) = \Delta G^{\dagger} + W_{ib}$, and $W_{ib} = W - W_{ipu}$;

hence, it is possible to approximate the work as $W_{ib} = W_{if} = W_i$.

The growth rate of the i-th sized nucleus (defined by the length of the pile-up) is

$$\frac{d\rho_i}{dt} = (k_f\rho)_{i-1} - \left|(k_f + k_b)\rho\right|_i + (k_b\rho)_{i+1} . \tag{7}$$

There are n of these equations; n is the largest pile-up which still constitutes a nucleus; any size larger than this is a growing crack. This system of first order differential equations constitutes a Markov-chain system. When k_f is not much different from k_b, it can be described by the Fokker-Planck equation of energy transfer, a mathematically and physically eminently satisfactory description

$$\frac{\partial \rho/\rho_t}{\partial t} = \frac{a^2}{2} \frac{\partial}{\partial X} (k_f + k_b) \frac{\partial \rho/\rho_t}{\partial X} . \tag{8}$$

This differential equation is widely studied. It corresponds to the diffusion equation when the diffusion coefficient is a function of the concentration ρ/ρ_t, where ρ_t is the total number of nuclei (Manning, 1968; Crank, 1970). In infinite and semi-infinite bodies the differential equation can be solved by the Boltzmann transformation. Substitution of $\eta = \frac{1}{2} Xt^{\frac{1}{2}}$ leads to the ordinary differential equation

$$-2\eta \frac{d\rho/\rho_t}{d\eta} = \frac{d}{d\eta}\left| \frac{a^2}{2} (k_f + k_b) \frac{d\rho/\rho_t}{d\eta} \right| \tag{9}$$

where X is the coordinate along the length of the nucleus. Solutions are available in functional forms as well as numerical methods for a wide variety of W_{pu} and boundary conditions. An alternative form

$$\frac{\partial \rho/\rho_t}{\partial t} = \frac{a^2}{2} (k_f + k_b) \frac{\partial^2 \rho/\rho_t}{\partial X^2} + \frac{a^2}{2} \frac{\partial k_f + k_b}{\partial \rho/\rho_t} \left(\frac{\partial \rho/\rho_t}{\partial X} \right)^2 \tag{10}$$

may be also a mathematically convenient expression (Jost, 1960; Bird et al., 1960). Then the Boltzmann transformation leads to

$$\frac{d^2\rho/\rho_t}{d\eta^2} + \frac{\eta}{a^2(k_f + k_b)} \frac{d\rho/\rho_t}{d\eta} + \frac{d\, \ell n(k_f + k_b)}{d\, \rho/\rho_t} \left(\frac{d\rho/\rho_t}{d\eta} \right)^2 = 0 \tag{11}$$

which has experimental advantages; for this the references should be consulted.

In previous studies, it was shown that subcritical crack growth is also probabilistic because thermally activated bond breaking is a stochastic physical process. This recognition leads to the description of crack size distribution. The probability density of crack size at time t is

$$P = \frac{1}{|2\pi a^2 (k_f + k_b)t|^{\frac{1}{2}}} \exp\left\{-\frac{|X - a(k_f - k_b)t|^2}{a^2(k_f + k_b)t}\right\}. \qquad (12)$$

This probabilistic physical process is always present: it is in the very nature of crack growth; the Weibull-type distribution, due to non-homogeneous material properties, is superimposed on this (Krausz and Krausz,1982). Similarly, there are two sources of the statistical character of the nuclei size distributions: (1) the always present physical reason, discussed here, and (2) the non-homogeneous character of commercial materials. Because both are probabilistic, strength distribution is observed as the function of the number of nuclei. The physical nucleus size distribution is superposed on the statistical flaw-size distribution (Fig. 6); both are "nearly" binomial.

The present stage of the investigation indicates that the physical probability distribution may lead to specimen-size independent strength: this behavior was indeed observed, in contradiction to the Weibull-type behavior (Kingery et al., 1976). The measured behavior is shown in Fig. 7. In these materials, when not dislocation pile-up controlled, the basic physical process is of the same description.

COMMENTS AND SUMMARY

During crack nucleation by dislocation conglomeration, the applied stress also affects the nucleus directly by straining the atomic bonds ahead of the nucleus tip, just the same way as the load always affects a crack. This causes the nucleus to grow exactly on the same physical principles as during the crack growth stage proper. At the submicroscopic stage, where nucleation takes place, the usual linear elastic fracture mechanics concepts are not valid, and the use of the stress intensity factor for crack growth analysis cannot be sustained. The use of the crack driving force, G, is somewhat better justified because it is not a quantity focussed on the crack tip. Nucleus growth, due to the mechanical work-imposed atomic bond breaking alone, may be described by the same relation as crack growth during the propagation stage,

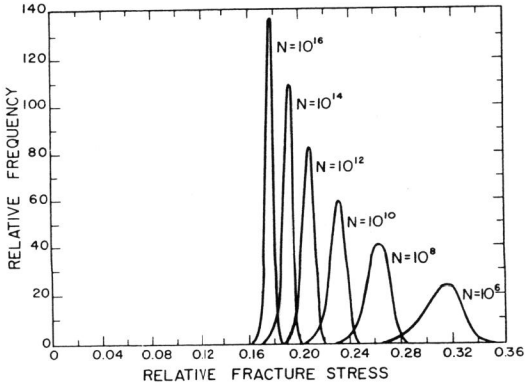

Fig. 6. Distribution of specimen strength containing N cracks, due to non-homogeneous materials structure.

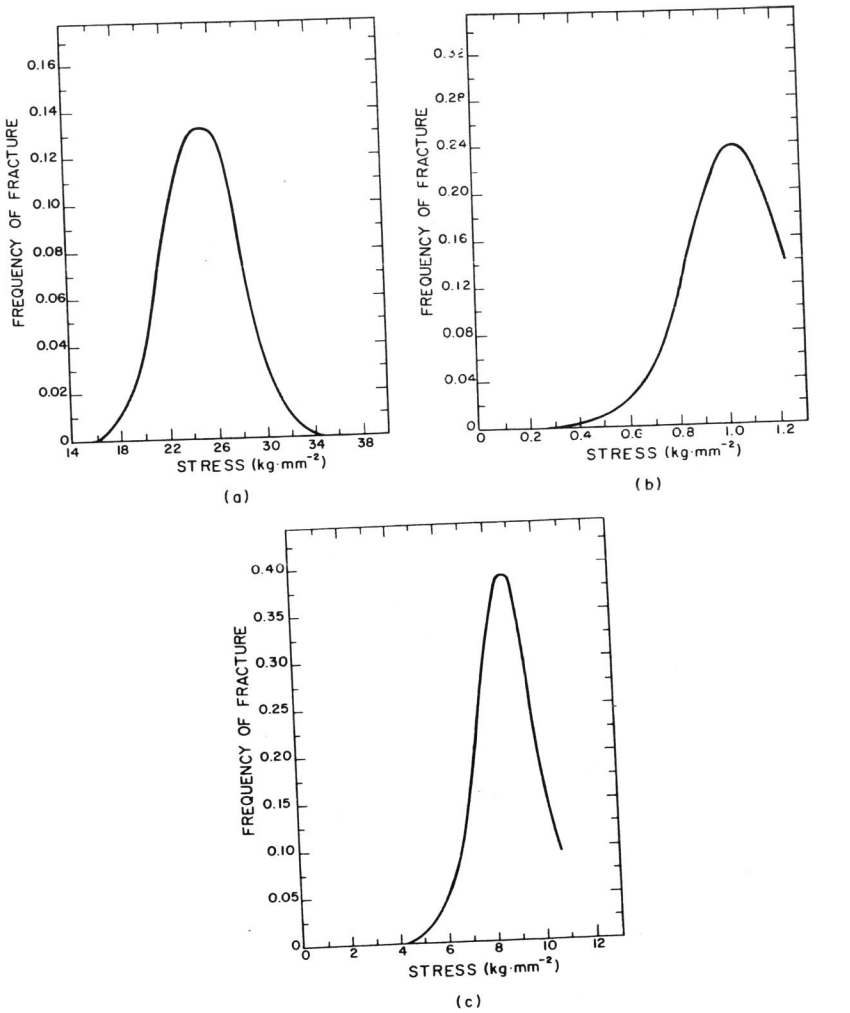

Fig. 7. Frequency of fracture, measured in (a) Portland cement (tensile; after Weibull) (b) plaster of Paris (bending; after Salmassy, Schwope and Duckworth) (c) porcelain (bending; after Weibull) (Kingery, 1976).

$$\text{growth velocity } v \propto G^m \qquad (13)$$

where m is an empirical quantity.

Eq.(13) is an empirical relation. It was shown in a series of papers that the growth process itself is probabilistic and is described by a function of the type (Krausz and Krausz, 1982, 1984, 1985)

$$v \propto \exp\left|-\frac{\Delta G^{\dagger} - W(G)}{kT}\right| \tag{14}$$

where $\Delta G^{\dagger}$ is the energy needed for atomic bond breaking; $W(G)$ is the mechanical work contributed by the crack driving force, $W \propto G$; T is the temperature in degree Kelvin; and k is the Boltzmann constant ($k = 1.38 \times 10^{-23} J\ K^{-1}$). Eq. (14) is a theoretical, rigorously derived expression, while Eq. (13), being an empirical relation, has its serious limitations. For some design purposes, however, the simplicity of the empirical expression can be of sufficient advantage to compensate for the dangers inherent in the use of non-theoretical relations in damage tolerant design. Eq. (14) is itself also a probabilistic relation.

Whichever of the two is selected, the well-known expression for the crack driving force can be used

$$G = Y^2\sigma^2 a \tag{15}$$

where Y is a geometrical and loading type dependent function, σ is the far-field normal stress, and a is the crack size.

Eqs. (3) and (13), or (14) and (15) constitute a full description of the probabilistic crack nucleation process for the fracture safety design of a single component. The crack growth stage, also in probabilistic context, was discussed in previous publications (Krausz and Krausz, 1982, 1984, 1985; Krausz et al., 1983; Krausz, 1979).

It is clear from the analysis that the important nuclei are not the deterministic ones: these are of average size only; the important nuclei, the ones that lead to cracks that may grow and eventually fracture are larger than average. Their size and distribution density can be determined by probabilistic analysis only.

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