

DEFECT POPULATION STATISTICS NEAR AND FAR FROM A CRITICAL EVENT

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ABSTRACT

We consider the defect size distributions at different stages of damage evolution, from the initial stage of defect nucleation and accumulation, through the intermediate stage of defect propagation and into the final stage leading to the appearance of the major crack. Critical events considered in this context are related to (a) the formation of microcracks exceeding the structural threshold associated with the grain size, and (b) the formation of a major crack that corresponds to the attainment of the maximum load. The significance of these two critical events is that they are often used to define the boundary between micro- and macro-mechanical analyses, and used in order to establish scale and size effects on material strength.

We consider the statistical distribution functions which are in widespread use for the description of cumulative defect size distributions, namely, the exponential, power law and the exponential-power law (also referred to as the Rosin-Rammler or Weibull) distributions. We note that the defect population statistics at different stages of evolution are best described by different statistical functions.

We discuss of the relationship between defect size distributions and the statistics of material strength. We point out that Weibull strength statistics *implies* power law defect size distribution, and note the direct correspondence between the power law defect size distribution exponent and the Weibull modulus in the statistics of strength, giving the relationship between these parameters.

We propose to use the transition between different distribution statistics as an indicator of the approach of a critical event. The effect of the structural size barrier associated with the grain size is to retard temporarily the crack growth beyond this critical size. This results in increasingly steep distribution curves, reflected in the increase of the Rosin-Rammler exponent parameter. Once crack growth proceeds beyond the structural barrier, a power law 'tail' of the crack size distribution appears. Microstructurally large defects evolve from the exponential towards power law cumulative size distributions. The appearance of the major crack is preceded by the decrease in the exponent of the power law 'tail'. Observations confirming these conclusions have been reported in materials science and seismology.

1 INTRODUCTION

Statistical analyses of defects and particles are used in various branches of science, such as materials science, seismology, fragmentation, planetology, etc (Rosin and Rammler [1], Kolmogoroff [2], Golombek and Rapp [3], Botvina and Oparina [4]). Defect population statistics and its evolution under loading provide a useful tool for the characterisation of damage accumulation and material progression towards failure. Processes of defect nucleation and growth can be considered at various scales (Korsunsky et al [5]): void nucleation and growth at the nanometre scale; microcrack nucleation and propagation at the micrometre scale; multiple cracking of quasibrittle materials, such as concrete, at the millimetre scale; and rock fracturing in the vicinity of faults in the Earth crust at the scale between centimetres and kilometres. Size distributions are also of particular value in the analysis of dynamic fragmentation and in the study of asteroids. Despite the fact that the phenomena enumerated above span twelve decades of length scales, certain aspects of size distributions observed under these extremely different circumstances possess similar features and obey certain general rules.

A simple classification of the types of cumulative defect size distributions can be introduced. Denoting by N_0 the total number of defects and by $N(c)$ the number of defects of size exceeding c , the simple exponential cumulative size distribution function can be written in the form (parameter a describes the steepness of the curve):

$$N(c) = N_0 \exp(-ac) \quad (1)$$

The power law cumulative size distribution function has the form

$$N(c) = N_0 (c / c_0)^b. \quad (2)$$

Here N_0 now denotes the total number of defects exceeding c_0 . Finally, often the cumulative defect size distribution is best described by a combination of exponential and power law functions, often referred to as the Rosin-Rammler [1], or Weibull [2] distribution:

$$N(c) = N_0 \exp[-(c / c_0)^d]. \quad (3)$$

When random sized defect populations are considered, the cumulative size distribution is most commonly described by empirical Rosin-Rammler [1] or lognormal (Kolmogoroff [2]) functions.

A key question in the mechanics of material strength concerns the relationship between the defect population statistics and the statistics of strength.

2 DEFECT SIZE DISTRIBUTIONS AND WEIBULL STATISTICS OF STRENGTH

We establish the correspondence between power law statistics of the large defect ‘tail’ of the cumulative size distribution curve, and the Weibull statistics of macroscopic strength.

The strength of a defect can then be described by a monotonically decreasing function of defect size. Griffith asserted that in brittle materials defect strength decreases proportionally to the root of defect size,

$$\mathbf{s} = K_{lc} (\mathbf{p}c)^{-1/2} \quad (4)$$

This is likely to hold qualitatively true in all materials: larger defects have lower strengths, with the relationship obeying a power law*:

$$\mathbf{s} = A / c^{1/k}, \text{ or } c\mathbf{s}^k = A. \quad (5)$$

Given the cumulative defect size distribution is given by $N(c)$, the number of defects of size $(c, c+dc)$ is given by $-(dN / dc)dc$. The same selection of defects possesses the strength $(\mathbf{s}, \mathbf{s}+d\mathbf{s})$ and can be written as $-(d\bar{N} / d\mathbf{s})d\mathbf{s}$. Therefore

$$d\bar{N} / d\mathbf{s} = (dN / dc)(dc / d\mathbf{s}). \quad (6)$$

Weibull postulated that the form of the low strength (large size) defect strength distribution is power law (also sometimes referred to as algebraic), given by

$$\bar{N}(\mathbf{s}) = N_0 (\mathbf{s} / \mathbf{s}_0)^{-m}. \quad (7)$$

This implies that the large size tail of the defect size distribution is also algebraic, and of the form

$$N(c) = N_0 (c / c_0)^{-b}. \quad (8)$$

Using equations (5), (6) and (7) together allow the relationship to be established between the Weibull modulus, m , to the power law exponent of the tail of the defect size distribution, b , and the strength scaling exponent, k . In order for the Weibull scaling of strength to be observed, the

underlying defect size distribution must obey a power law. This stands in contradiction to the observation that defects of randomly distributed sizes most closely obey an exponential type distribution. This is likely to signify that during defect growth and interaction the size distribution evolves from exponential towards power law type. In order to validate this conclusion we develop and apply a simple defect population evolution model.

2 FACTORS INFLUENCING DEFECT POPULATION KINETICS

Evolution of defect population is controlled by the following factors: material structure and properties, loading conditions, and specimen geometry. These factors in turn determine the pre-existing distribution of defect nuclei and the nucleation rate, and the defect growth rate, which is affected by the presence of structural barriers, the nature of defect interaction and coalescence (Botvina and Korsunsky [7]).

The most commonly discussed example of a structural barrier to defect growth is the grain size of the material. It is well known that microstructurally short cracks exhibit ‘anomalous’ behaviour compared with long cracks. Namely, the growth rate of short cracks exhibits a minimum when the crack size approaches the size of the grain, giving rise to the fatigue crack growth threshold on the Paris’ kinetic diagram. A model aimed at describing the transition between the stages of short and long crack growth must account for this effect.

The growth rate of long cracks may exhibit different dependence on the crack size, usually described by a power law. The exponent of this dependence under monotonic and cyclic loading conditions provides an indication of the brittleness (high exponent) versus ductility (low exponent) of the material response. Defect growth rate may also become strongly affected by defect interaction when the defect density becomes sufficiently large. The extreme manifestation of this interaction is the process of defect coalescence, which leads to the appearance of larger defects at the expense of smaller ones.

3 MODELLING THE EVOLUTION OF DEFECT POPULATION

In order to analyse the influence of the various factors discussed above we develop a simple model of defect growth from a fixed number of pre-existing nuclei, and their subsequent interaction. No account is taken of the process of defect nucleation during growth, nor do we consider defect coalescence. In developing the model we deliberately do not attempt to capture the fine details of defect growth and interaction, but rather aim to reveal the general nature of the dependence of the properties of the population evolution, such as the cumulative defect size distribution and the defect size spectrum, on the underlying mechanisms common to a wide variety of processes.

The model assumes the number of defects to remain equal to the number of pre-existing flaws. The sizes of defect nuclei are chosen at randomly in the interval (0,1) and their location is prescribed at random within the two-dimensional unit box. The distance between defects is assumed to be given by the distance between their centres.

At each step of the growth simulation the defect size is incremented by:

$$\Delta l_i = C s_0 l_i^b (1 + a p), \quad (10)$$

where l_i is the size of i -th defect, b is the exponent of the defect growth power law, p is the term reflecting the presence of defect interaction, and a is the scaling factor describing its intensity (no interaction when $a=0$). We assume that each defect interacts only with three of its nearest neighbours. For a given defect the presence of its neighbours is assumed to produce an increase in stress proportional to the remotely applied stress s_0 with the coefficient

$$p = \sum_{n=1,2,3} \sqrt{l_n / r_n}, \quad (11)$$

where r_n denotes the distance to one of the three nearest neighbours ($n=1,2,3$). This simple relationship is chosen on the basis of the linear elastic fracture mechanics expression for the stress field in the vicinity of a tensile crack. We use an array of 500 nuclei in the simulation, which was found to be sufficient to reveal the statistical information about the defect population.

4 DEFECT POPULATION MODELLING AND STAGES OF DAMAGE ACCUMULATION

The initial cumulative crack size distribution is best approximated by exponential-type functions (Rosin-Rammler or simple exponential).

Let us consider the effect of growth law on the population statistics by varying the defect growth exponent \mathbf{b} in equation (11) within the range $0.5 < \mathbf{b} < 1.5$. Notionally low values of \mathbf{b} (e.g. $\mathbf{b}=0.5$) may correspond to slow defect growth, as perhaps in a ductile metal; intermediate value of \mathbf{b} ($\mathbf{b}=1$) may be thought to correspond to semi-brittle material response, while the higher values of \mathbf{b} ($\mathbf{b}=1.5$) are likely to be associated with the brittle state of material.

The case of $\mathbf{b}=0.5$ (notionally ductile type of material behaviour) in the absence of defect interaction ($\mathbf{a}=0$) leads to an exponential-type defect distribution, similar to the first curve in Fig.1a. However, during subsequent growth (not shown in the Figure) the distribution curve becomes progressively steeper, as smaller defects grow relatively faster than larger ones. This has a levelling effect on the defect sizes, and appears to reinforce uniformly distributed damage and to avoid localisation. Introducing even fairly weak defect interaction ($\mathbf{a}=0.1$) leads to the evolution of the distribution away from the exponential-type and towards a distribution with a power law 'tail' (Fig.1a). Fig.1b shows the defect size spectra corresponding respectively to the first and last curve in Fig.1a. It illustrates the phenomenon of multiple fracture taking place, with many defects growing at similar rates. However, it is possible to identify faster growing defects which are likely to correspond either to larger sized nuclei or to locations favouring strong interaction. In the long run these defects outgrow the rest and form the major crack.

The case of $\mathbf{b}=1$ (notionally semi-brittle type of material behaviour) without defect interaction ($\mathbf{a}=0$) a stable exponential-type defect distribution (first curve in Fig. 1c) is permanently maintained, i.e. the defect distribution displays perfect self-similarity during growth. In the presence of defect interaction ($\mathbf{a}=0.05$) the 'tail' of the distribution becomes less steep, and the entire distribution evolves towards the power law distribution (Fig.1c). The final spectrum of defect sizes is characterised by the presence of one or two large defects (Fig.1d).

In the case of $\mathbf{b}=1.5$ (brittle type of material behaviour) even in the absence of defect interaction ($\mathbf{a}=0$) the distribution evolves towards the power law type (Fig.1e). The slope of this distribution for large defect sizes decreases, while that for small defect sizes increases. The spectrum of defect sizes (Fig.1f) shows a fairly uniform size distribution across the scale of defect sizes. Switching on interaction in this case rapidly leads to the appearance of a major crack.

The general trend observed in all cases of defect population evolution is from exponential type distribution towards power law scaling of cumulative defect number with defect size. The exponent of the power law 'tail' corresponding to large size defects progressively decreases as defect growth proceeds.

The analysis of cumulative defect size distribution curves allows the identification of two distinct regimes of damage accumulation. The first regime of distributed multiple damage is characterised by self-similarity of defect size spectrum and the stability of the exponential type cumulative distribution during defect growth.

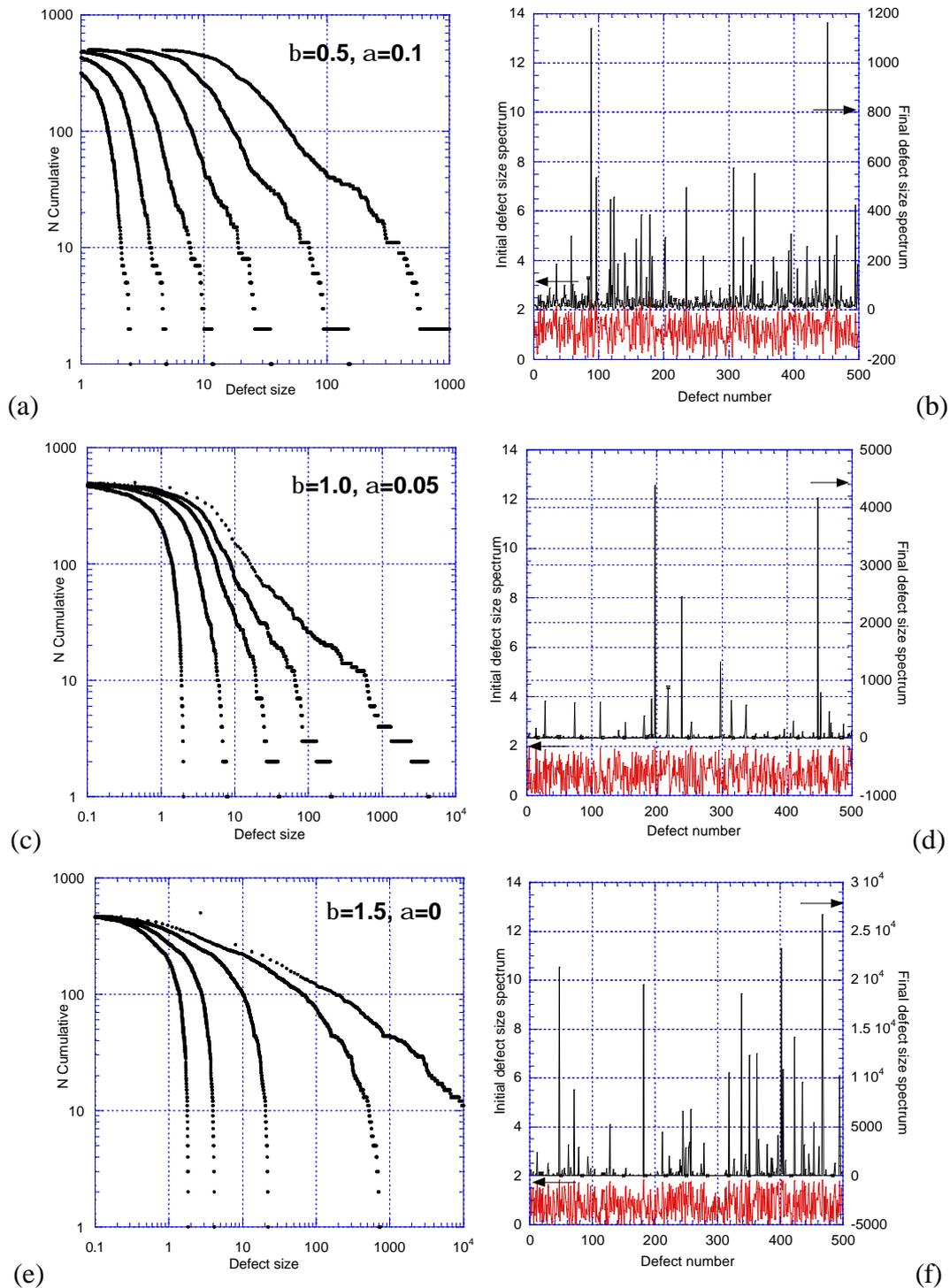


Figure 1: Cumulative defect size distributions and size spectra during defect growth (see text).

The second regime of localised damage accumulation corresponds to the appearance of power law segments on the cumulative size distribution curve, particularly in the region of the largest sized defects. This power law 'tail' of the defect size distribution is responsible for the frequently observed Weibull scaling of strength. Defect size spectra emerging after defect growth reveal the appearance of a few dominant defects that outgrow the rest. This phenomenon is connected with the transition from distributed to localised damage and fracture, and with the scale transition from micromechanical multiple short crack regime to the macromechanical regime of single major crack growth.

During the transition from the first regime (distributed damage) to the second regime (localised damage) the self-similarity of defect size distribution curves and defect size spectrum is broken. As defect growth progresses the new defect distribution follows power law and also maintains self-similarity during subsequent damage accumulation. While in the first self-similar regime the distribution is exponential, in the second self-similar regime the distribution is power law. The approach of the critical event associated with the formation of a single dominant defect is characterised by the reduction in the power law exponent b .

5 DISCUSSION

We have discussed the relationship between strength scaling and defect size distributions, and considered the evolution of the latter during defect growth. We demonstrated using defect growth and interaction modelling that the approach to a critical event is characterised by the following phenomena:

1. The self-similarity of the initial exponential defect size distribution is broken, and is replaced with power law distribution, particularly in the region of large defect sizes.
2. The fast growth of larger defects leads to the reduction in the slope (power law exponent) of the defect size distribution. This change in the distribution parameter (b) can serve as an indicator of the onset of damage localisation.
3. The onset of localised damage is also reflected in the appearance of dominant defects in the defect size spectrum.

The above observations suggest that these aspects of defect population evolution can be used as criteria for the identification of the transition from micromechanical to macromechanical damage regime, i.e. from microcracking to large crack propagation phenomena.

REFERENCES

- [1] Rosin, P. and E. Rammler, The laws governing the fineness of powdered coal, *J. Inst. Fuel*, **7**, 29-36, 1933.
- [2] Kolmogoroff, A.N., About the logarithmic-normal law of distribution of particle dimensions generated by disintegration. *Proc. Acad. Sci. USSR* **31**, 99-101, 1941.
- [3] Golombek, M., D. Rapp, Size-frequency distributions of rocks on Mars and Earth analog sites: Implications for future landed missions. *J. Geophys. Res.*, **102**, 4117-4129, 1997.
- [4] Botvina L.R. and I.B. Oparina, Kinetics of different scale multiple fracture. *Doklady Physics* **43**, 644-647, 1998.
- [5] Korsunsky A.M, K. Kim, L.R. Botvina, An analysis of defect size evolution. *Intl. J. Fracture* **125-130**, 2004.
- [6] Weibull W., The phenomenon of rupture in solids. *Proc. Royal Swedish Inst. of Engng. Research (Ingeniers Vetenskaps Akademien Handlingar)* **153**, 1-55, 1939.
- [7] Botvina L.R. and A.M. Korsunsky, On the structure of plastic and damage zones in different materials and at various scales. *Proc. XIth Intl. Conf. on Fracture*, Turin, 2005.