Reliability Assessment from Fatigue Micro-Crack Data

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Key Words — **Bayes inference, Coalescence, Fatigue, Gibb's sampling, Hierarchical model, Kernel density estimate, Micro-crack, Propagation**

Summary & Conclusions — **Micro-cracks are generally defined to be cracks less than 1 mm in length, which propagate under cyclic stresses until they grow large and cause failure in an item (*eg*, component or structure). This paper proposes a method of using data on 'fatigue micro-crack growth in a material' to predict its reliability. It is increasingly important to model such cracks effectively. Their growth properties, which differ in several respects from larger cracks, are discussed.**

The paper develops a hierarchical model for the propagation of micro-cracks in a material. This stochastic model attempts to model the dependence of growth on local conditions, varying throughout the material, that causes variation in growth rates across the specimen. Given the model, data on micro-crack growth are used to compute posterior distributions of model parameters, from which a predictive distribution for reliability can be calculated. Computation of the posterior distributions is by Gibb's sampling and kernel density estimation. The methodology is illustrated with two data sets, one simulated and the other from a cast-iron specimen. Some possibilities for further work are presented.

1. INTRODUCTION & OVERVIEW

Acronym[1]

MCMC Monte Carlo Markov chain.

When a metal item (*eg*, structure or component) is subject to a cyclic load, it generally fails eventually[2]. Thus it is important — from a safety, legal, financial, and academic perspective — to predict when this fatigue failure is likely to occur. Fatigue failure of a metallic item occurs because cracks propagate through it, and this propagation is a function of several internal & external factors: *eg*, size of load, microstructural properties of the material, temperature, humidity.

Broadly speaking, crack propagation has 5 phases.

1. Dormant. There are no cracks in the material.
2. Nucleation. The crack is initially formed.
3. Micro-crack growth. The crack grows rather haphazardly up to about 1 mm in length.
4. Macro-crack growth. The crack continues to propagate before its growth rate finally increases dramatically.
5. Failure. The component fails; this occurs very quickly, relative to the other phases, and can be ignored as a factor in determining reliability. ◄

Out of the many cracks that nucleate and become micro-cracks in a specimen, usually there is only one that becomes dominant and causes failure. The fact that only one macro-crack is important makes the modeling of phase #4 rather easier than the others. There are many situations in which the macro-crack phase #4 is the longest phase in the specimen life. Thus, most of the considerable body of work on crack propagation is devoted to macro-cracks.

Nevertheless, the micro-crack phase can form a very sizeable proportion of the failure time — 60% is typical for some materials — particularly in situations of relatively low stress levels where lifetimes are long. Figure 1 [1] shows this for two specimens of a molybdenum steel. Such situations are very common where, for example, components have been designed to withstand stresses considerably above those that they actually encounter. Because the reliability of many components is improving, micro-crack behavior is becoming a critical factor in determining reliability. So in terms of quantifying component lifetime and as a factor to be considered in the design process, models for the micro-crack phase are increasingly important.

Once a crack has attained a certain threshold size, failure occurs very rapidly. So, to determine component reliability, a model for crack propagation is proposed and used to calculate when the length of the largest crack exceeds the threshold.

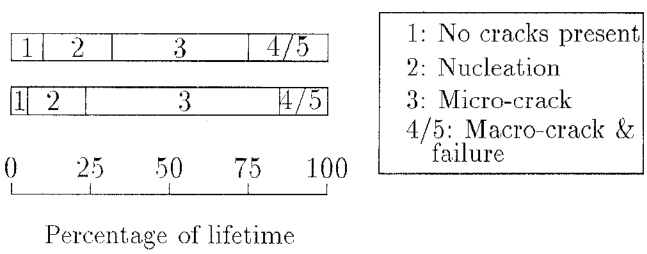

Figure 1. Time Spent in Phases of Crack Growth
[for two specimens of molybdenum alloy]

Three properties of micro-cracks make macro-crack models inappropriate:

1. The usual models for macro-cracks cannot accommodate the various features of micro-crack growth. Section 2 proposes a modification of the usual macro-crack model that accounts for these differences.
2. There are many micro-cracks in the specimen that must be modeled collectively, as opposed to one dominant macro-crack.

[1]The singular & plural of an acronym are always spelled the same.
[2]Some ferrous materials appear to have a fatigue limit, below which the item does not fail.

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3. Micro-crack growth is a function of varying local conditions in the material. ◄

Section 3 argues that a stochastic hierarchical model is a good first step in modeling the randomness & *s*-dependencies between the collection of micro-cracks. Section 4 describes how statistical inference and reliability prediction can be conducted using MCMC, and provides two illustrations using data on micro-crack growth.

Notation

a, $a(t)$ crack length at time t
ΔK stress intensity range
C, n, Q material specific constants
$\Delta\sigma$ stress range
a_0 initial crack length
d diameter of a grain in the material microstructure
D distance from the point of crack nucleation to where the crack encounters the first grain boundary
N number of micro-cracks in a specimen
$f(a,d;\ \theta)$ empirical function of a, d, and parameter θ
m, ϕ grain boundary specific constants, $0 \le \phi \le 1$
i index for cracks; $i=1,2,\ldots,N$ unless otherwise specified
j index for times; $j=1,2,\ldots,k$ unless otherwise specified
m_i, ϕ_i $[m, \phi]$ for crack i
$\text{logit}(\phi_i)$ $\log(\phi_i) - \log(1-\phi_i)$
$a_{i,j}$ observed crack length for crack i at time j
$A_i(t)$ length of crack i at time t, a r.v.
$\mathbf{A}$ $\{a_{i,j}:\ i=1,\ldots,N;\ j=1,\ldots k\}$.

Other, standard notation is given in "Information for Readers & Authors" at the rear of each issue.

2. MICRO-CRACK PROPAGATION: WORK TO DATE

2.1 Previous Work

The usual model for large macro-crack growth is the Paris-Erdogan equation [2: chapter 1] which defines:

$$\frac{da(t)}{dt} = C\cdot(\Delta K)^n, \qquad (1)$$

$$a(0) = a_0, \qquad (2)$$

where, usually,

$$\Delta K = Q\cdot\Delta\sigma\cdot\sqrt{\pi\cdot a}.$$

To solve (1) uniquely, a_0 is needed. This model has been used successfully to describe the observed propagation of a dominant macro-crack in many experiments and the values of C & n have been established for a wide range of materials.

The growth of a macro-crack is as smooth as the use of such a differential equation model implies. This is in stark contrast to what we observe for micro-cracks, whose progression can be smooth but can involve periods of stationarity and the possibility of being stopped altogether. This can be observed by plotting crack-growth *vs* crack-length for a set of cracks in a metal; figure 2 [3] is a typical plot. This widely observed phenomenon is caused by the crack encountering a boundary between grains in the material microstructure; at such a boundary, growth rate is slowed by a factor that depends on local conditions. In this way, some micro-cracks propagate to become macro-cracks with hardly any delay while others are held back for some time or even stopped altogether. The difference in the length at which cracks slow down is due to the different distance that the cracks progress before hitting a grain boundary.

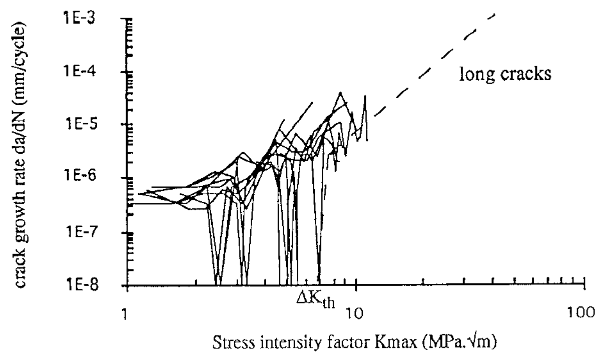

Figure 2. Typical Growth Behavior of Micro-Cracks

The general approach to modeling the effect of a grain boundary is to take the Paris-Erdogan equation and multiply the r.h.s by a factor that accounts for the local conditions at the first grain boundary:

$$\frac{da}{dt} = C\cdot(\Delta K)^n\cdot f(a,d;\ \theta), \qquad (3)$$

The $f(a,d;\ \theta)$ is usually increasing in the distance from the first grain boundary. A variety of forms for f have been proposed that empirically capture this property; *eg*, Miller *et al* simply propose [4]:

$$f = a-d, \text{ for } a < d,$$

while Plumtree & Schäfer suggest [5]:

$$f = 1 - \phi\cdot((d-a)/d)^2, \text{ for a constant } \phi.$$

However, there is no consensus on the best form for f: it appears to vary for different materials.

2.2 Micro-Crack Model with an Exponential Local Term

One model of the form in (3) is:

$$\frac{da(t)}{dt} = C\cdot(\Delta K)^n\cdot[1 - \phi\cdot\exp(-m\cdot(a-D)^2)], \qquad (4)$$

$$a(0) = a_0, \qquad (5)$$

D is a function of d.

Eq (4) & (5) for da/dt is the Paris-Erdogan rule multiplied by the local factor:

$$1 - \phi \cdot \exp(-m \cdot (a-D)^2).$$

The size of the slowdown in growth at the grain boundary is governed by ϕ:

- If $\phi=0$ then there is no local effect and the crack moves according to Paris-Erdogan.
- If $\phi=1$ then when $a=D$ (when the crack hits the first grain boundary), $da(t)/dt=0$ and the crack is stopped.

The m is a scaling factor that controls how far away from the boundary the local effect is important:

- If m is small, then the crack slows down a long distance from the boundary.
- If m is large, then the crack slows down a short distance from the boundary.

The use of an exponential measure of distance for $f(a, d; \theta)$ is new. The advantage of such a measure is that it is increasing but bounded in the distance from D. Thus, as a progresses beyond D, the $\exp(-m \cdot (a-D)^2)$ becomes smaller and $da(t)/dt$ becomes closer & closer to the usual Paris-Erdogan equation for macro-cracks. However it remains empirical and, like all proposed forms for f, has not been derived by considering more fundamental processes of crack growth.

A solution for a(t) is not available in closed form but can be efficiently obtained with a second order finite difference approximation. The solution is shown in figure 3 for:

- 5 values of ϕ = 0.6 (the fastest growing), 0.7, 0.8, 0.9, 1 (the slowest growing)
- $C = 0.2$, $\Delta\sigma = 10$, $n = 1$, $m = 0.02$, $Q = 1$, $D = 80$.

The crack growth does indeed slow around the value of D, with the extent of the slowdown, depending on the size of ϕ.

3. EXTENDING TO A RANDOM MODEL FOR MANY MICRO-CRACKS

There has been some work on random models for micro-crack propagation, although the work is small compared with that for macro-cracks. Cox & Morris define a model through a growth-control parameter that evolves as a Markov chain [6]. Taylor has introduced the concept of a *P-a* plot to describe the probability of growth of a crack in a given number cycles as a function of crack length [7]. Our approach treats the parameters of the deterministic model as r.v. This concept has been used for macro-crack models, such as the work of Paluszny & Nicholls on a model for crack growth in ceramics [8]. To our knowledge, the idea has not been applied to micro-crack models.

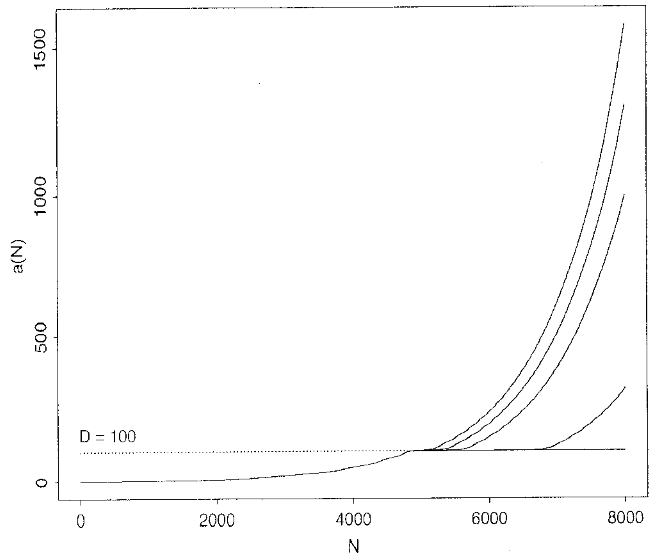

Figure 3. Solution for $a(t)$ vs ϕ

3.1 General

We have established a deterministic model for a single micro-crack in terms of parameters: $C, n, m, \phi, \ldots$. Stage #2 of the modeling process is to extend the model to many cracks, growing broadly in the same manner but with variations according to local conditions. A simple tractable form for such a collection of similar entities is a hierarchical model, which describes the cracks as a set of random, exchangeable objects, conditionally *s*-independent of each other, given local conditions around each crack.

Assumptions

1. N is a constant for a given specimen.
2. n, C, $\Delta\sigma$, are known.
3. The local conditions at each crack are described by the local parameters m_i, D_i, ϕ_i.
4. Conditional on the local parameters,

a. each crack is *s*-independent.

b. the deterministic model of (5) gives a solution for $a_i(t)$.

5. $A_i(t)$ has a Gaussian distribution with mean $a_i(t)$ and standard deviation $\sigma \cdot a_i(t)$.
6. The use of multiplicative error for $A_i(t)$ is necessary because crack lengths vary over several orders of magnitude with time.

7a. The local parameters are r.v. that come from some underlying common probability distribution.

7b. The $\log(m_i)$ are *s*-independent and have a Gaussian distribution with mean M and standard deviation σ_m.

7c. The logit(ϕ_i) have a Gaussian distribution with mean Φ and standard deviation σ_ϕ.

8. Statistical inference is Bayes[3]. Thus prior degrees-of-belief on M, σ_m^2, Φ, σ_ϕ^2, d, σ^2 are required. ◄

[3]Bayes theory uses probability as degree-of-belief, and has no relation to probability as relative frequency.

The distribution of the D_i can be obtained from geometrical considerations and is a function of grain diameter d. The evaluation of this distribution is addressed in section 3.2. This hierarchical model is often visualized as a directed graph which represents all the quantities of interest in the model and their influences on each other. Each node represents one part of the model and is s-independent of all other nodes in the graph, conditional on its parents (the nodes that point directly to it).

- A solid line between nodes indicates a random relationship between nodes (the parent is a parameter in the distribution of the child).
- A dotted line indicates a logical or deterministic relationship between the two connected nodes.
- A box around nodes indicates a set of variables that are conditionally s-independent given their parents. ◄

Figure 4 is the directed graph that represents this model.

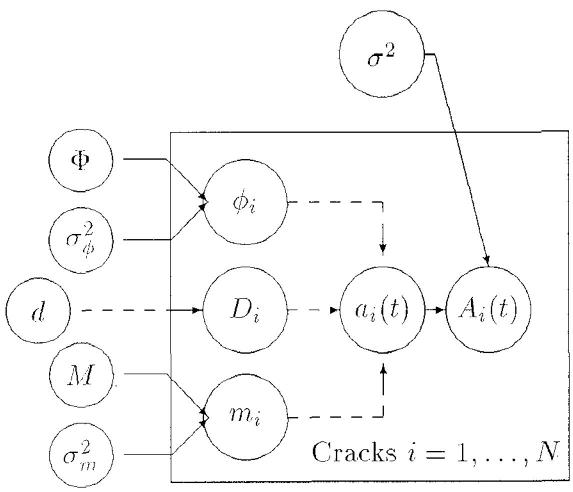

Figure 4. Directed-Graph Representation of the Hierarchical Model

The strengths of the hierarchical model are not only in its tractability. The cracks are unconditionally s-dependent, but the similarity between each crack is maintained since the marginal distribution of $A_i(t)$ is the same for all i (a result of assumptions #4a, #5, #7a).

3.2 Prior Distribution for D

A very simple example shows how we find our prior degree-of-belief.

Example

There are 2 dimensions, and the grains are circular with a diameter d. A crack nucleates at a point in the circle at a position (R, θ) in polar co-ordinates. It then proceeds at an angle ψ (clockwise from the positive x-axis) until it hits the boundary of the circle. The length of the line from nucleation point to circle perimeter is D. Thus (by the cosine rule):

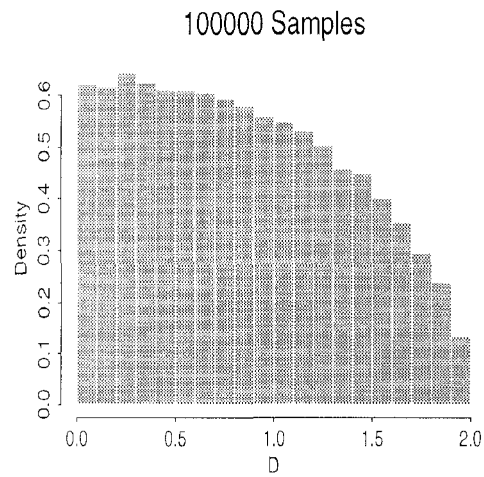

Figure 5. Simulated Density of D [d=1, circular grains]

$$D = -R\cdot\cos(\theta - \psi) + [\tfrac{1}{4}d^2 - R^2\cdot\sin^2(\theta-\psi)]^{1/2}, \qquad (6)$$

In the absence of more specific information for this example, assume that R, θ, ψ are uniformly distributed r.v. over their possible values, then one can generate values from the distribution of D by direct simulation. Figure 5 is a histogram of the resulting values of D when d is fixed at 1. ◄

More generally, d itself varies; indeed, the distribution of grain diameters is easily observed and has been quantified for many materials. This generalization presents no problem to the direct simulation of the distribution of D.

Other, perhaps more realistic, geometries for the grains could be used, *eg*, Voronoi tessellations. Direct simulation of a distribution for D is available, although more complex. The problem can be considered in all 3 dimensions, and used with spheres or 3-dimensional Voronoi tessellations. However, since crack growth often occurs in one direction, perpendicular to the stress axis, a 2-dimensional geometry is usually sufficient. We are interested only in a prior distribution for D that is updated, given our data on crack growth, the use of the simpler prior from an assumption of circular grains might be all that is needed.

4. STATISTICAL INFERENCE AND RELIABILITY ASSESSMENT

Assumptions

9. We have data on N cracks. The length of each crack is observed at times $t_1, t_2, \ldots, t_k$.

10. To simplify, $a_{i,1} = a_0$ of the crack, as required to solve (5).[4] ◄

[4]One could of course allow a_0 to be a r.v. and incorporate it into the inference.

Given the data, the statistical analysis has 3 objectives:

- Estimate model parameters. Because we adopted Bayes inference, the goal is to obtain posterior distributions of the parameters, conditional on $\boldsymbol{A}$.
- Predict the progression of cracks in other specimens of the same material.
- Predict the future propagation of the observed cracks. This is important because it can be used to predict the reliability, or time to failure, of the specimen. ◄

To conduct *s*-inference with this model, obtaining posterior distributions of parameters and predictive distributions, is a computational challenge. Recent advances in stochastic simulation techniques — in particular, MCMC — meet the challenge; *s*-inference is quite feasible using a machine of moderate computational power, *eg*, the results in section 4.3 took a few hours on a Pentium PC.

4.1 Parameter Estimation

The model has many parameters:

- Each crack has 3 parameters — m_i, D_i, ϕ_i.
- The global distributions of m_i, D_i, ϕ_i are described by parameters M, σ_m^2, d, Φ, σ_ϕ^2.
- The multiplicative error σ^2. ◄

Thus, for N cracks, there are $3N + 6$ parameters.

The parameters are partitioned in 2 groups: local and global. On the local level, crack i is described by its 3 local parameters; estimation of m_i, D_i, ϕ_i, σ^2 yields specific information about the performance of each crack. On the global level, the distribution of the population of local parameters in the specimen is estimated, *ie*, M, σ_m^2, d, Φ, σ_ϕ^2.

MCMC for simple hierarchical models is usually performed with the Gibb's sampler, and we use it here [9: and its references]. The sampler does not require one to be able to sample from the posterior distribution of each parameter, but rather the *full conditionals* for each parameter, or the distribution conditional on the data and all other parameters. The full conditional for any parameter can be obtained by looking at the joint distribution of data and parameters as a function of the parameter in question; in this paper, combining all the distributional and *s*-independence assumptions in section 3 (*viz*, assumptions #1, #2, #4, #5, #7b, #7c, #8 - #10), this joint distribution is:

$$f(a_{i,j}, m_i, D_i, \phi_i; \quad i=1,\ldots,N,\ j=1,\ldots,k;\ \sigma^2, M, \sigma_m^2, d, \Phi, \sigma_\phi^2)$$

$$= \left[\prod_{i=1}^{N} \zeta_{i,k} \cdot f_m(m_i|M, \sigma_m^2) \cdot f_\phi(\phi_i|\Phi, \sigma_\phi^2) \cdot f_D(D_i|d)\right] \cdot \pi(\sigma^2)\cdot\pi(M)\cdot\pi(\sigma_m^2)\cdot\pi(\Phi)\cdot\pi(\sigma_\phi^2)\cdot\pi(d), \tag{7}$$

$$\zeta_{i,k} \equiv \prod_{j=2}^{k} \frac{1}{\sqrt{2\pi}\cdot\sigma\cdot a_i(t_j)} \cdot \exp\left(-\frac{(a_{i,j} - a_i(t_j))^2}{2\sigma^2\cdot a_i(t_j)^2}\right).$$

$a_i(t_j)$ = solution to the model (5) with m_i, D_i, ϕ_i, and $a_0 = a_{i,1}$,

a form for $f(D_i|\mathrm{d})$ is explained in section 3.1

$\pi()$ denotes the prior distributions on hyper-parameters.

A sample from each full conditional distribution is calculated differently. For the full conditionals of m_i, D_i, ϕ_i, calculation of the pdf requires that $a_i(t_j)$, for $i=1,\ldots,k$, be computed; this is a slow process. Thus, for these parameters, the *griddy* Gibb's sampler is used [10], evaluating the full conditional at 5 points. For the hyper-parameters, the pdf's are of a form that is easy to evaluate, and a sampling is done from a discrete approximation to the continuous distribution.

The output from the sampler is a set of values of each parameter that are random samples from the relevant posterior distribution. These values can be used to estimate the posterior distribution, either by combining them into a histogram or by using one of the kernel density estimation techniques [9, 11]. Predictive pdf's for future values of crack length can be obtained in a similar manner.

4.2 Predicting Reliability

Notation

A_{th}	a given threshold size
T	life-length of specimen
$^{(j)}$	implies: sample j, $j=1,2,\ldots,L$
L	number of samples produced by Gibb's sampler from posterior distributions of the local parameters.

Assumption

11. Specimen reliability is estimated by predicting the time at which the first crack reaches A_{th}, conditional on $\boldsymbol{A}$.

$$\Pr\{T > t|\boldsymbol{A}\} = \Pr\{\max_i\{\boldsymbol{A_i(t)}\} \le A_{\mathrm{th}}|\boldsymbol{A}\}$$

$$= \Pr\{A_1(t) \le A_{\mathrm{th}}, \ldots, A_N(t) \le A_{\mathrm{th}}|\boldsymbol{A}\}. \tag{8}$$

The conditional *s*-independence of the A_i are used to estimate the joint posterior distribution of all the crack lengths at any time t with the kernel estimate:

$$\Pr\{A_1(t) \le A_1, \ldots, A_N(t) \le A_N|\boldsymbol{A}\}$$

$$= \iiint \left[\prod_{i=1}^{N} \Pr\{A_i(t) \le A_i|m_i, D_i, \phi_i, \sigma^2\}\right] \cdot \pi(m, D, \phi|\boldsymbol{A})\ dm\ dD\ d\phi$$

$$= \mathrm{E}\left\{\prod_{i=1}^{N} Pr\{A_i(t) \le A_i|m_i, D_i, \phi_i, \sigma^2\}\right\}$$

$$\approx \frac{1}{L}\cdot\sum_{j=1}^{L}\prod_{i=1}^{N} \mathrm{gauf}\left(\frac{A_i - a_i(t)^{(j)}}{a_i(t)^{(j)}\cdot\sigma^{(j)}}\right), \tag{9}$$

$a_i(t)^{(j)}$ is the solution to (5) with parameters $m_i^{(j)}$, $D_i^{(j)}$, $\phi_i^{(j)}$.

Use this approximation in (8); the reliability is:

$$\Pr\{T > t|A\} \approx \frac{1}{L} \cdot \sum_{j=1}^{L} \prod_{i=1}^{N} \text{gauf}\left(\frac{A_{\text{th}} - a_i(t)^{(j)}}{a_i(t)^{(j)} \cdot \sigma^{(j)}} \right). \quad (10)$$

4.3 Application to Data

Two sets of data are analyzed. In both cases, vague prior distributions were placed on the hyper-parameters:

- a Gaussian distribution with mean 0 and standard deviation 1000 on M and Φ,
- inverse Gamma distributions with 'scale parameter = 0.5' and 'shape parameter = 0.5' for σ^2, σ_m^2 and σ_Φ^2. For the prior distribution of D, we assumed little prior information available on the grain diameters d, except that an upper bound to d was 500; thus (6) was used to form the prior distribution on each D_i from a uniform distribution on $[0, 2\pi]$; where θ, ψ, R were chosen uniformly on [0,500].

4.3.1 Data Set #1

This is a simulated set of lengths from $N = 10$ cracks, taken from a solution to (5). The crack lengths were observed at $k = 10$ time points. Figure 6 shows the 10 cracks with the observed-lengths marked.

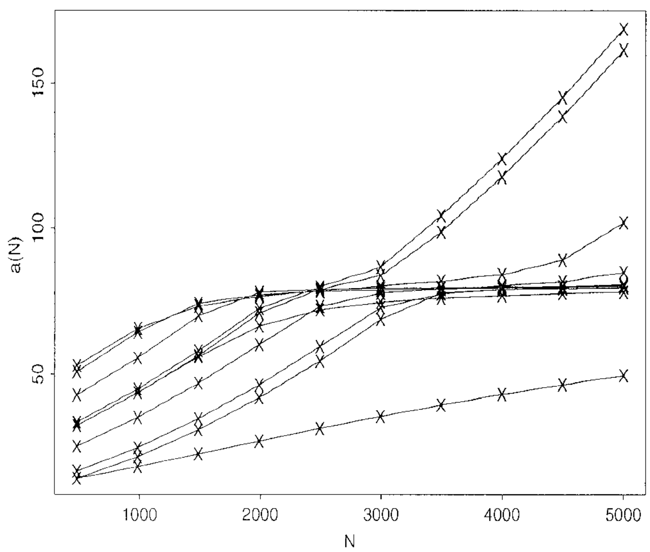

Figure 6. Simulated Data

The data were analyzed using the Gibb's sampler; 10^3 samples from all the posterior distributions were generated. The first 300 were ignored and the results calculated using the remaining 700 samples. With N=10, there are 36 parameters to be estimated from 100 data points, so that the posterior distributions for the crack specific parameters m, D, ϕ were not very informative. Figure 7 shows the kernel pdf estimates of the posterior distributions of the mean & variance of $\log(m)$ and $\text{logit}(\phi)$. Figure 8 shows the estimate of the future reliability, with $A_{\text{th}}=1000$, of the specimen to be fairly precise, with failure predicted to occur "almost certainly" between $t=14$ and $t=16$.

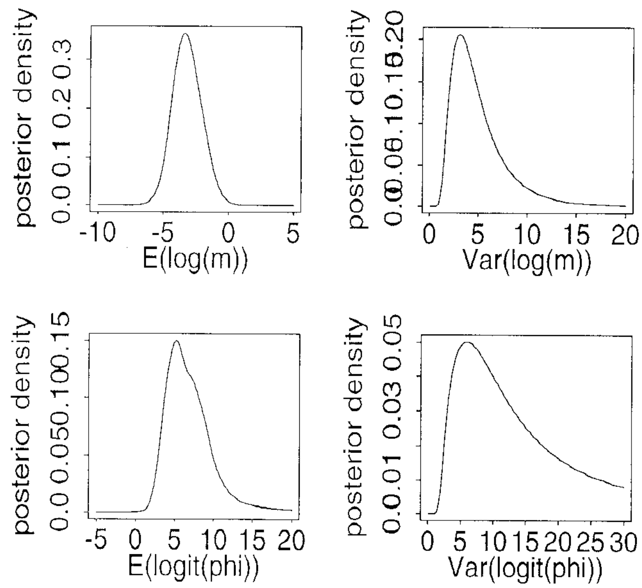

Figure 7. Kernel Posterior pdf Estimates for 4 Global Parameters
[given the data from the simulated specimen with 10 micro-cracks]

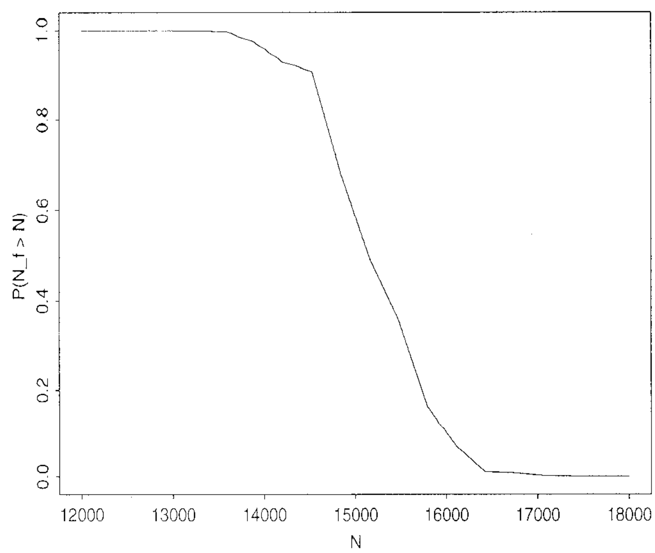

Figure 8. Estimated Reliability of Simulated Specimen
[with: 10 micro-cracks, $A_{\text{th}}=1000$]

4.3.2 Data Set #2

This is an experiment on a specimen of cast iron. The specimen was subjected to a cyclic load at a constant $\Delta\sigma$ and the growth of cracks measured with the aid of a microscope. Figure 9 shows the observed lengths of 190 micro-cracks in the specimen. The lengths were observed at only 4 points; thus our model is over-parameterized as regards estimation of individual crack properties (since there are 3 parameters per crack). So we concentrate on the 6 global parameters and the reliability prediction. Figure 10 shows the predicted reliability, with $A_{th}=1000$.

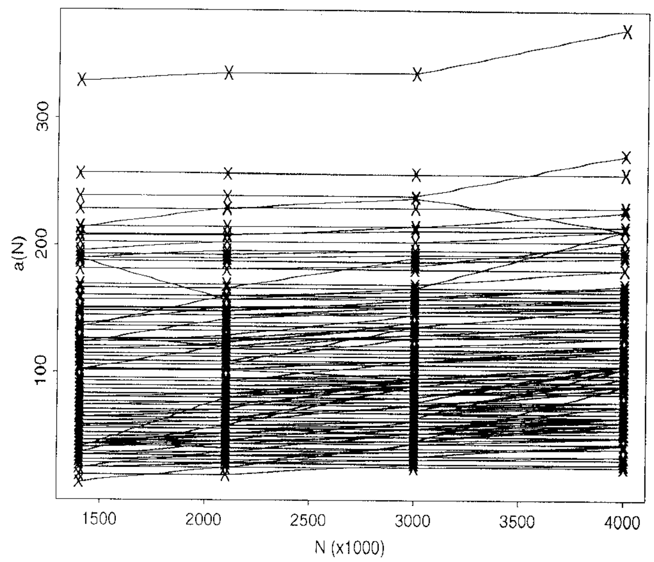

Figure 9. Micro-Crack Data
[from a cast-iron specimen]

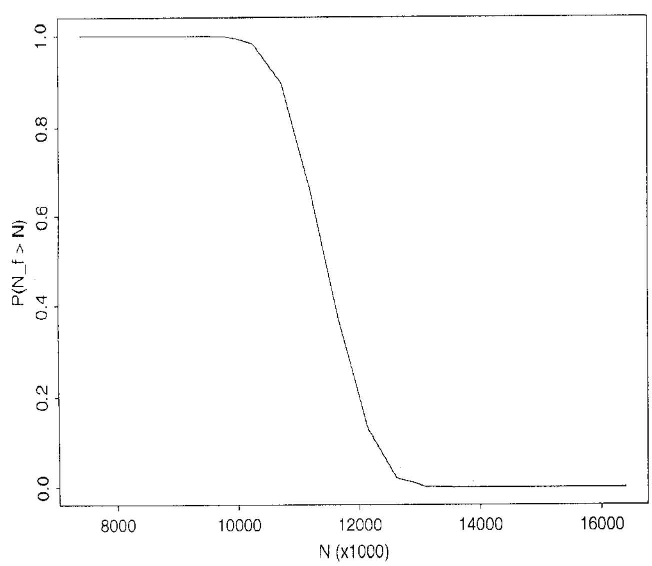

Figure 10. Estimated Reliability of Cast-Iron Specimen
[with: $A_{th}=1000$]

Figure 9 shows that there is one dominant crack that is larger than the others; thus, in contrast to the simulated data, the reliability prediction is almost entirely dependent on the predicted growth of this crack alone.

5. CLOSING REMARKS

One important aspect of micro-crack growth has been ignored in this approach: there is often a large spatial-dependence between micro-cracks. For example, neighboring cracks can coalesce, and the presence of a large crack can inhibit growth of cracks nearby. In some materials the main cause of growth in the micro-crack phase is coalescence. Coalescence occurred in some of the cracks of data set #2, and was resolved by considering all the cracks that subsequently coalesced as one crack with length the sum of its constituents. This rather crude approach can be improved upon, and presents an interesting modeling problem.

A practical reason for not incorporating a spatial component into the model, apart from the prospect of computational problems, is that the data on micro-crack growth does not provide any information on the location of each crack in the specimen. This reflects the difficulty of 1) observing such small objects, and 2) accurately measuring them on a specimen. Even locating the same crack that was measured previously can be a problem. However, improvements in experimental techniques mean that spatial data ought to become possible to collect, at which point a spatial model approach can be pursued.

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