Statistical Analysis of Slow Crack Growth Experiments

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Abstract

A common approach for the determination of Slow Crack Growth (SCG) parameters are the static and dynamic loading method. Since materials with small Weibull module show a large variability in strength, a correct statistical analysis of the data is indispensable. In this work we propose the use of the Maximum Likelihood method and a Baysian analysis, which, in contrast to the standard procedures, take into account that failure strengths are Weibull distributed. The analysis provides estimates for the SCG parameters, the Weibull module, and the corresponding confidence intervals and overcomes the necessity of manual differentiation between inert and fatigue strength data. We compare the methods to a Least Squares approach, which can be considered the standard procedure. The results for dynamic loading data from the glass sealing of MEMS devices show that the assumptions inherent to the standard approach lead to significantly different estimates.

Key words: Slow Crack Growth, Weibull distribution, Maximum Likelihood, Bayesian Analysis

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1 Introduction

Subcritical crack growth is a well known phenomenon for a large variety of glass and ceramic materials. A widely used empirical relation models the stress intensity at the crack tip and the rate of crack growth by a simple power law (Munz and Fett, 2001). The model covers slow crack growth rates which are most interesting for lifetime prediction:

$$v = A\left(\frac{K_I}{K_{IC}}\right)^n \tag{1}$$

with v representing the crack growth rate, $\frac{K_I}{K_{IC}}$ the ratio of actual and critical stress intensity at the crack tip and the material and environmental dependent *slow crack growth parameters* (SCG) A and n. The determination of the SCG parameters of structural glass and ceramic components is therefore an essential part in assessing the reliability of industrial products. Various methods to determine these parameters exist, which can be related to two different approaches.

The *double torsion*, *double cantilever* and *compact tension* method count among the first approach. It uses special test samples with artificially induced macroscopic cracks, and allows for a relatively comfortable and direct —mostly optical— observation of the crack propagation. The drawback of this group of methods is, besides the need for special test samples and equipment, the fact that macroscopic cracks might show a different SCG behavior than natural microscopic flaws.

The second approach makes use of the fact that material subject to subcritical growth of initial defects shows time dependent strength (Munz and Fett, 2001). This property consequently leads to finite lifetimes in tests under static loading conditions:

$$t_f = B\sigma_i^{n-2}\sigma^{-n}\left[1-\left(\frac{\sigma}{\sigma_i}\right)^{n-2}\right] \tag{2}$$

The time to failure is denoted by t_f, B contains some fracture mechanical quantities including A, σ is the applied load, and σ_i the inert strength. In tests under dynamic loading conditions the fracture strength is dependent on the applied loading rate

$$\sigma_o^{n+1} = B\sigma_i^{n-2}\dot{\sigma}(n+1)\left[1-\left(\frac{\sigma_o}{\sigma_i}\right)^{n-2}\right] \; , \tag{3}$$

where σ_o denotes the characteristic fracture strength, $\dot{\sigma}$ the loading rate in the dynamic loading test. Both methods are efficient in the determination of the dependency in (1) using samples with natural microscopic defects. They are often applied to determine the SCG parameters of glasses and ceramics as

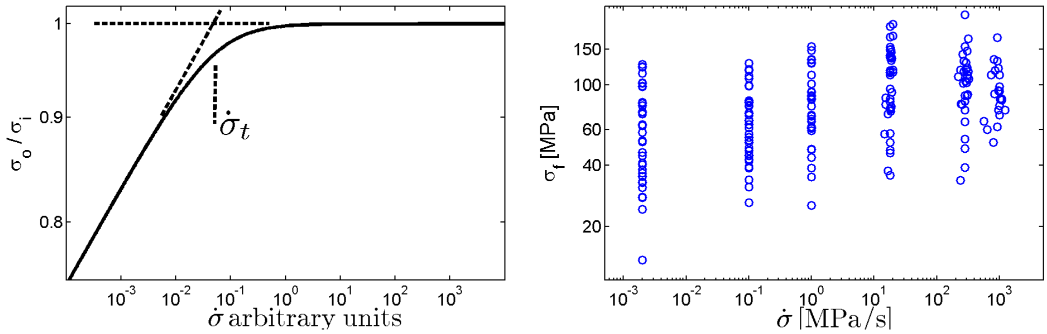

Fig. 1. The left plot shows the dependency (3) between loading rate $\dot{\sigma}$ and characteristic failure strength σ_o with asymptotes (5). For materials with small Weibull parameter it can be hard to localize the plateau region from experimental data as shown by the right plot (RB-data, see Sec. 4 for details).

they overcome the mentioned drawbacks of the above approach. The analysis of both, static and dynamic loading experiments, simplifies the SCG behavior of the material assuming the power law relation in (1). In principle one needs to take into account all three stages operant in ceramics and glasses as well as the threshold stress intensity below which no SCG behavior can be observed. In comparison to dynamic configurations static loading tests provide more lifetime relevant results since they are less affected by the stages two and three of the SCG (Sudreau et al., 1994). The 'lifetime tests with modified evaluation' given by Fett et. al. does not require any assumption on the SCG law (Munz and Fett, 2001). However, to use this method one needs to know the inert strength and lifetime distributions and one has to ensure that both are determined by the same flaw distribution. Especially for tests that have to be applied on device level this can be difficult to ensure.

In this paper we focus on the analysis of dynamic loading measurements (3) comparing several methods to determine the SCG parameters when strengths are Weibull distributed. Model (2) for static loading experiments is equivalent and the analysis can be performed in the same manner — thus retaining all advantages as described in the following [1]. We present dynamic tensile loading measurements of the glass sealing of Micro Electro Mechanical Components. Figure 1 schematically depicts relation (3), the according quantities can be determined using relatively simple mechanical test methods and the measurements can be performed in an industrial environment. For details on the experimental setup we refer to Glien et al. (2004).

Being a probabilistic quantity the strength of ceramics and glasses can show large scattering. Therefore, a reasonable amount of samples has to be measured and a correct statistical analysis needs to be conducted. Most often the

[1] Thanks to the referee for pointing this out.

examined strength data σ_f are Weibull distributed:

$$\sigma_f \sim \mathrm{WB}(\sigma_f|\sigma_o, m) = m\,{\sigma_o}^{-m}{\sigma_f}^{m-1}e^{-\left(\frac{\sigma_f}{\sigma_o}\right)^m}\ , \tag{4}$$

where σ_o denotes the characteristic fracture strength and the Weibull module m describes the amount of variation. The smaller the Weibull module of the considered material, the more important an accurate statistical analysis becomes. An accurate analysis needs to account for the Weibull distribution and therefore inhibits the use of standard methods. Since m is in good approximation independent of the loading rate equation (3) can be simplified by regarding only the two asymptotes shown in Figure 1

$$\log\sigma_o(\dot{\sigma}) = \begin{cases} \left[\frac{1}{1+n}\log\dot{\sigma} + \log D\right] & \text{for} \quad \log\dot{\sigma} \le \dot{\sigma}_t \\ \frac{\dot{\sigma}_t}{1+n} + \log D & \text{for} \quad \log\dot{\sigma} > \dot{\sigma}_t \end{cases}\ , \tag{5}$$

where $\dot{\sigma}_t$ denotes the intersection of the two asymptotes

$$\dot{\sigma}_t = \frac{\sigma_i^3}{B(N+1)} \qquad \text{with} \qquad B = \frac{D^{n+1}}{n+1}\sigma_i^{2-n}\ . \tag{6}$$

We propose to use the *Maximum Likelihood* method which explicitly takes into account the Weibull distribution of the strengths. The standard procedure C 1368–01 given by (ASTM, 2001) uses a Least Squares fit which leads to significantly different results. In a further step we describe how a *Bayesian analysis* provides the opportunity to fit the measured data to the entire model (5). This method liberates us from the need to exclude data from the plateau-region where inert strength is observed, and also yields exact confidence intervals that all other methods fail to provide. As the implementation of those common statistical methods is relatively tedious we provide a MatLab [2] code at `www.tuebingen.mpg.de/~tpfingst/FBMCode.zip`.

2 Statistical parameter-estimation

In the following section we introduce the basic concepts for statistical parameter estimation which we use to analyze the experimental data. We start with a closer look at Maximum Likelihood estimations and relate them to Least Squares fits which are often used in SCG experiments due to their simplicity. We proceed describing a Bayesian analysis that not only delivers point estimates of parameters, but also provides us with confidence intervals.

[2] MatLab is a trademark of The MathWorks, Inc.

Let us assume that some quantities y and x are dependent via a mapping f

$$y(x) = f(x; \theta_1, \theta_2 \ldots) \tag{7}$$

and one tries to determine the parameters $\theta_1, \theta_2 \ldots$ empirically by measuring N samples $\mathcal{D} = \{x_1, y_1, \ldots x_N, y_N\}$. Due to measurement uncertainty and variations in test samples the measurements are corrupted. Thus the observations y_i are distributed according to the specific scattering mechanism

$$y \sim p(x|f, \boldsymbol{\theta}) \ , \tag{8}$$

where all parameters are collected in a vector $\boldsymbol{\theta}$. In SCG experiments, for example, the failure strengths are Weibull distributed around σ_o as given in eq. (4).

The Maximum Likelihood method (see e.g. Duda et al. (2001)) uses the distribution in (8) to find the most plausible parameters by maximizing the *Likelihood* $\mathcal{L}(\boldsymbol{\theta})$ which is by definition the probability of observing the data under the condition that the parameters $\boldsymbol{\theta}$ are known

$$\mathcal{L}(\boldsymbol{\theta}) = p(\mathcal{D}|f, \boldsymbol{\theta}) \ . \tag{9}$$

The maximization can be performed using standard algorithms such as conjugate gradient ascent (Press et al., 1986, chap. 10.6).

The Maximum Likelihood method reduces to a Least Squares fit when the noise is Normal, i.e.

$$y = f(x; \theta_1, \theta_2 \ldots) + \epsilon \qquad \text{with} \qquad \epsilon \sim \mathcal{N}(0, \sigma^2_{\text{Noise}}) \ . \tag{10}$$

The residuals $\epsilon_i = y_i - f(x_i; \theta_1, \theta_2 \ldots)$ are then Gaussian variables and the Likelihood is a product of Gaussian distributions

$$\mathcal{L}(\boldsymbol{\theta}) = \prod_{i=1}^{N} p(y_i, x_i | f, \boldsymbol{\theta}) = \prod_{i=1}^{N} \mathcal{N}\left(\epsilon_i, \ \sigma^2_{\text{Noise}}\right) \ . \tag{11}$$

One can easily show that in this case the Maximum Likelihood solution is given by a Least Squares fit by considering the logarithm of the Likelihood

$$\log \mathcal{L}(\boldsymbol{\theta}) = -\frac{N}{2} \log(2\pi\sigma^2_{\text{Noise}}) - \frac{1}{2\sigma^2_{\text{Noise}}} \left(\sum_{i=1}^{N} \epsilon_i^2 \right) \tag{12}$$

which is maximized when the sum of squared residuals (rightmost term) is minimal. The Least Squares fit therefore corresponds to the implicit assumption that the observed quantity is corrupted by Normal noise.

The Maximum Likelihood method and the special case of Least Squares fits estimate a sensible set of parameters but fail to provide a notion of uncertainty that remains after the experiment. Bayesian theory, in contrast, enables us to use the data to update our knowledge about the parameters and quantifies the remaining uncertainty. For details we refer to standard literature such as (Duda et al., 2001; Jaynes, 2003).

Before conducting any experiment, we always have some vague knowledge about the parameters $\boldsymbol{\theta}$, which we code in a *prior* distribution $p_o(\boldsymbol{\theta})$. Here we use uninformative priors for all parameters that only constrain them to physically meaningful values. Using Bayes' rule we can formally compute what we learn about the parameters by exploiting the measured data $\mathcal{D}$:

$$p(\boldsymbol{\theta}|\mathcal{D}) = \frac{p(\mathcal{D}|\boldsymbol{\theta})p_o(\boldsymbol{\theta})}{\mathcal{Z}} \tag{13}$$

where $p(\mathcal{D}|\boldsymbol{\theta})$ is the likelihood $\mathcal{L}(\boldsymbol{\theta})$ from (9) and $\mathcal{Z}$ denotes the normalizing constant

$$\mathcal{Z} = \int p(\boldsymbol{\theta}|\mathcal{D}) \, \mathrm{d}\boldsymbol{\theta} \; . \tag{14}$$

The so-called *posterior* distribution $p(\boldsymbol{\theta}|\mathcal{D})$ — the probability distribution of $\boldsymbol{\theta}$ *given* the data — contains all information we have about the parameters. All quantities of interest $\langle g \rangle$ such as expected values or variances of the parameters $\boldsymbol{\theta}$ can be calculated according to

$$\langle g \rangle = \mathrm{E}_{p(\boldsymbol{\theta}|\mathcal{D})} \left[g(\boldsymbol{\theta}) \right] = \int p(\boldsymbol{\theta}|\mathcal{D}) \; g(\boldsymbol{\theta}) \, \mathrm{d}\boldsymbol{\theta} \; . \tag{15}$$

Unfortunately the integrals (14) and (15) cannot be calculated analytically for most models, but Markov Chain Monte Carlo Sampling (MCMC) yields good approximations that are guaranteed to converge. For excellent introductory texts on MCMC see MacKay (2003) and Neal (1993). The idea of sampling methods is to approximate the integrals in (15) by sums over M samples $\boldsymbol{\theta}_n$ from the posterior distribution:

$$\langle g \rangle = \int p(\boldsymbol{\theta}|\mathcal{D}) \; g(\boldsymbol{\theta}) \, \mathrm{d}\boldsymbol{\theta} \; \approx \; \sum_{n=1}^{M} g(\boldsymbol{\theta}_n) \qquad \text{where} \qquad \boldsymbol{\theta}_n \sim p(\boldsymbol{\theta}|\mathcal{D}) \; . \tag{16}$$

For $M \to \infty$ the approximation approaches the integral and for finite sample sizes good estimates can be obtained. We draw the samples $(\boldsymbol{\theta}_n)_{n=1\ldots M}$ from the posterior distribution using the *Metropolis-Hastings Method.*

The Metropolis-Hastings Method constructs a Markov Chain with $p(\boldsymbol{\theta}|\mathcal{D})$ being its equilibrium distribution rather than drawing independent samples from $p(\boldsymbol{\theta}|\mathcal{D})$. Starting at some $\boldsymbol{\theta}_1$, in each step n a proposal for a following chain link $\boldsymbol{\theta}_{n+1}$ is drawn from a *proposal distribution* $Q(\boldsymbol{\theta}_n, \boldsymbol{\theta}_{n+1})$ and is accepted if the ratio

$$a = \frac{p(\boldsymbol{\theta}_{n+1}|\mathcal{D})}{p(\boldsymbol{\theta}_n|\mathcal{D})} \frac{Q(\boldsymbol{\theta}_n, \boldsymbol{\theta}_{n+1})}{Q(\boldsymbol{\theta}_{n+1}, \boldsymbol{\theta}_n)} \tag{17}$$

exceeds one; if $a \leq 1$ it is accepted with probability a. It can be shown that for all positive Q the probability of $\boldsymbol{\theta}_n$ approaches its equilibrium. A closer look at (17) shows that the normalizing constant $\mathcal{Z}$ cancels out in the ratio a. Thus we only need to be able to calculate $p(\mathcal{D}|\boldsymbol{\theta})$ and $p_o(\boldsymbol{\theta})$. As a proposal distribution we choose a Gaussian distribution

$$Q(\boldsymbol{\theta}, \boldsymbol{\theta}') = \frac{1}{\sqrt{2\pi|\boldsymbol{\Sigma}|}} e^{(\boldsymbol{\theta}-\boldsymbol{\theta}')^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{\theta}-\boldsymbol{\theta}')} \tag{18}$$

with diagonal covariance matrix $\boldsymbol{\Sigma}$ that we can adjust to obtain optimal convergence rates. Note that for this just as for other symmetric proposal functions Q cancels in the ratio (17). MacKay (2003, chap. 29) provides a detailed description including a short pseudocode. Details on the convergence of Markov Chains are given by Cowles and Carlin (1996).

3 Assessment of SCG parameters

In the preceding section we have described the concepts of Least Squares, Maximum Likelihood and Bayesian Analysis in general. In the following we relate these common statistical methods to the determination of SCG parameters. We describe the procedure according to the standard C 1368–01 (ASTM, 2001) and compare it to the Maximum Likelihood solution. Furthermore we show how a Bayesian Analysis puts aside the need to discard data in the range of inert strength and provides confidence intervals to all parameters.

3.1 Standard procedures

Several different techniques to estimate the SCG parameters exist that greatly vary in simplicity. All methods have in common that they require the loading rates to lie below the region where inert strength is approached — according to (5) $\log \dot{\sigma}$ is required to be below $\dot{\sigma}_t$. The logarithm of σ_o is then simply a linear function of the log loading rate with slope $\frac{1}{n+1}$ and axis intercept $\log D$.

The arithmetic mean method (AMM) uses the mean failure stress at given stress rates in combination with a Least Squares fit to obtain slope and axis intercept. In the individual data method (IDM) the fit is done directly on all data without preprocessing. A Monte Carlo simulation is presented by Ritter (1981, 1979) which uses a method similar to the AMM but replacing the mean by the median failure stress. Other methods are the Weibull median, median deviation, homologous stress, bivariant, and trivariant methods (Choi et al., 1997).

A comparison in Choi et al. (1997) shows that IDM is to be preferred to AMM. IDM is also the standard given by (ASTM, 2001). We therefore compare the methods proposed in this work to IDM as a baseline procedure.

3.2 Maximum Likelihood Method

As shown in the previous section the Least Squares fit applied by the standard procedures such as IDM does not reflect that the failure strengths σ_f are Weibull distributed. We therefore use a Maximum Likelihood Method (MLM), also restricting the data to the part below inert strength.
Note that Maximum Likelihood is a common procedure when it comes to fit the parameters of a *single* Weibull distribution to data (Gross et al., 1996), the MLM which we present here is used to find the SCG parameters n and D as well as the Weibull module m.

3.3 Full Bayesian Analysis

While the MLM overcomes the implicit assumption of normal noise one still faces the problem that (log) loadings rates have to be restricted to values below $\dot{\sigma}_t$. It can be very hard to clearly ascertain the unknown $\dot{\sigma}_t$ and results may depend on its choice. We propose to use the Full Bayesian Analysis (FBM) as given in Section 2.2 to find *all* parameters n, D as well as m and $\dot{\sigma}_t$ including the corresponding confidence intervals. We estimate the parameters as the medians of the respective posterior distributions and state 95% confidence intervals bounded by the 2.5 and 97.5 percentiles.

4 Results and Conclusions

In the following we present the results of the proposed methods on two experimental data sets. The *RB-data* represents dynamic tensile loading measurements we did on the sealing of Micro Mechanical Components, the *GS-data* was taken from Gross et al. (1996). Figure 2 shows the data together with the predicted σ_o given by FBM and Table 1 summarizes the results of all methods. Note that in the RB-data we had to discard all measurements beyond loading rates of 10^2 MPa/s—for IDM and MLM— due to the fact that the

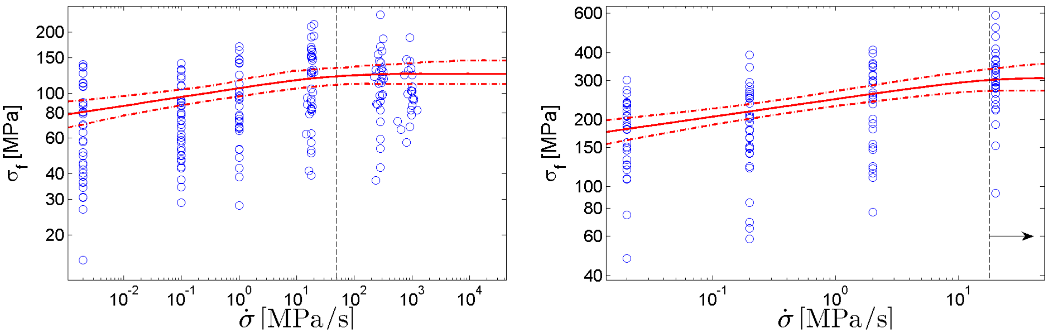

Fig. 2. Results for the data sets RB-data (left) and GS-data (right). Experimental data (○) together with the median σ_o predicted by FBM (—) and a 95% confidence interval (···) are shown. FBM detects where inert strengths are observed; the start of the plateau area is indicated by (--). Note that the RB-data shows a pronounced saturation region, while for the GS-data the plateau is correctly found to lie to the right of the measurements.

inert strength might have been observed there. The GS-data apparently does not attain this region.

The first striking fact is that the IDM prediction for D lies off the confidence intervals in both cases. This discrepancy reflects the deviation of the Weibull-scattering from IDMs assumption of Normal noise while n is only slightly affected. The MLM predictions do not differ significantly from the FBM.

When applying dynamic or static loading experiments one has to make sure that the simplification introduced by (1) is justified when using the SCG parameters for lifetime prediction. Once this is clarified a correct Bayesian treatment of the data is to be favored over the traditional IDM method and the MLM. When using IDM on dynamic loading data one has to additionally estimate the Weibull module m in a separate Weibull analysis for a fixed loading rate. Furthermore the simplification of Least Squares is unnecessary now that powerful computers are widely available. MLM gives results that are comparable to those of FBM but still requires constraining the loading rates in a preprocessing stage and confidence intervals are not automatically obtained. We provide the code for the FBM and MLM method at `www.tuebingen.mpg.de/~tpfingst/FBMCode.zip` which makes their

RB	IDM	MLM	FBM	95% conf.i.
D	85.8	106.0	105.8	[96.4, 115.7]
n	15.5	18.5	22.6	[12.8, 37.9]
m	—	2.50	2.59	[2.26, 2.97]

GS	IDM	MLM	FBM	95% conf.i.
D	222	268	247	[229, 268]
n	11.2	11.9	11.7	[7.5, 17.4]
m	—	3.05	2.98	[2.54, 3.48]

Table 1
Results of the compared methods. On the RB-data (left) MLM and IDM were run on the data for loading rates below 10^2MPa/s while the complete GS-data (right) was used for all methods.

use straightforward.

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