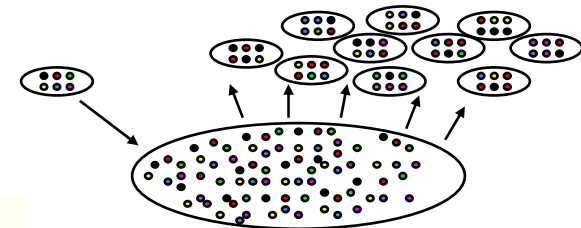
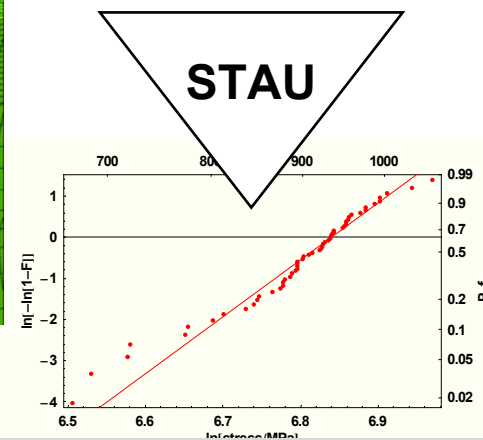
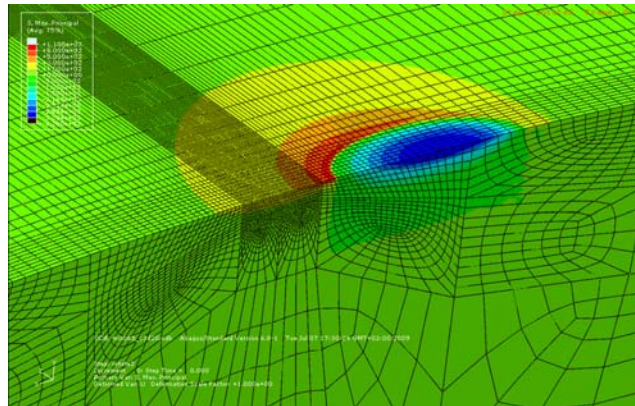


# Uncertainties in Mechanics and Materials Research – Application in the field of Materials Research

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Karlsruhe Institute of Technology (KIT), Institute for Applied Materials (IAM)



# Outline

- Scope; historical account
- About ceramics...
- The Weakest Link approach and Fracture Mechanics
- STAU – the interface to Finite Elements
- Uncertainty analysis: Bootstrap & Bayes' methods
- Reducing uncertainties by pooling
- ( uncertainty: predictions/boundary conditions )
- Summary

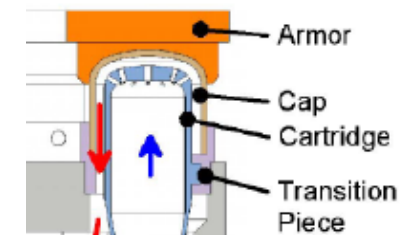
# Scope I

## ■ Reliability of brittle materials

ceramics



tungsten



glass

steel (ferrite)

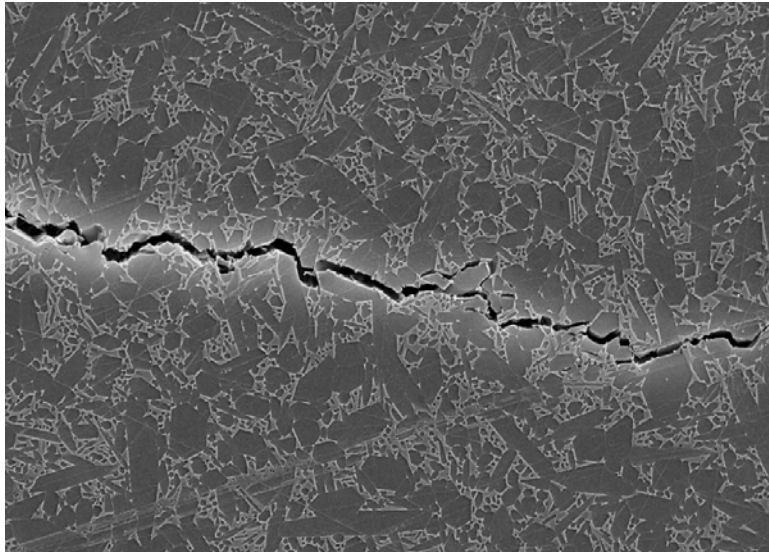


## ■ high strength, low wear, heat resistance, chemical inertness

## Scope II

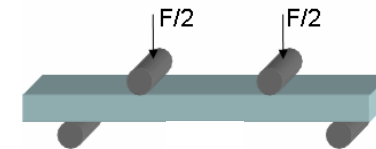
- fields of interest

microstructure (silicon nitride  $\text{Si}_3\text{N}_4$ )



failure behaviour

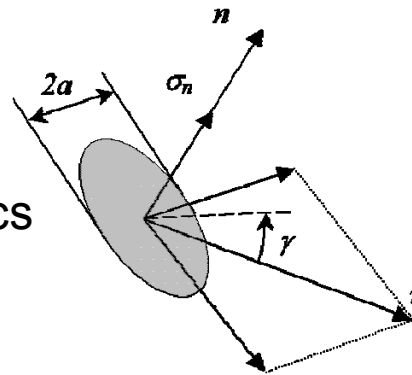
mechanical properties



# Scope III

■ methods

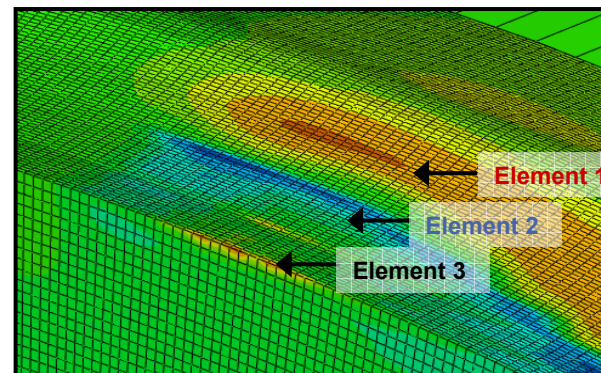
fracture mechanics



probability theory



engineering



# From then to now (history)

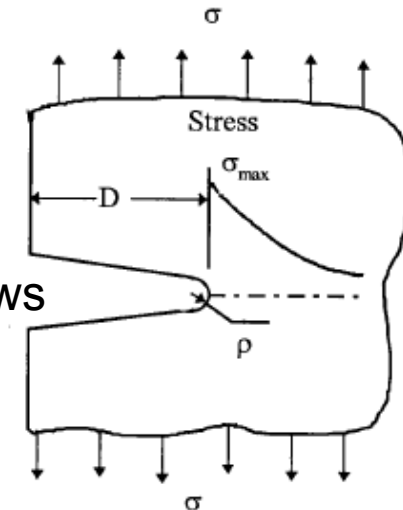
- fracture of materials (mechanics)

Griffith (~1920)

Irwin (~1960)

the importance of material flaws

Hutchinson, Rice (~1970)



- fracture of materials (statistics)

Weibull (~1930)

Freudenthal (~1950)

Batdorf, Evans, Matsuo (~1980-90)

fracture mechanics based weakest link approach

- material flaws as stress raisers

# From then to now II

- computers (engineering)

Finite elements

stress analysis under complex loads

stress analysis for complex geometries

(microstructure)

- FE postprocessing (CARES, STAU)

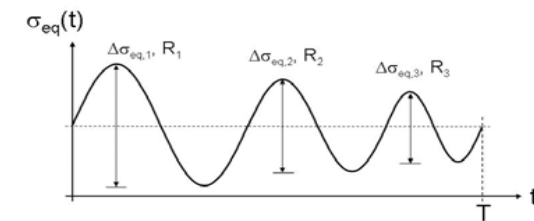
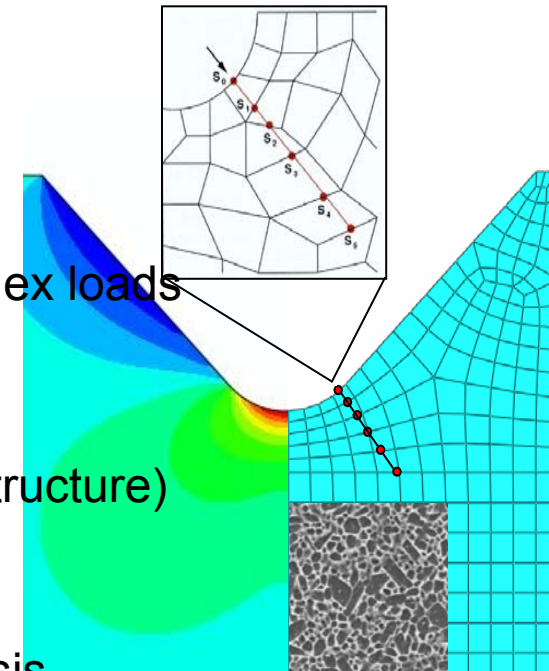
link between stress analysis and reliability analysis

spontaneous fracture

delayed (time-dependant) fracture

cyclic loading

- the importance of microstructure



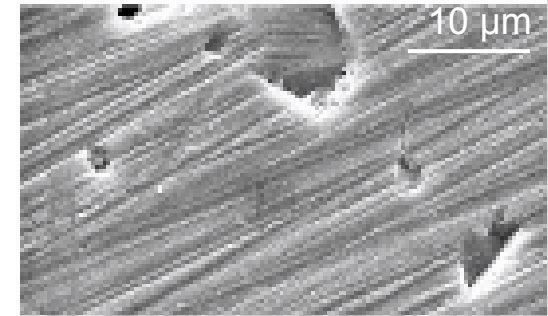
# The importance of microstructure

- the importance of microstructure (high strength ceramics)

sintering: pores, inclusions, grain boundaries

phases, fibres, ...

machining: surface flaws



(surface treatment; hardening)

- FE postprocessing & microstructure

crack propagation

critical crack size; fracture toughness

crack resistance

contact loading; thermal shock



# Aspects of uncertainty

- material behaviour (inherent scatter)

strength: characteristic strength, scatter

crack propagation: power law parameters

lifetime: strength & crack propagation parameters

(surface treatment; hardening)

- material characterization (data uncertainties)

limited amount of data

data from different sources

- modelling; analysis

unknown boundary conditions

various models for strength, lifetime, crack propagation

# Reliability uncertainty

- Failure probability

obtained by numerical analysis of mechanical stress field

including routines for crack propagation

uncertainty in input parameters transforms to results

- lifetime prediction

dito

data from different sources

- size effect

mechanisms of fracture (microcrack failure)

**Data base uncertainties**



**prediction uncertainties**

# Strategies for uncertainty assessment

- material behaviour (inherent scatter)

strength: use appropriate pdf

crack propagation: assess parameter uncertainty

lifetime: use stress/lifetime approach via suitable pdf

- material characterization (data uncertainties)

pooling: transferring of data to reference conditions

use data from different sources

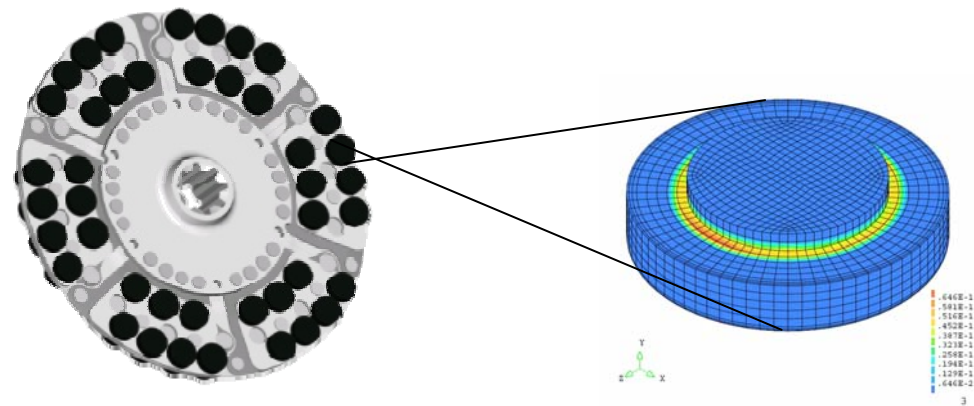
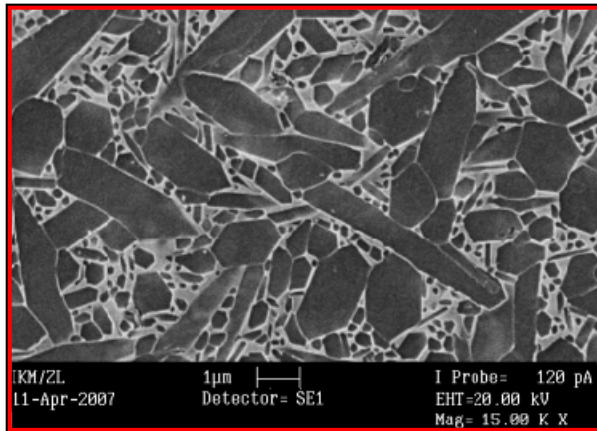
- modelling; analysis

parametric studies...

both, probabilistic and non-probabilistic approaches !!

# About ceramics

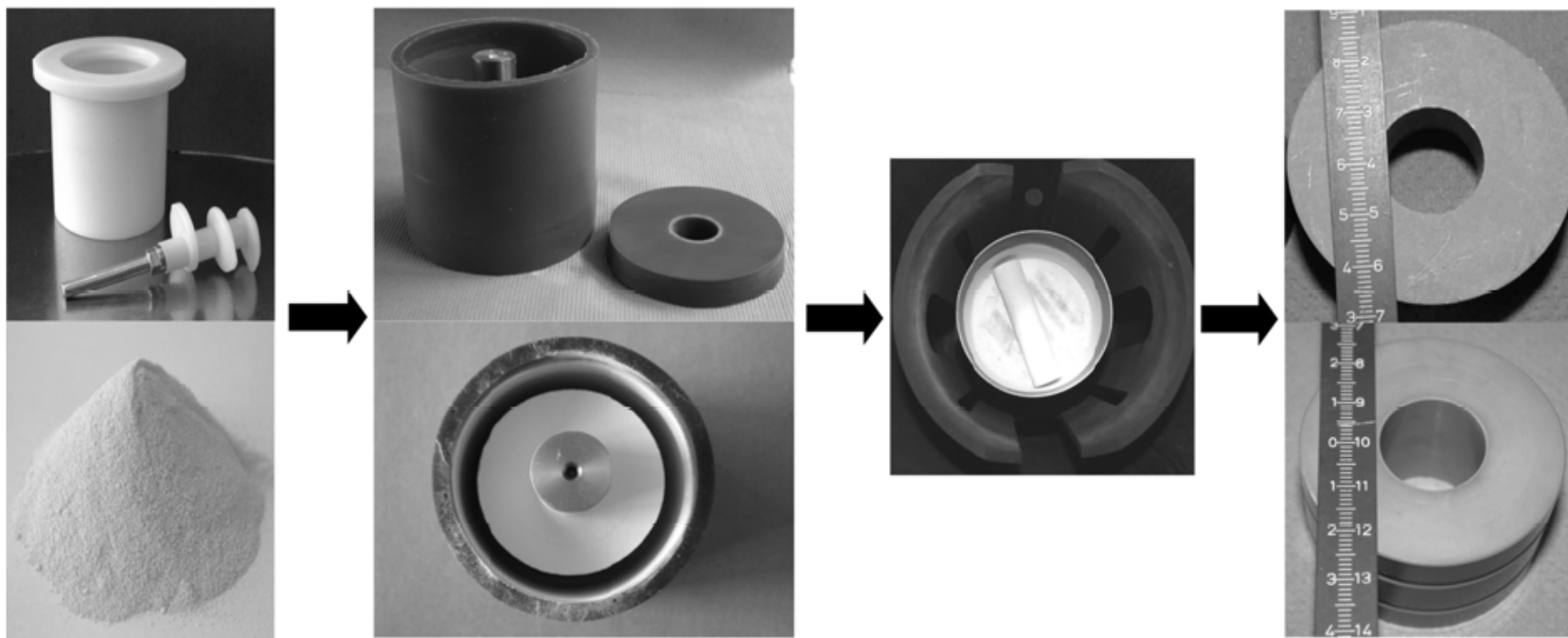
High performance *sfb* 483  
sliding and friction systems  
based on advanced ceramics



# About ceramics II

from powder to product: typical steps in ceramic processing

High performance **sfb 483**  
sliding and friction systems  
based on advanced ceramics

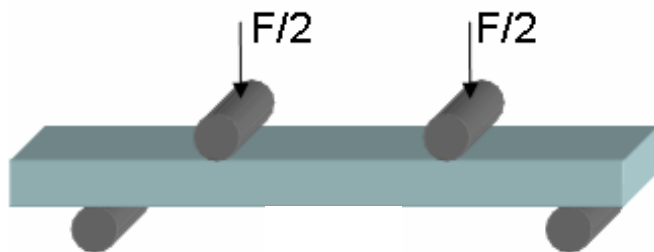


*Bild 7: Schema der Keramikherstellung am IKM am Beispiel Keramikwalzen*

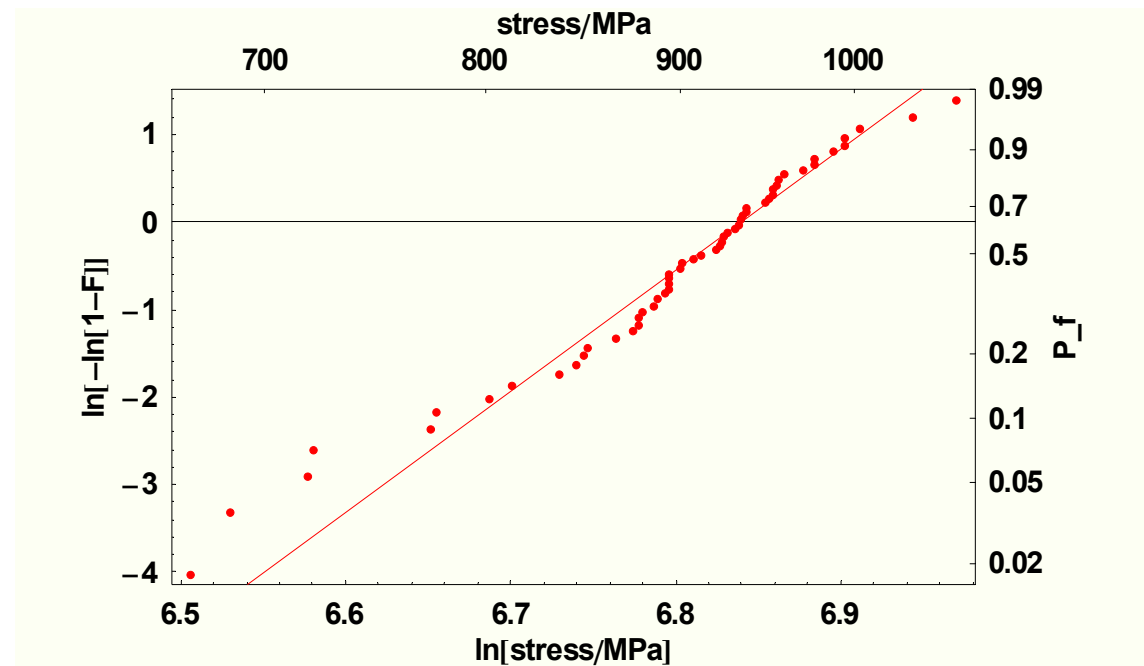
# About ceramics III

after sintering: grinding to final geometry → surface flaws

material characterization: four-point bend test  
 (inert strength, lifetime under static & cyclic loads)

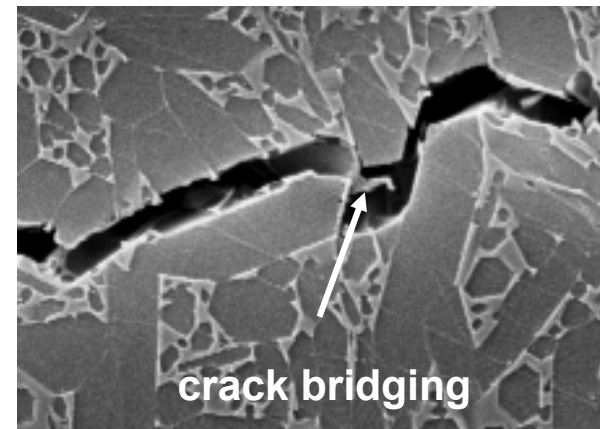
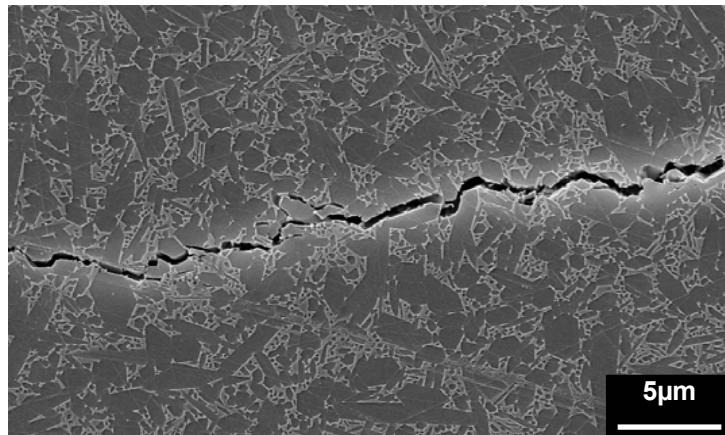


typical Weibull diagram for  
 4PB fracture strength of  
 $\text{Si}_3\text{N}_4$  ceramic;  $F=i/(n+1)$ :



# About ceramics IV

high strength ceramics: strengthening mechanisms



crack bridging stresses affects critical crack size: „R-curve effect“

# About ceramics V

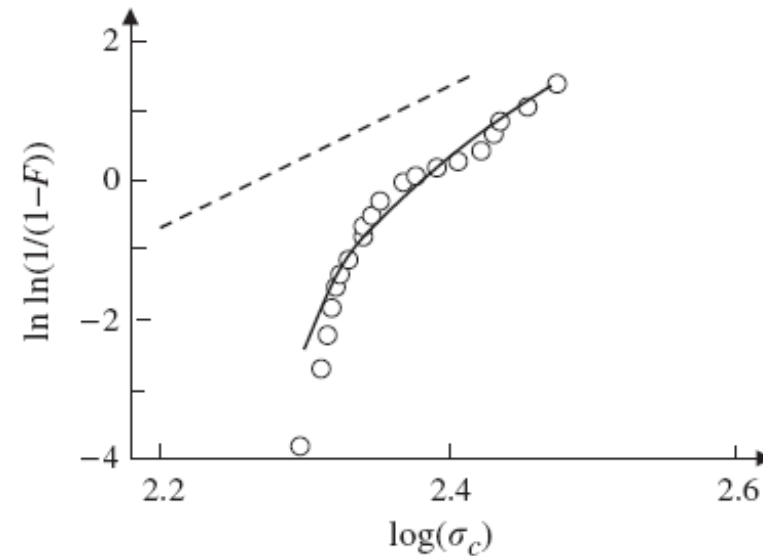


Fig. 23. Weibull plot of the strength for an  $\text{Al}_2\text{O}_3$  (full line: calculated from bridging relation; broken line: corresponding distribution for a flat  $R$  curve, Fett and Munz<sup>143</sup>).

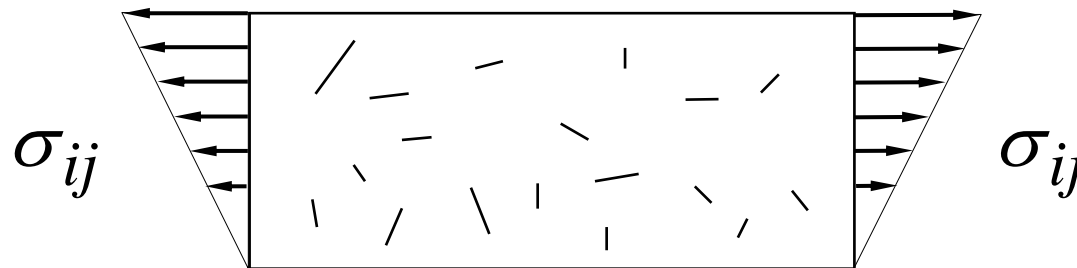
crack bridging stresses affects critical crack size: „R-curve effect“



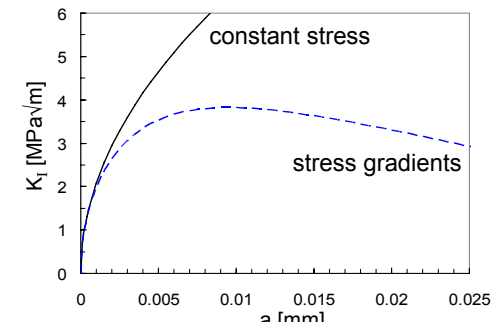
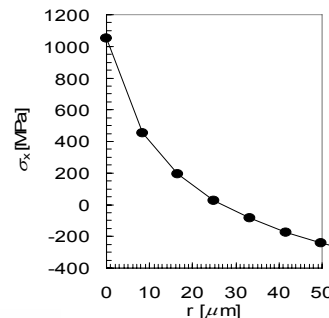
# About ceramics VI

critical crack size with respect to local stress field

inert strength; K-concept:  $K_{I,eq} = \sigma_{eq} Y_I \sqrt{a}$   $\longrightarrow$   $\sigma_{eq} = \frac{K_{I,eq}}{Y_I \sqrt{a}}$



inert strength; strongly varying local stresses (contact; thermal shock):



$$K_I(a) = \int_0^a \left( h_I^{(1)}(x, a) \cdot \sigma(x) + h_I^{(2)}(x, a) \cdot \tau(x) \right) dx$$

$$h_I^{(i)}(x, a) = \sqrt{\frac{2}{\pi a}} \sum_{m=0}^{\infty} D_{I,m}^{(i)} \cdot \left(1 - \frac{x}{a}\right)^{m-\frac{1}{2}}$$

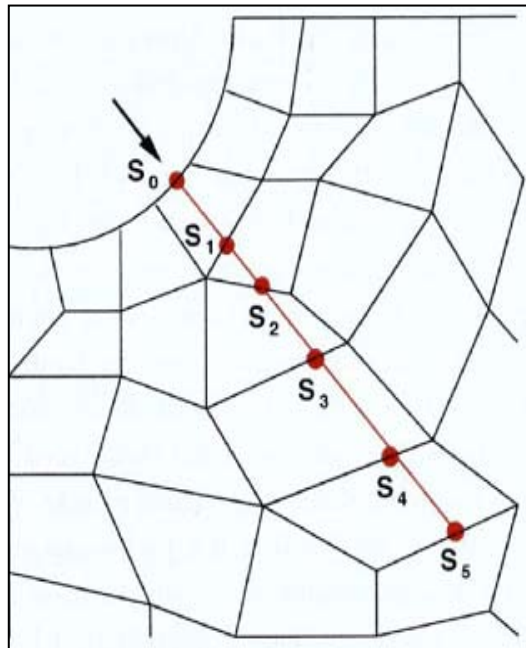
## About ceramics VII

inert strength; R-curve behaviour:

$$K_{tip}(a) = K_{appl}(a) - K_{br}(a) = \int_0^a h(x, a) \sigma_{appl}(x) dx - \int_0^a h(x, a) \sigma_{br}(x) dx$$

iterative procedure for critical crack size necessary:

$$K_{tip}(a_c) = K_{Ic}$$



# Basic ideas of the weakest link approach

Basic idea (components & system): system failure, if weakest link fails



- isotropy; i.e. flaws are uniformly distributed
- size and orientation are random
- flaws are independent (no interaction)

probabilistic model

- fracture mechanics: flaws as planar cracks
- most unfavourable combination of stress, flaw size and orientation determines failure of a component

failure model

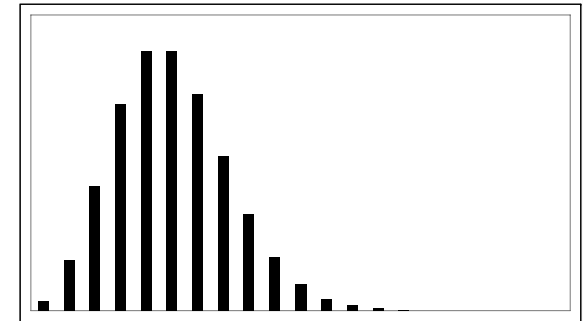
## The weakest link approach in brief

$$1 - Q_n = (1 - Q_1)^n$$



$$P_f = 1 - \exp[-M Q_1]$$

$$p_n = \frac{M^n}{n!} e^{-M}$$



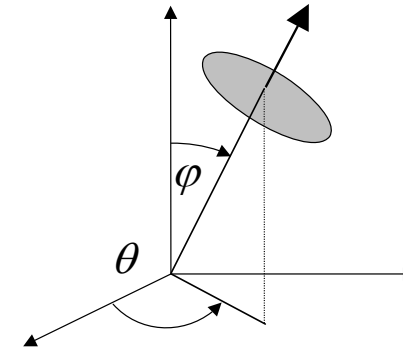
failure of individual flaws:  $Q_1$

flaw population:  $p_n$

# The weakest link approach in detail (enter fracture mechanics)

## 1st step (individual flaw) - $k=1$

e.g. flaw at location  $(x, y, z)$  with given orientation but random size  $a$



failure, if  $a \geq a_c(\vec{x}, \theta, \varphi)$  since  $a$  random variate with distribution  $F(a)$

i.e. with probability 
$$P(a \geq a_c(\vec{x}, \theta, \varphi)) = \int_{a_c}^{\infty} f(a) da = 1 - F(a_c(\vec{x}, \theta, \varphi))$$

If location and orientation are also random: 
$$Q_1 = \frac{1}{V} \int_V \frac{1}{4\pi} \int_{\Omega} (1 - F(a_c)) d\Omega dV$$

$Q_1$  is the failure probability for a component with exactly one flaw of random size and orientation at a random location of the component !!

# The weakest link approach in detail (enter fracture mechanics)

2nd step (fixed number of flaws/dislocations/extrusions/...) -  $k=n$

flaws are independent (no interaction)



1 component with  $n$  flaws ==  $n$  components, each with 1 flaw

consider  $n$  components each with 1 flaw: each component fails with probability  $Q_1$



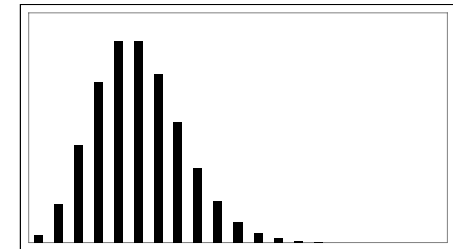
→ survival probability  $1-Q_n$  for  $n$  components:

$$1 - Q_n = (1 - Q_1)^n$$

number of flaws follows a Poisson distribution:

$$p_n = \frac{M^n}{n!} e^{-M}$$

$M$  - average number of flaws per component



→ probability that a component has exactly  $n$  flaws and fails:  $p_n Q_n$

# The weakest link approach in detail (enter fracture mechanics)

## 3rd step (summing it all up ...)

component with random number of flaws has failure probability:

$$P_f = \sum_{n=0}^{\infty} p_n Q_n = 1 - \sum_{n=0}^{\infty} \frac{M^n}{n!} e^{-M} (1 - Q_1)^n = 1 - e^{-M} e^{M(1-Q_1)} = 1 - \exp(-MQ_1)$$

$MQ_1$  is just the average number of critical flaws in the component

Now we need some information about the flaw size distribution  $F(a)$ :  $F(a) \propto a^{-r} \propto \sigma_{eq}^{2r}$

$$P_f = 1 - \exp \left[ - \frac{1}{V_0} \int_V \frac{1}{4\pi} \int_{\Omega} \left( \frac{\sigma_{eq}}{\sigma_0} \right)^m d\Omega dV \right]$$

↑  
fracture mechanics



and finally we obtain a **size effect** relation:

$$P_f = 1 - \exp \left[ - \frac{1}{V_0} \int_V \frac{1}{4\pi} \int_{\Omega} \left( \frac{\sigma_{eq}}{\sigma^*} \right)^m d\Omega dV \left( \frac{\sigma^*}{\sigma_0} \right)^m \right] = 1 - \exp \left[ - \frac{V_{eff}}{V_0} \left( \frac{\sigma^*}{\sigma_0} \right)^m \right] = 1 - \exp \left[ - \left( \frac{\sigma^*}{b} \right)^m \right]$$

# The size effect in the weakest link approach

a look at geometry...



what we learn from the final result:

$$P_f = 1 - \exp \left[ - \frac{1}{V_0} \int_V \frac{1}{4\pi} \int_{\Omega} \left( \frac{\sigma_{eq}}{\sigma^*} \right)^m d\Omega dV \left( \frac{\sigma^*}{\sigma_0} \right)^m \right] = 1 - \exp \left[ - \frac{V_{eff}}{V_0} \left( \frac{\sigma^*}{\sigma_0} \right)^m \right] = 1 - \exp \left[ - \left( \frac{\sigma^*}{b} \right)^m \right]$$

the component strength distribution is a Weibull distribution with parameters  $m$  and  $b$

the component size leads to a geometry dependence of the distribution parameter  $b$

it is possible to define a geometry-independent distribution parameter  $\sigma_0$

the size effect is described by the volume integral  $V_{eff}$  using a reference stress value  $\sigma^*$



# The weakest link model – ready for FE use

Numerical integration of stress field:

$$P_f(t) = 1 - \exp \left[ - \frac{1}{V_0} \int_V \frac{1}{4\pi} \int_{\Omega} \max_{\tau \in [0, t]} \left\{ \left[ \left( \frac{\sigma_{eq}}{\sigma_0} \right)^{n-2} + \Psi \right]^m \right\} d\Omega dV \right]$$

spontaneous failure                      Sub-critical crack growth

Fracture at time  $t$  is governed by the maximum load in  $[0, t]$ !

$$\Psi = \frac{\sigma_0}{B} \int_0^{\tau} \left( \frac{\sigma_{eq}(t')}{\sigma_0} \right)^n dt'$$

Calculation of  $P_f(t)$  by FE-Postprocessing (self-developed STAU postprocessor)  
 - non-linear problem!

# The local risk of rupture – a design tool

Consider partial volume  $V_t$

$$\pi(\vec{x}) = \lim_{V_t \rightarrow 0} \frac{P(\text{critical flaw in } V_t)}{P(\text{critical flaw in } V)} = \lim_{V_t \rightarrow 0} \frac{P(FK)}{P(K)}$$

using the following events:

$F$ : given flaw is located in  $V_t$      $P(F) = V_t/V$   
 and     $K$ : given flaw is critical     $P(K) = Q_1$

We need the probability  $P(F|K)$ :

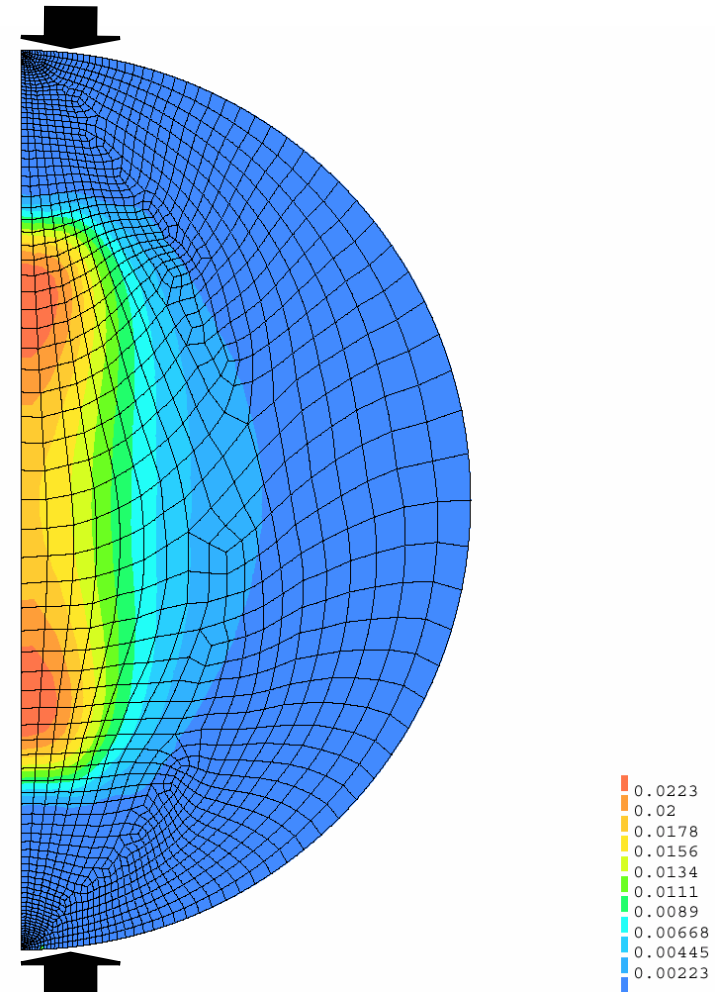
$$P(F|K) = P(FK)/P(K) \quad (\text{Bayes' theorem})$$

We obtain the probability  $P(FK)$  from:

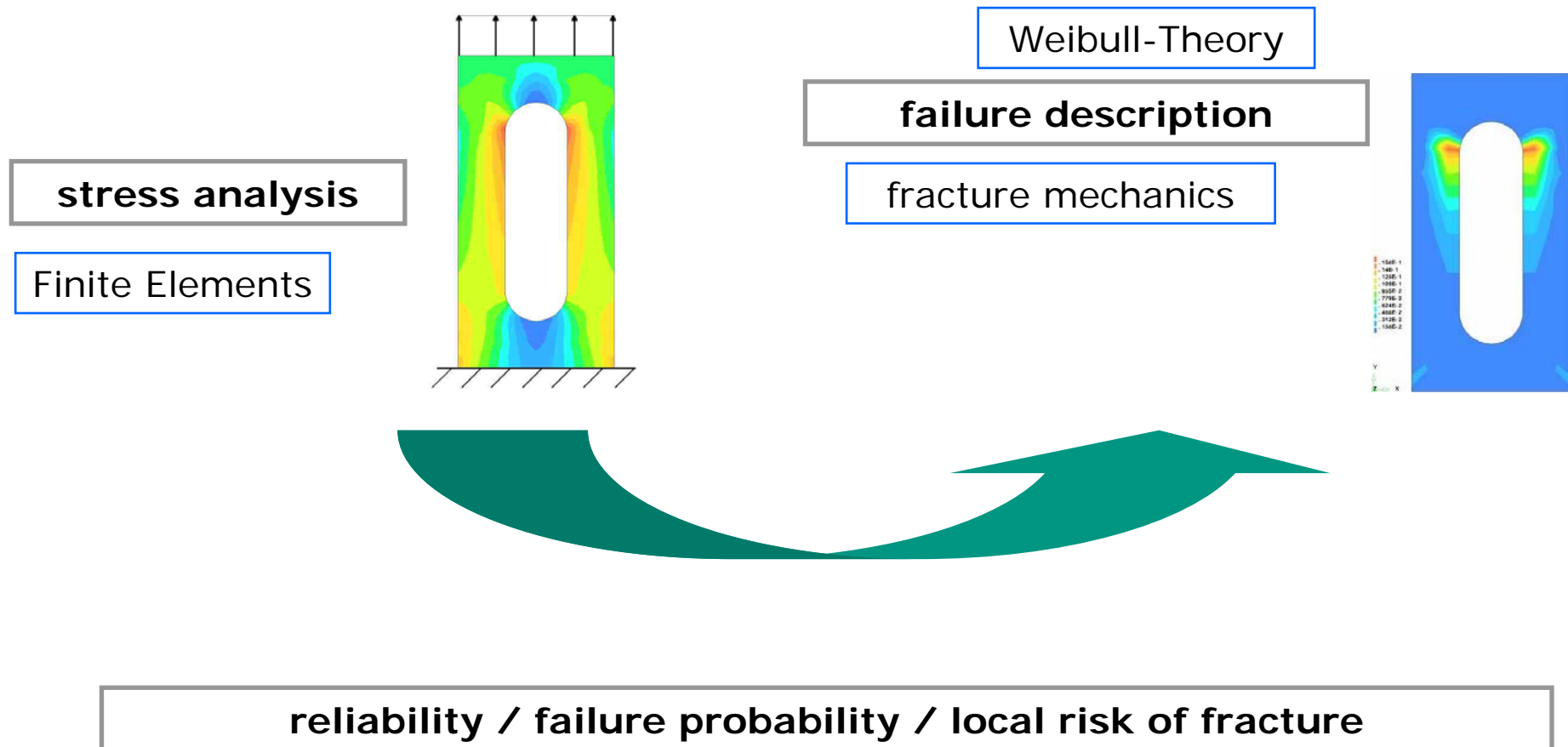
$$P(FK) = \frac{1}{V} \int_{V_t} \frac{1}{4\pi} \int_{\Omega} (1 - F_a(a_c)) \, d\Omega \, dV.$$

and thus:

$$\pi(\vec{x}) = \frac{\frac{1}{4\pi} \int_{\Omega} \left(\frac{\sigma_{eq}}{\sigma_0}\right)^m \, d\Omega}{\frac{1}{V} \int_V \frac{1}{4\pi} \int_{\Omega} \left(\frac{\sigma_{eq}}{\sigma_0}\right)^m \, d\Omega \, dV}$$



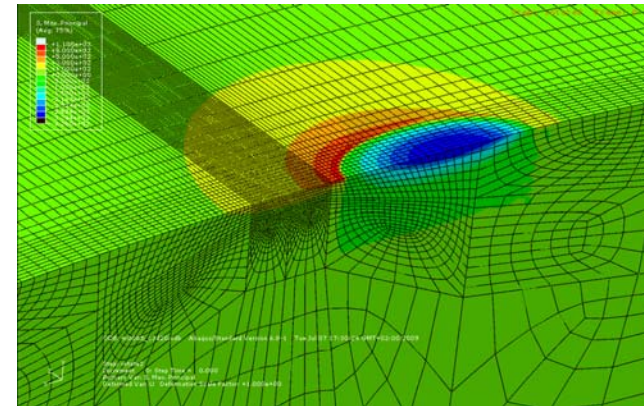
# The basic idea of STAU (FE interface)



# The interface to Finite Elements

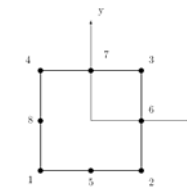
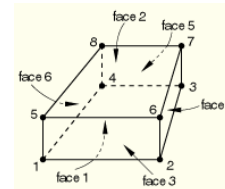
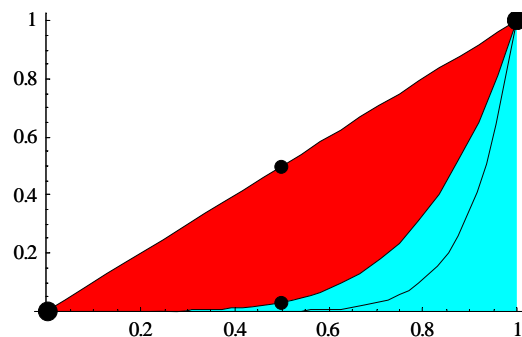
what we have to calculate (simple case):

$$P_f = 1 - \exp \left[ - \frac{1}{V_0} \int_V \frac{1}{4\pi} \int_{\Omega} \left( \frac{\sigma_{eq}(x, y, z, \alpha, \beta)}{\sigma_0} \right)^m d\Omega dV \right]$$



from Finite Element stress analysis we obtain stress tensor at node  $n$ :

$$\sigma_{ij}(x_n, y_n, z_n)$$



large difference (red) between linear interpolation and  $m=5 \dots 10$  curves!

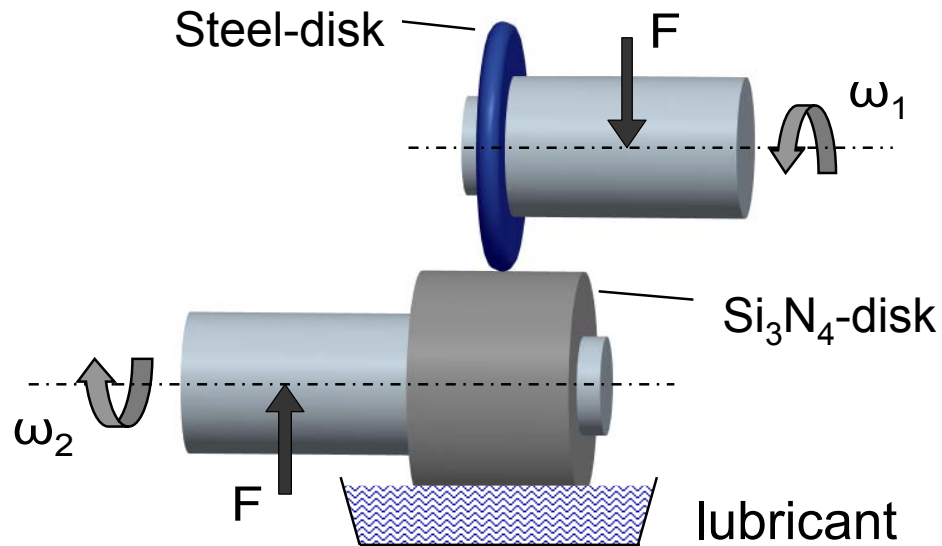
→ integration of  $\sigma^m$  would be very inaccurate!

we use the interpolation functions to generate additional integration points

# The options for Finite Element models

geometry:	2D model (plane stress, plane strain) 3D model axisymmetric model
analysis:	surface flaws volume flaws interfaces
options:	spontaneous fracture sub-critical crack propagation cyclic crack propagation stress gradients R-curve behaviour <i>(not all to combine!)</i>

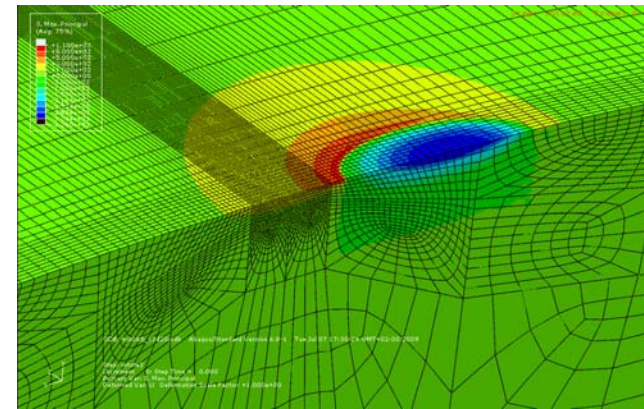
# Results: Rolling contact fatigue (RCF) test



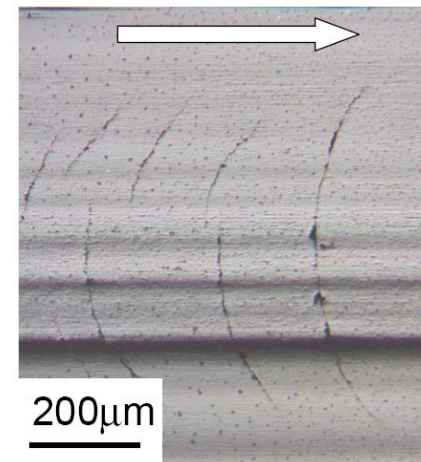
- lubricant: friction coefficient  $\mu=0.085$
- $F=1700\text{N}$
- relative slip:  $\sim 22\%$
- max. principal stress:  $\sim 1100\text{ MPa}$

RCF tests: Iyas Khader, Fraunhofer Institute IWM, Freiburg

Stress distribution

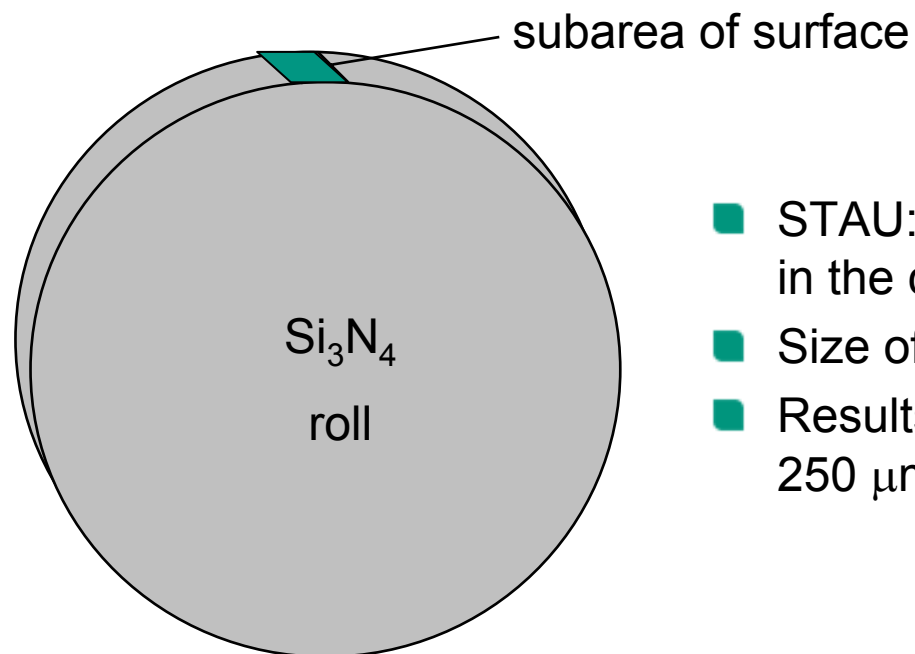
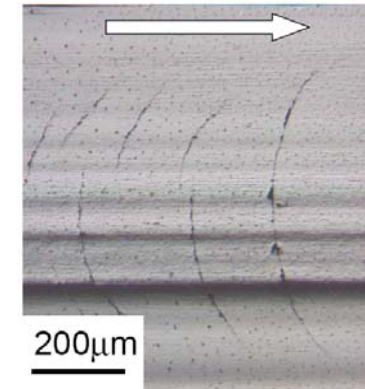


Damage after  $10^5$  rotations



## Results: STAU analysis

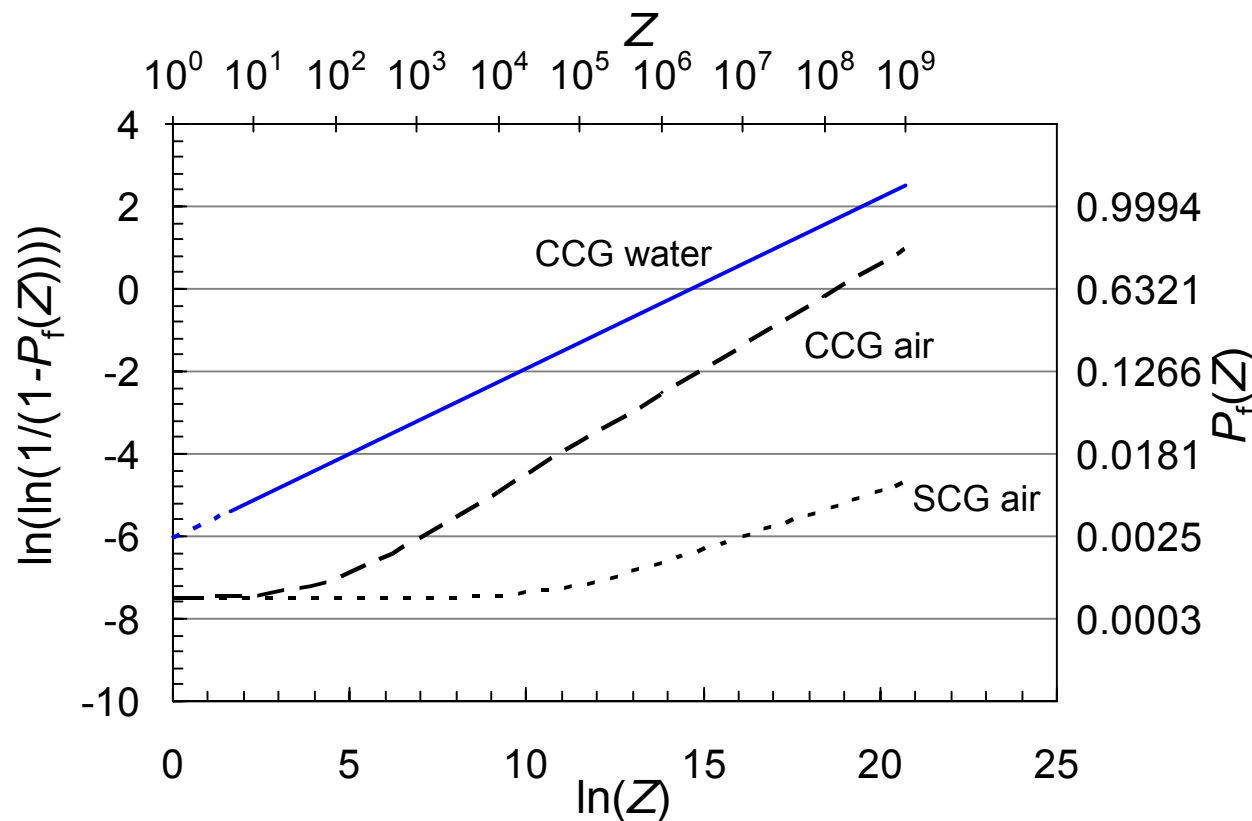
- Contact damage: initiation of macroscopic flaws
- Predicting of a certain flaw density on the surface



- STAU: probability of the initiation of one flaw in the considered subarea
- Size of subarea ↔ crack density
- Results refer to crack density of 1 crack per 250 μm along the circumference

# Results: Failure probability

- Probability to initiate one macroscopic crack every 250 μm



- Weibull CDF

$$P_f = 1 - \exp \left[ - \left( \frac{Z}{N_0} \right)^m \right]$$

$m$  – slope of the curve

$N_0$  - characteristic lifetime  
(63%-quantile)

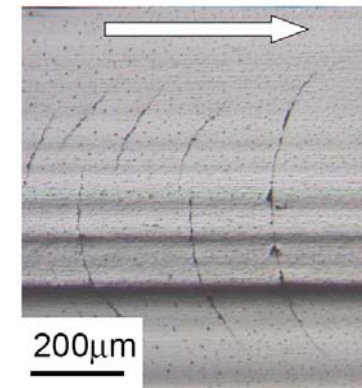
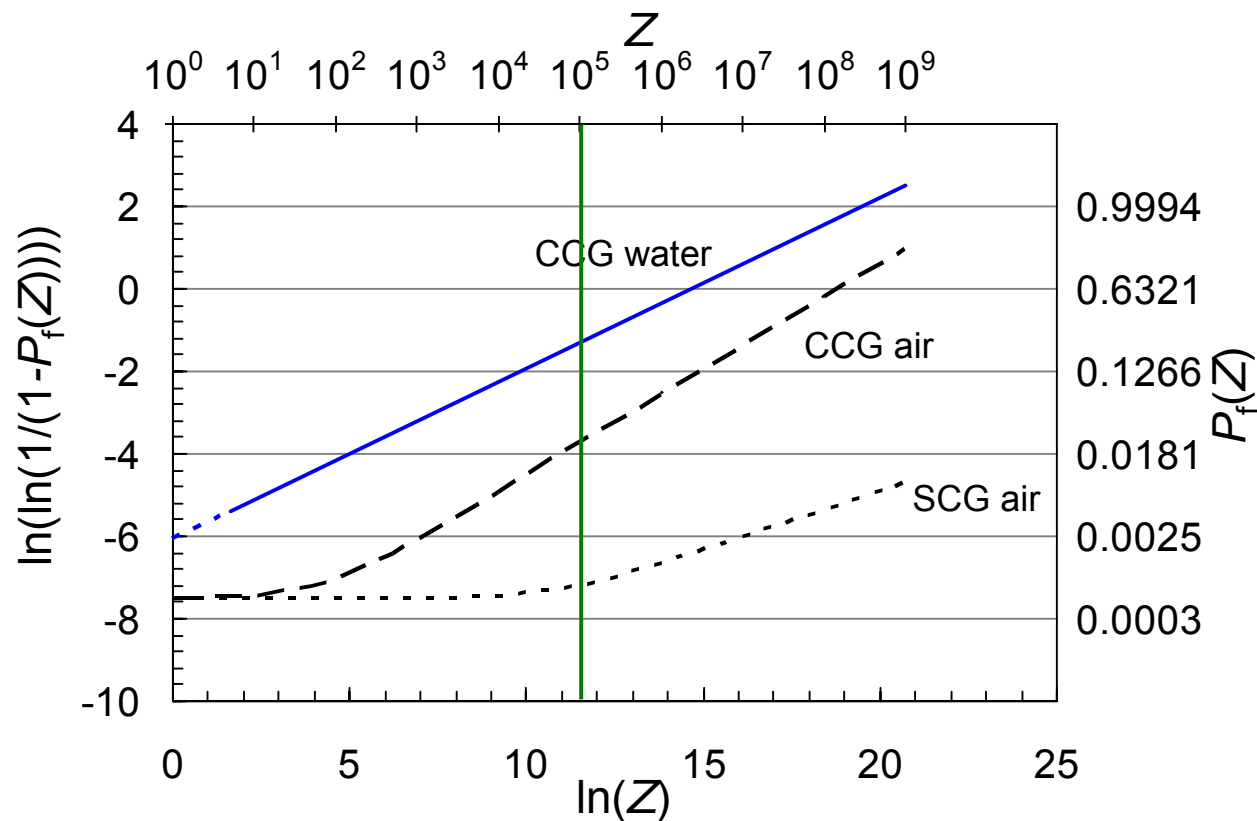
$Z$  – no. of rotations

- Highest failure probability obtained for fatigue parameters in water.



# Results: Failure probability

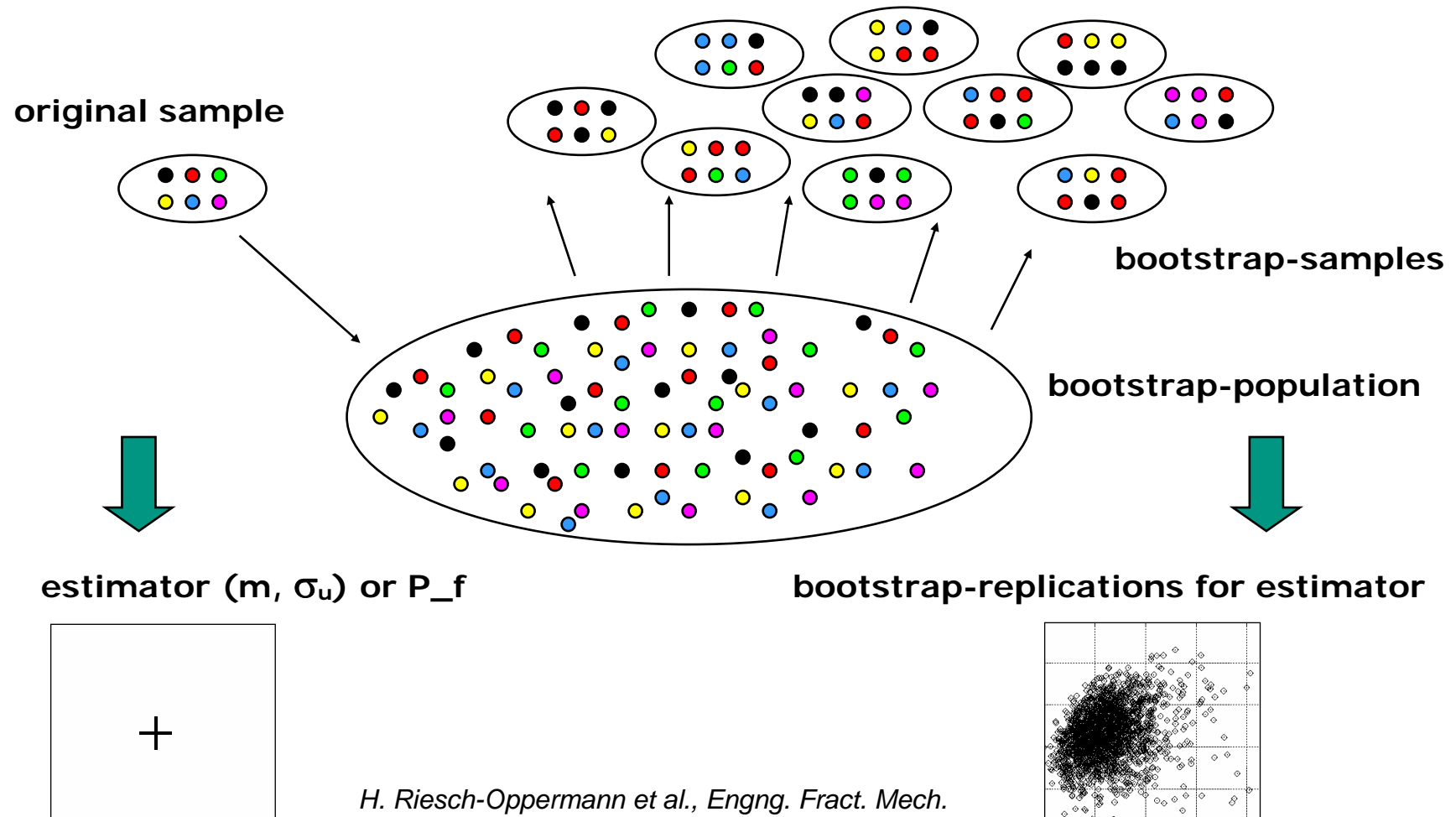
- Relation with experimental crack density after 10 h



- Initiation probability low for parameters in (air)

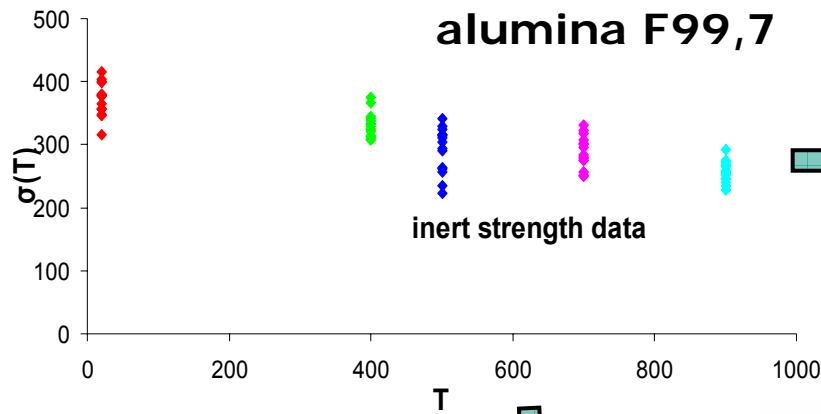
# Bootstrapping: assessing the uncertainty by resampling

Use original sample to get confidence intervals for failure probability



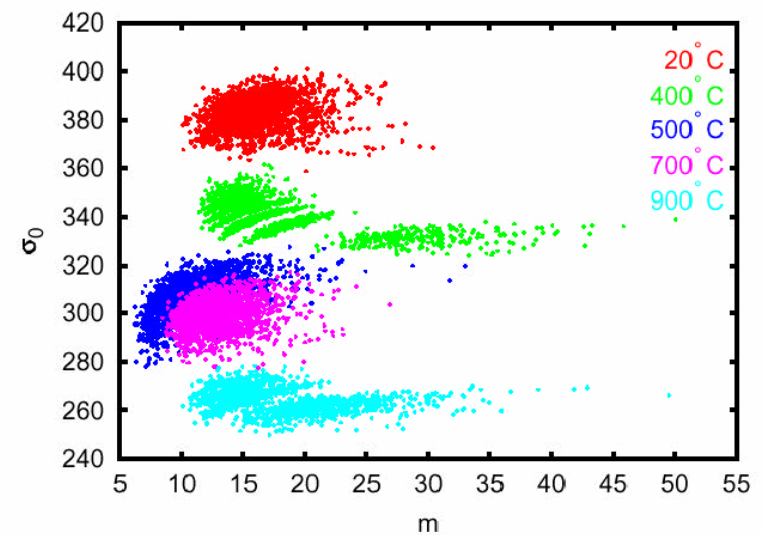
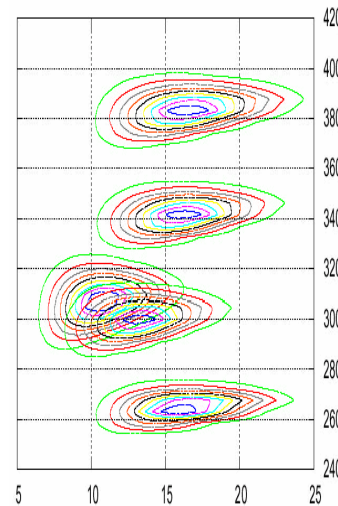
*H. Riesch-Oppermann et al., Engng. Fract. Mech.*

# Assessment of material uncertainties – statistical evaluation



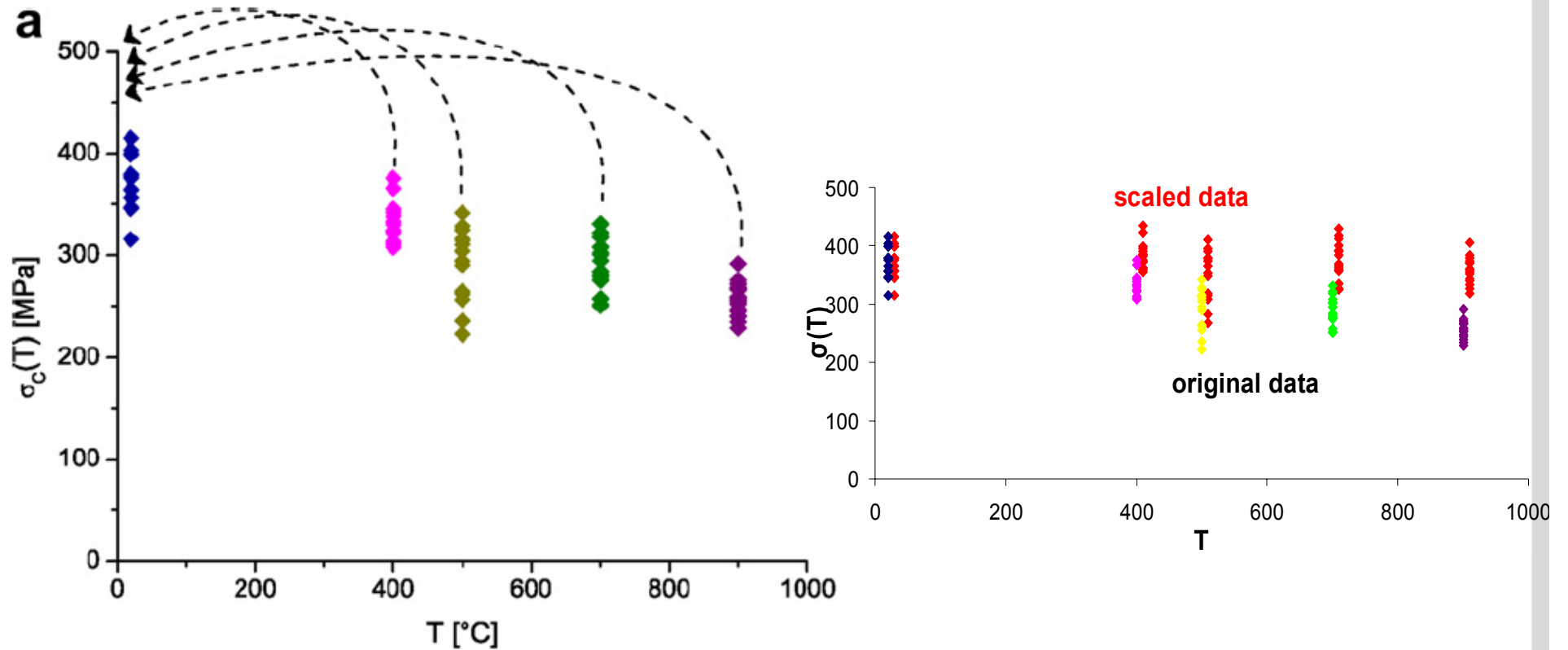
**bootstrap  
resampling**

**Bayesian posteriori  
analysis**  
(generalized Maximum-  
Likelihood method)



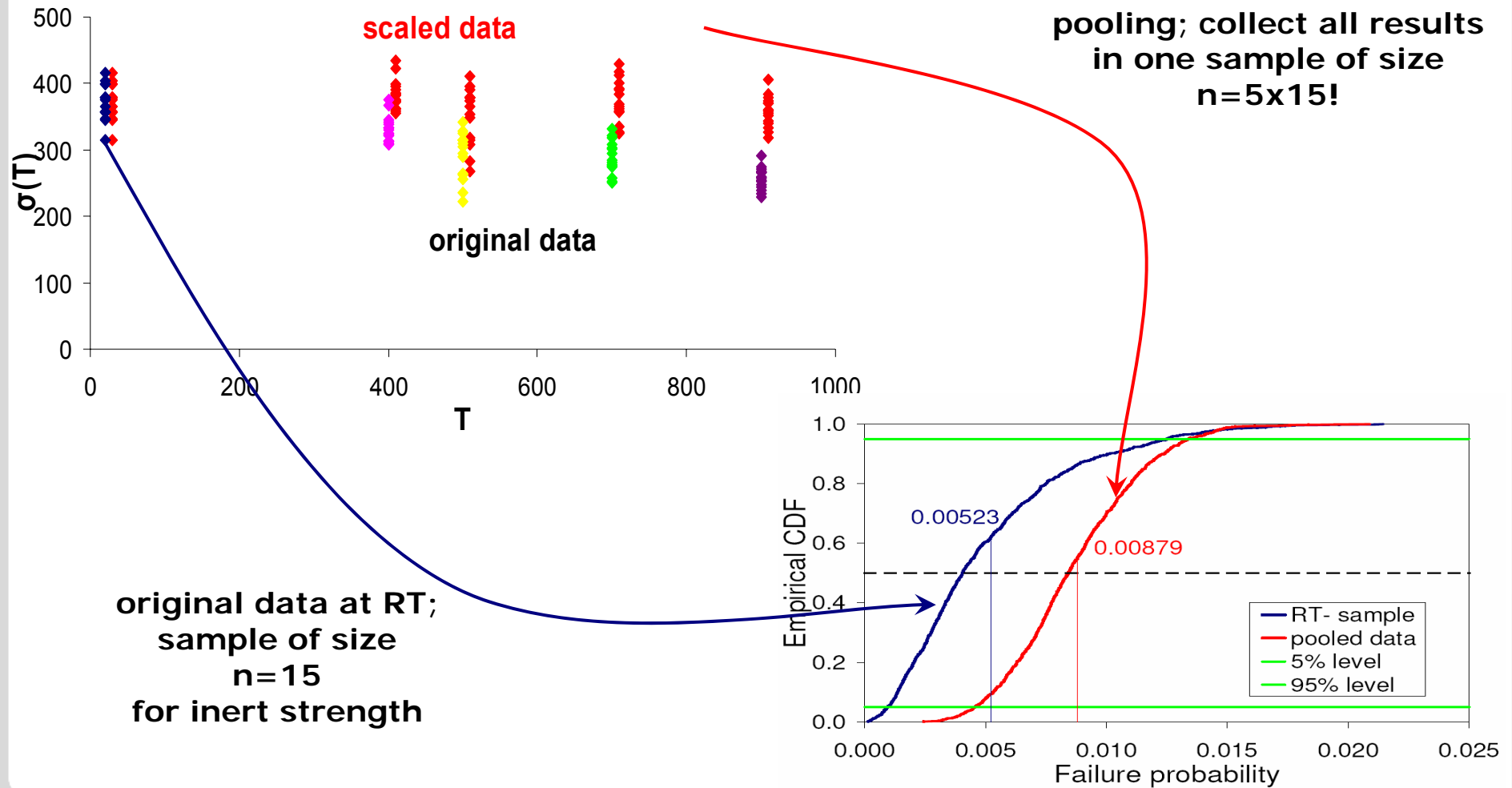
# Pooling: reduction in uncertainty by combining samples

Scaling of strength data to ambient temperature

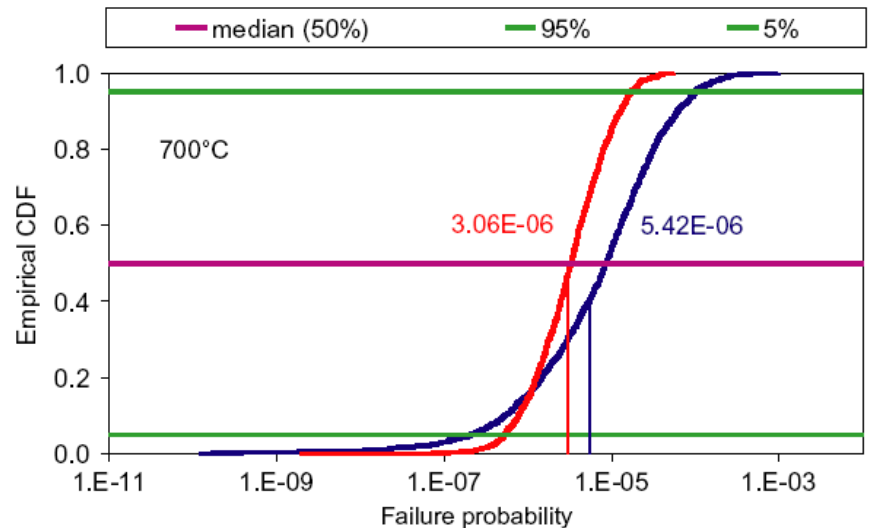
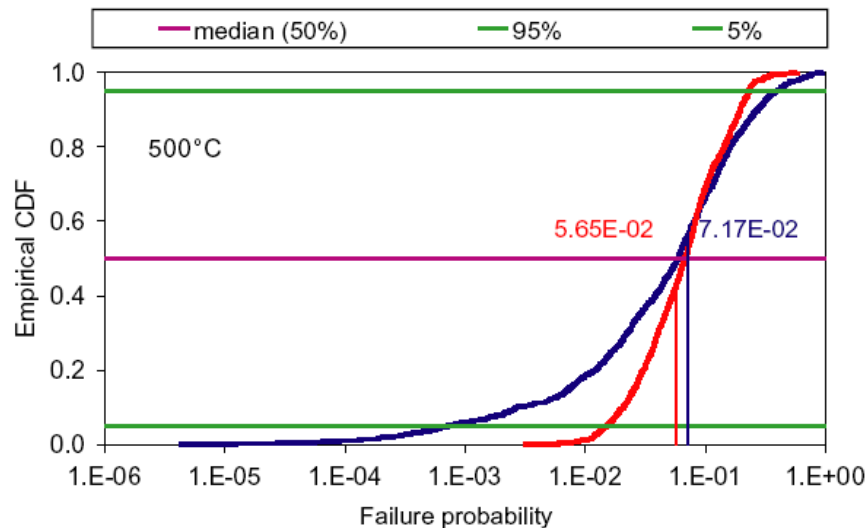
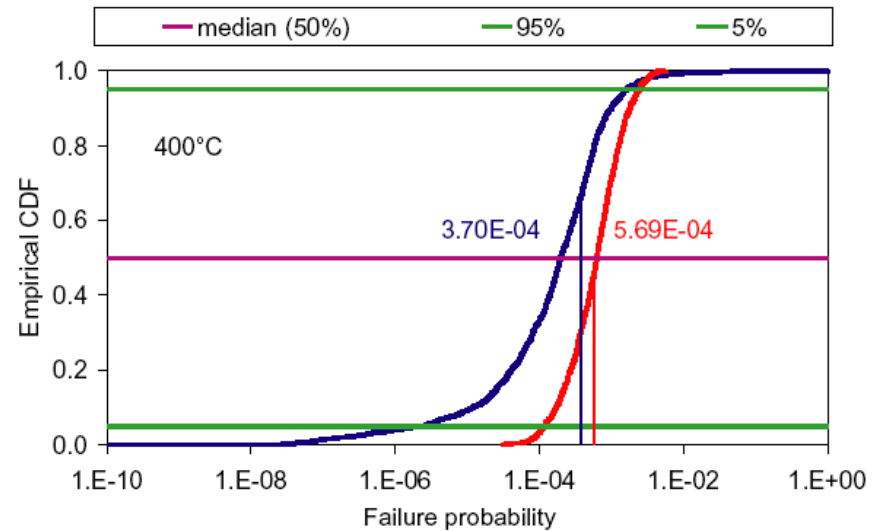
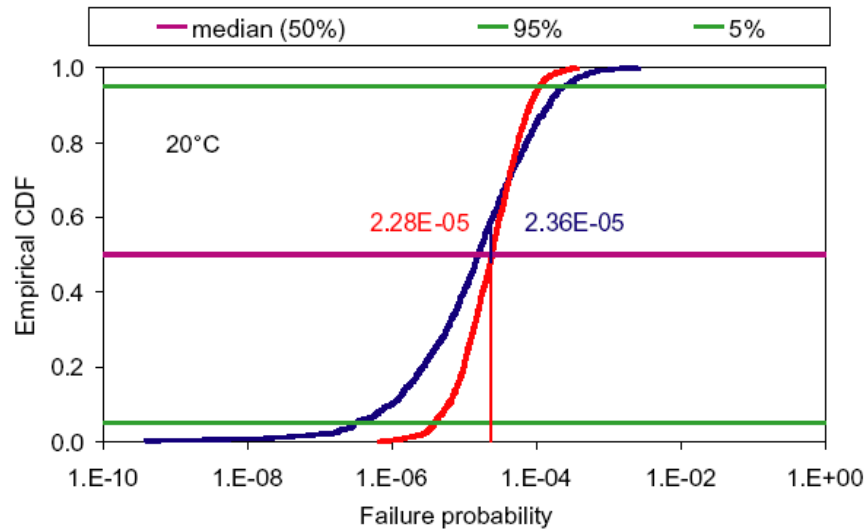


Sample size enlarged by pooling

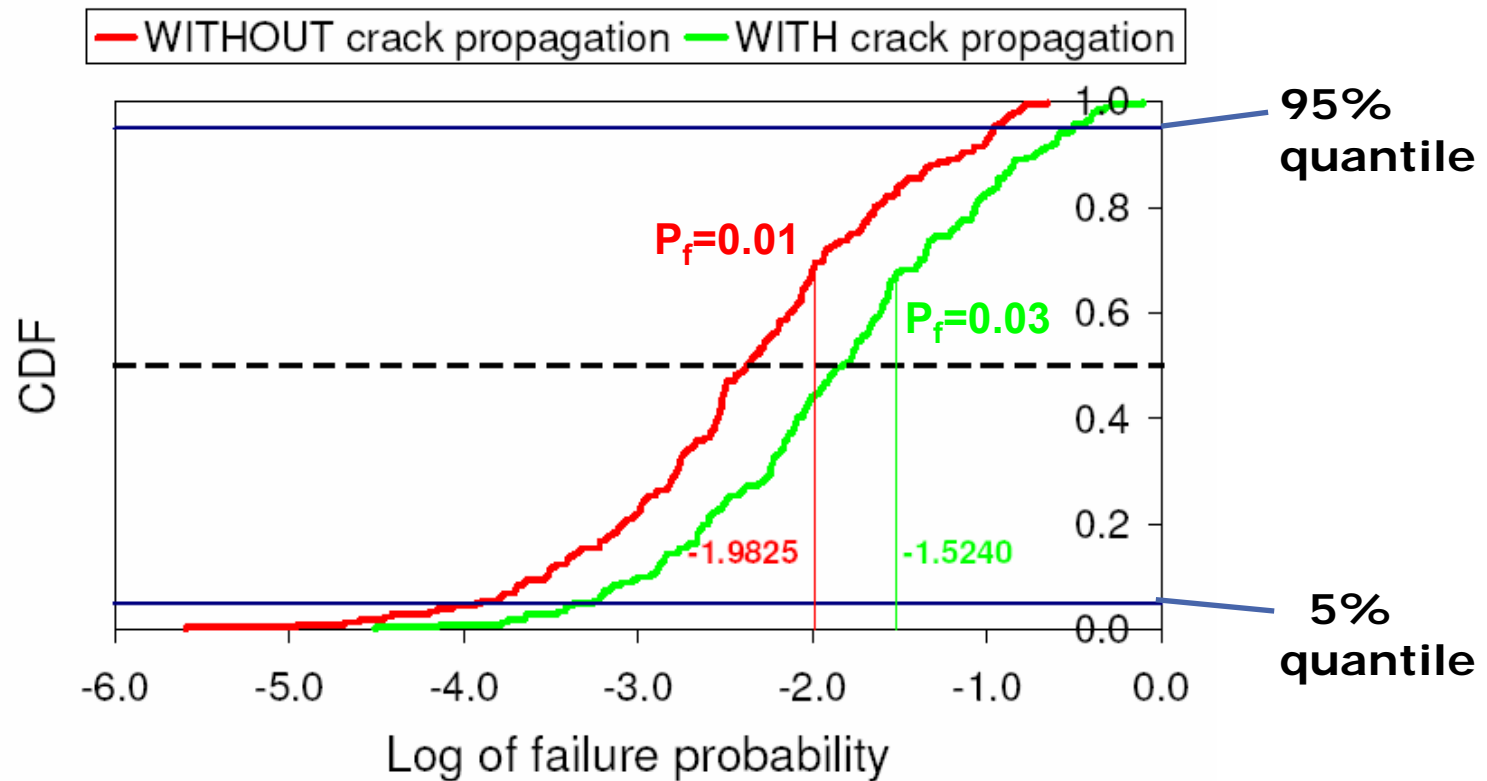
# Reduction of scatter by intelligent pooling – ceramic component



# Uncertainty assessment and reduction by pooling & resampling



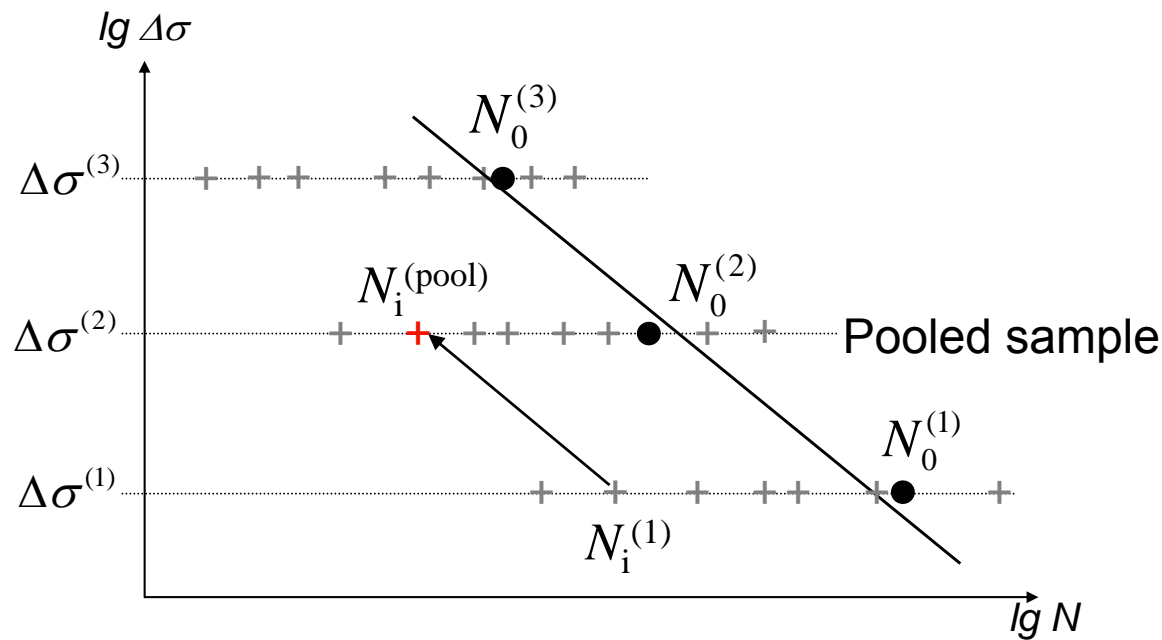
# Prediction of scatter in Pf – bootstrap results



**note: large impact of crack propagation and 2-3 mag's uncertainty in results!**

# Pooling: reduction in uncertainty by combining samples

- Increase number of data available for one load level



- Conversion using Weibull-distribution:

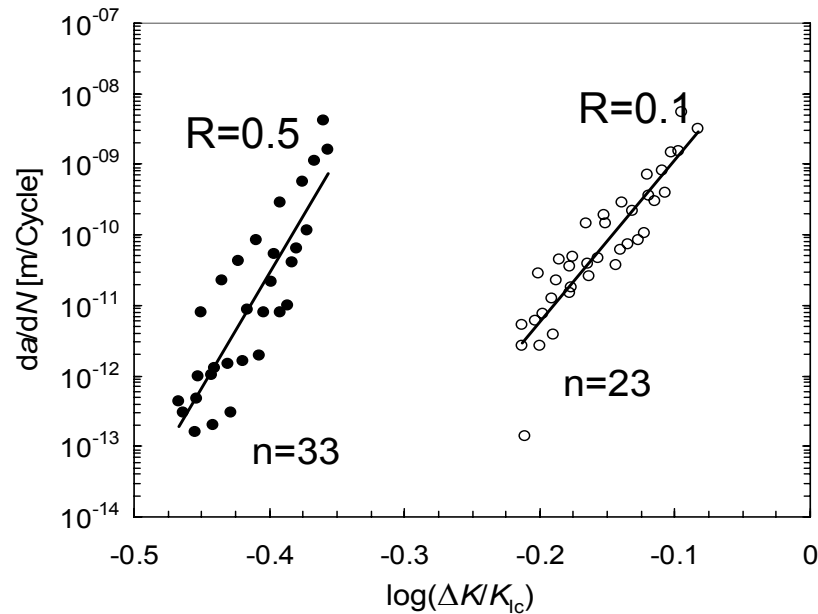
$$N_i^{(pool)} = N_i^{(1)} \left( \frac{N_0^{(pool)}}{N_0^{(1)}} \right)$$

- Relation between  $\Delta\sigma$  and  $N_0$  follows from S-N-curve fit

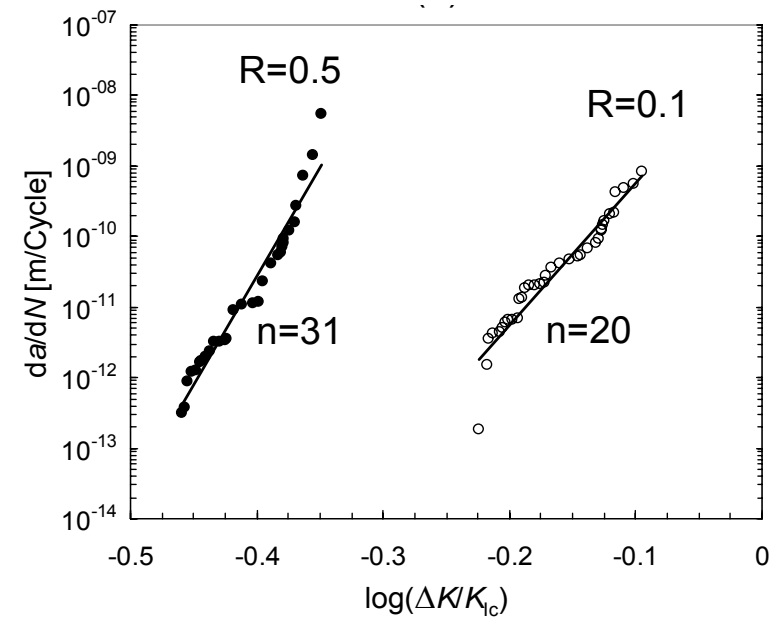


# Pooled crack growth curves

## unpooled



## pooled



- Scatter (uncertainty in  $n$ ) is decreased by pooling
- variation of  $n$  with  $R$  remains

M. Härtelt et al., J.Am.Ceram.Soc., (2011), in press

# Summary

- Ceramics
- WLT statistics
- fracture mechanics
- the role of microstructure
  
- pooling:           using data efficiently  
                          getting an idea about possible inhomogeneities
  
- uncertainties: (bootstrap) and Bayes
  
- (modelling uncertainties)

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