German Aerospace Center (DLR e.V.)
Institute of Test and Simulation for Gas Turbines, Augsburg

Size Effect in Intermetallics: Experiments and Numerics

Dr.-Ing. Arun Raina

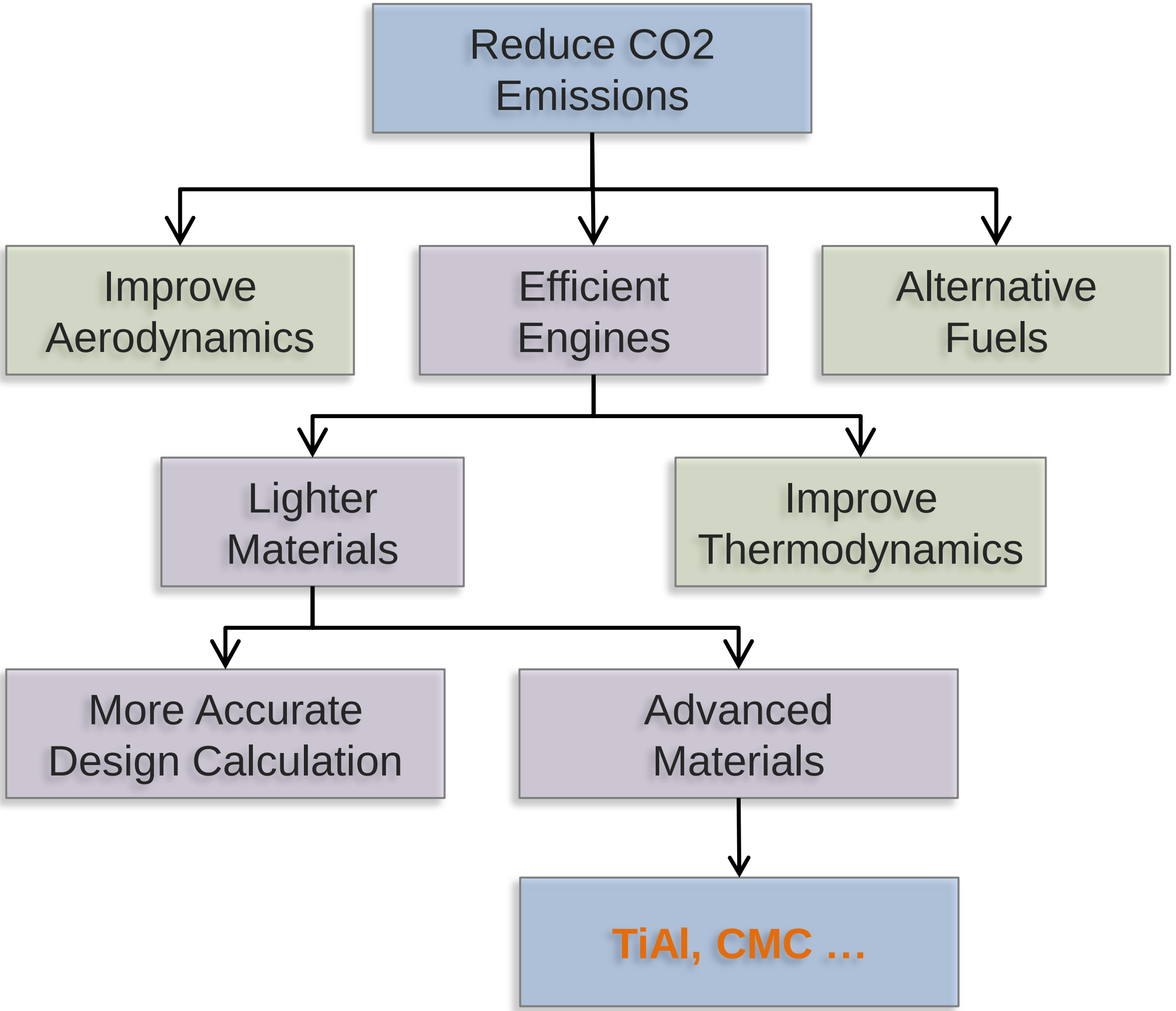
DLR

Contents

Contents

Motivation

- Aviation accounts for ≈ 2.1% of global CO_2 emissions - roughly equivalent to Germany's total emissions [1].
- EU aims to reduce its domestic CO_2 emissions by 80% by 2050 compared to 1990 levels [2].
- For aviation industry, goal is halving aviation CO_2 emissions relative to 2005 levels by 2050 [3].

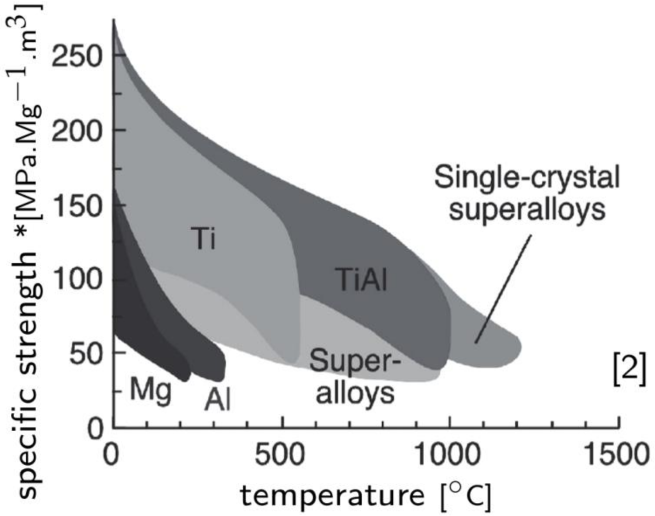


[1] EPRS BRI(2017)603925_EN. [2] EUR-Lex - 52011DC0112 (2011) [3] EUR-Lex - 32017R2392.

Background

Why Intermetallics?

[1] Rolls-Royce



	σ_{UTS} [MPa]	σ_Y [MPa]	ρ [g/cm^3]	σ_{UTS}/ρ [*]	E [GPa]	ε_f [%]	T_{oxid} [°C]
Stainless Steel AISI 304 [3]	505	215	8	63	200	70	850
Ni-based super alloy [4]	1500	1200	8.5	176	210	35	900
Titanium Aluminide [5]	600	450	3.8	158	170	<1	1000

[2] Appel et al. (2011) [3] asm.matweb.com [4] Pollock & Tim (2006) [5] Kim (1989)

Overview

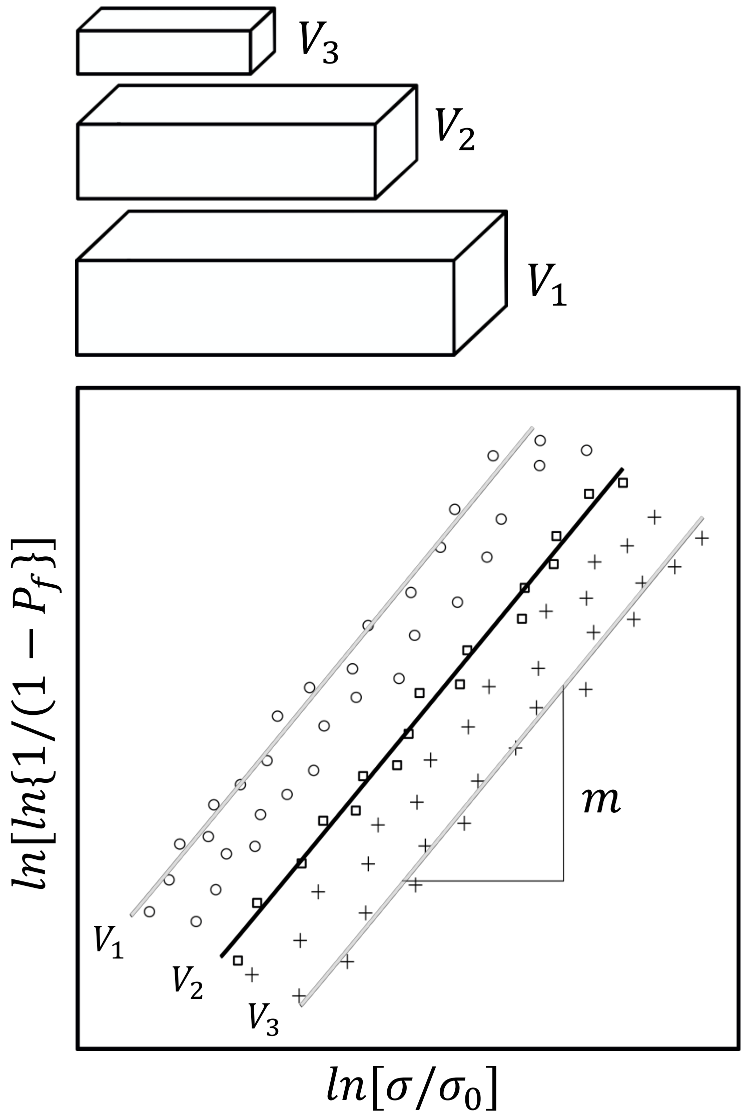
Weakest link Weibull model

- Failure probability[1] is written as

$$P = 1 - \exp\left\{- \int \mathfrak{s}(\sigma) dV\right\}$$

$$\mathfrak{s}(\sigma) = \frac{1}{V_0} \cdot \left(\frac{\sigma}{\sigma_0}\right)^m$$

- Empirical relation for stochastic failure strength
- Empirical relation for volume effect
- FE implementation tells if – not – where failure occurs!
- Scaling may not be applicable to all materials e.g. TiAl, CMC
- Failure probability in terms of fracture energy more suitable for materials with SSY.



[1] Weibull (1951)

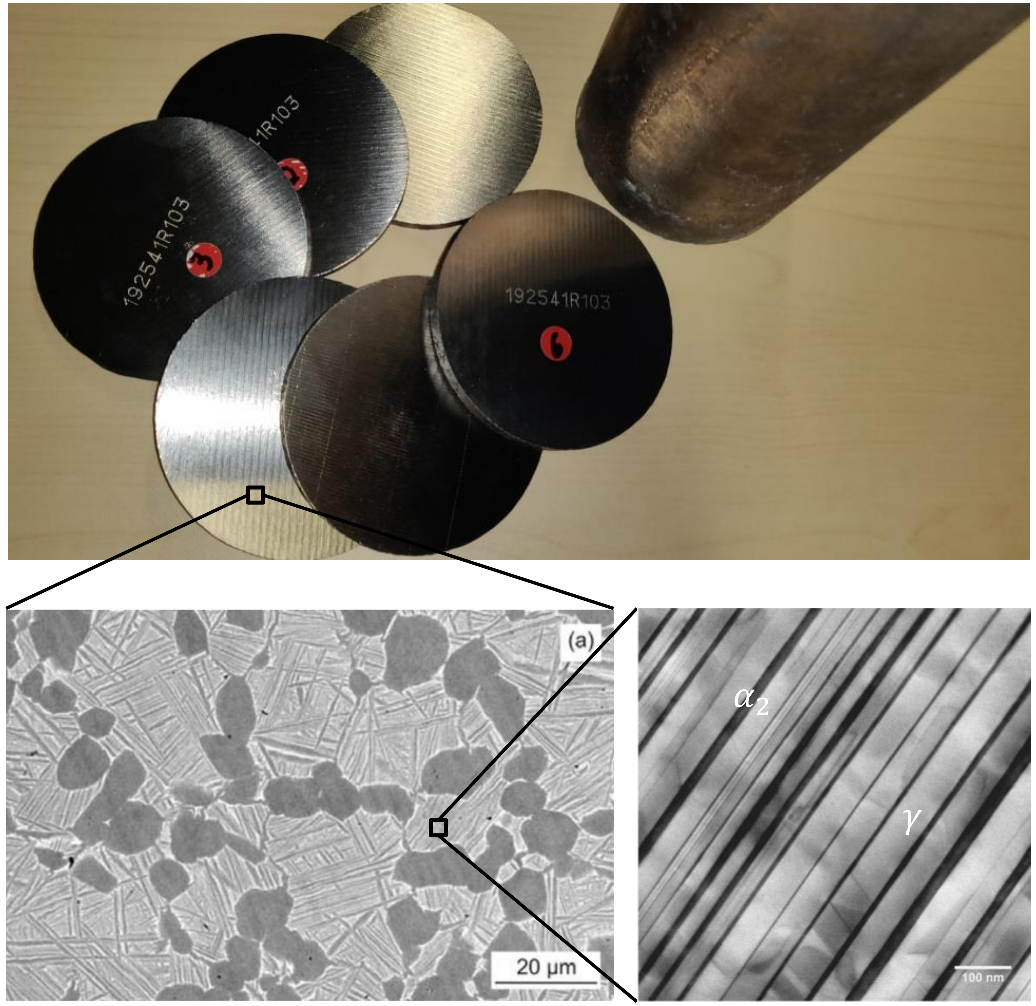
Contents

Titanium Aluminide alloy as test material

- Titanium Aluminide (TiAl) Typ GE48-2-2
- Titanium Aluminium Chromium Niobium

  48 : 48 : 2 : 2 at% and 59.8 : 32.8 : 2.55 : 4.85 wt%
- TiAl 48-2-2 remelt stocks are manufactured by Vacuum Arc Remelting (VAR)
- Manufacturer provided properties:

Fracture toughness	15 – 18 MPa$\sqrt{\mathrm{m}}$
Fracture strength	450 – 500 MPa
Density	3.97 g/cm^3
Hardness	285 HV10
Young's Modulus	160 GPa
Yield strength	430 MPa



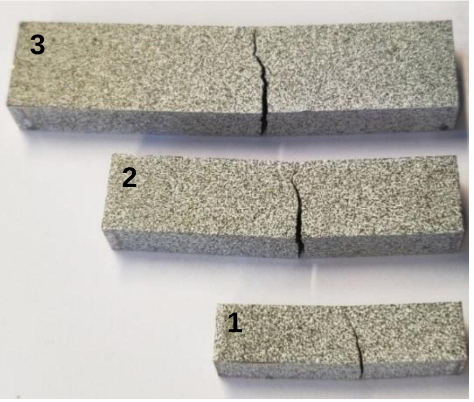
Duplex with lamellar colonies

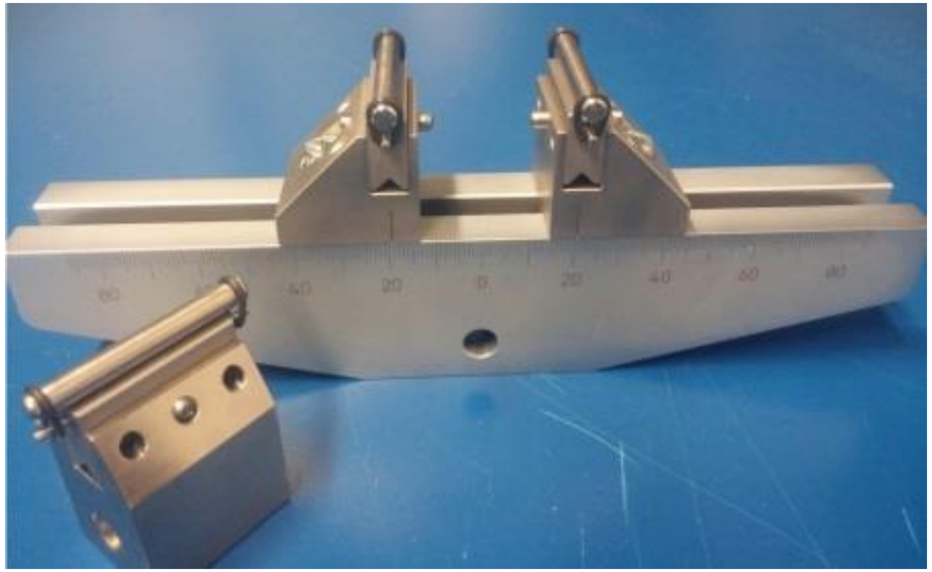
Specimen preparation and test configuration

- Three point bending tests are performed
- Specimens are cut using the Electrical Discharge Machining process.
- Dimensional tolerance and surface finish as per ASTM E399.
- For each specimen, force and DIC data are recorded. Strain rate fixed at 0.5% min^{-1}.
- Three geometrically identical sizes are selected.

	Length (L)	**Height** (H)	**Width** (B)	**Count** (n)
Size 1	25.2	6.0	6.0	11
Size 2	37.8	9.0	6.0	14
Size 3	50.4	12.0	6.0	4

All dimensions in mm





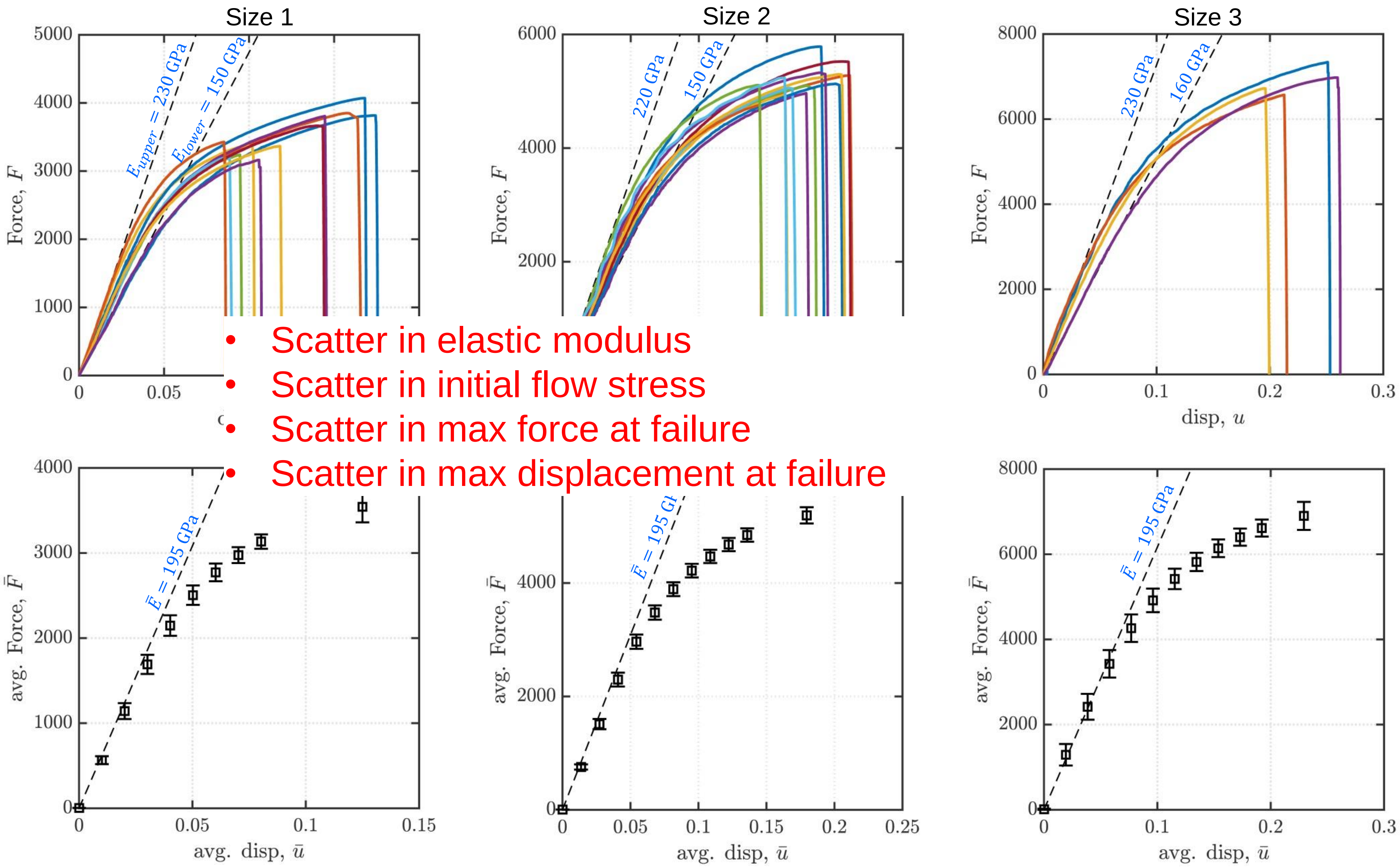
Force displacement data

Experiment data
Upper and lower bounds for elastic modulus are computed using analytical relation

$$u = \frac{FL^3}{48EI} + \frac{FLH^2}{40GI}$$

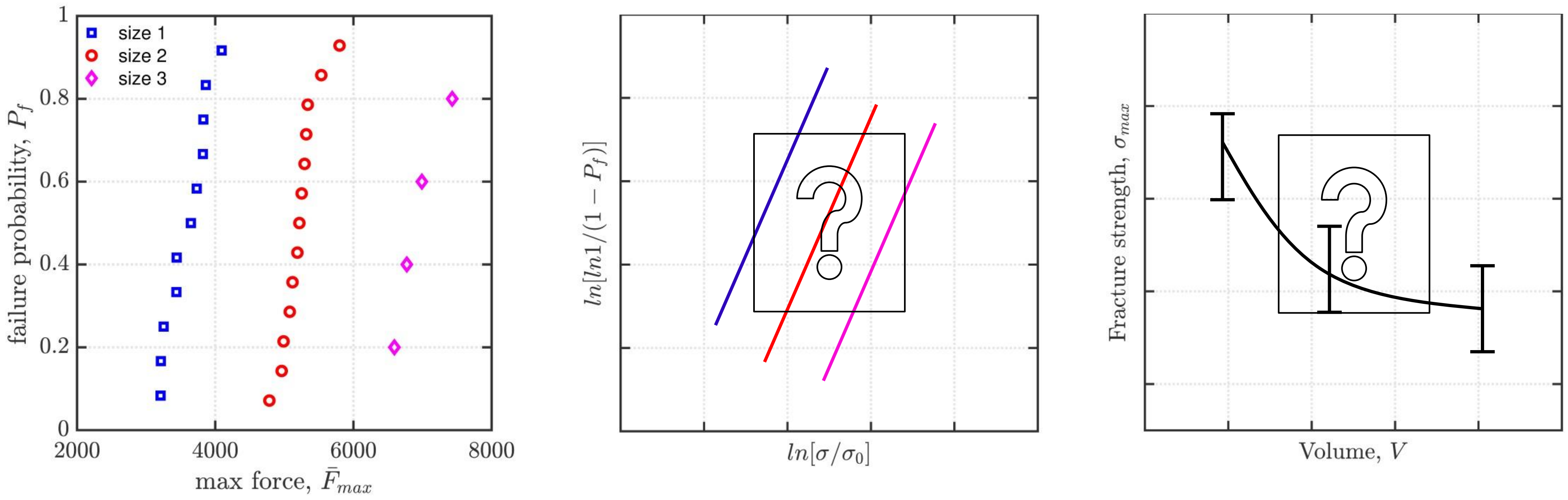
Averaged data
95 % confidence intervals are computed as

$$CI = \pm 1.96 \frac{sd}{\sqrt{n}}$$



- Scatter in elastic modulus
- Scatter in initial flow stress
- Scatter in max force at failure
- Scatter in max displacement at failure

Distribution in fracture stress



- Cumulative density function for failure probability is obtained from sorted sample of size N as [1]

$$P_f = \frac{i - 0.3}{N + 0.4}$$

- Analytical relation for flexural stress is only valid in linear elastic region

$$\sigma = \frac{3FL}{2BH^2}$$

[1] C. Przybilla et al (2011)

Contents

DLR

Phase field modeling of elastic-plastic fracture [1]

$\boldsymbol{\varepsilon}$, total strain
$\boldsymbol{\varepsilon}^{\mathrm{p}}$, plastic strain
α, equi. Plastic strain
d, crack phase field

- Define the space-time accumulated work density as

$$\mathcal{W} = \int_V \left(\int_0^T \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} \, dt \right) dV = \int_V \left[\underbrace{\widehat{W}(\mathfrak{C})}_{\text{rate-indep.}} + \underbrace{\mathfrak{D}}_{\text{rate-dep.}} \right] dV$$

where $\mathfrak{C} = \{\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^{\mathrm{p}}, \alpha, \nabla\alpha, d, \nabla d\}$ is the constitutive set.

- Make the energetic-dissipative split

$$\widehat{W} = \underbrace{\psi^e(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{\mathrm{p}}, d)}_{\text{stored energy}} + \underbrace{\mathcal{D}^{pf}(\alpha, \nabla\alpha, d, \nabla \mathrm{d})}_{\text{dissipation}}$$

- Stored energy takes the form

$$\psi^e(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{\mathrm{p}}, d) = g(d) w_e = g(d) \left[\frac{\kappa}{2} \mathrm{tr}^2[\boldsymbol{\varepsilon}^e] + \mu \, \mathrm{tr}[\mathrm{dev}(\boldsymbol{\varepsilon}^e)^2] \right]$$

- Dissipation due to gradient-plasticity and fracture takes the form

$$\mathcal{D}^{pf}(\alpha, \nabla\alpha, d, \nabla d) = g(d) w_p(\alpha, \nabla\alpha) + \big(1 - g(d)\big) w_c + 2 l_f \gamma(d, \nabla d) w_c$$

[1] C. Miehe, F. Aldakheel, A. Raina (2016)

Phase field modeling of elastic-plastic fracture [1] …

- Define a dissipation potential function

$$\widehat{\mathrm{V}}(\dot{\mathfrak{C}}) = \underbrace{\sup}_{\boldsymbol{f}^p, r^p, f^f - r^r} \underbrace{\sup}_{\lambda^p, \lambda^f} \left[\boldsymbol{f}^p : \dot{\boldsymbol{\varepsilon}}^p - r^p \dot{\alpha} + \left(f^f - r^r\right)\dot{d} - \lambda^p \phi^p - \lambda^f \phi^f\right]$$

$$\begin{aligned} \boldsymbol{f}^p &= -\partial_{\boldsymbol{\varepsilon}^p}\psi^e \\ r^p &= \delta_\alpha \mathcal{D}^{pf} \\ f^f &= -\partial_d \psi^e \\ r^r &= \delta_d \mathcal{D}^{pf} \end{aligned}$$

- Define the global rate potential of coupled gradient-plasticity-gradient damage

$$\Pi = \int_V \left(\int_t \frac{d}{dt}\widehat{W}(\mathfrak{C}) + \widehat{\mathrm{V}}(\dot{\mathfrak{C}})\right) - \mathcal{P}_{ext}(\dot{\boldsymbol{u}})$$

- The global *minimization* of the *multi-field problem* yields the primary unknowns

$$\left\{\dot{\boldsymbol{u}}, \dot{\alpha}, \dot{d}, \dot{\boldsymbol{\varepsilon}}^p\right\} = \mathrm{Arg}\left\{ \underbrace{\inf}_{\dot{\boldsymbol{u}}, \dot{\alpha}, \dot{d}, \dot{\boldsymbol{\varepsilon}}^p} \Pi \right\}$$

- Of particular interest is the Euler equation derived for the evolution of phase field fracture

$$\dot{d} = (1-d)\mathcal{H} - [d - l_f^2 \Delta d] \qquad \textit{where} \qquad \mathcal{H} = \underbrace{\max}_{s \in [0,t]} \mathfrak{P} \geq 0$$

- The dimensionless *crack driving state function* is

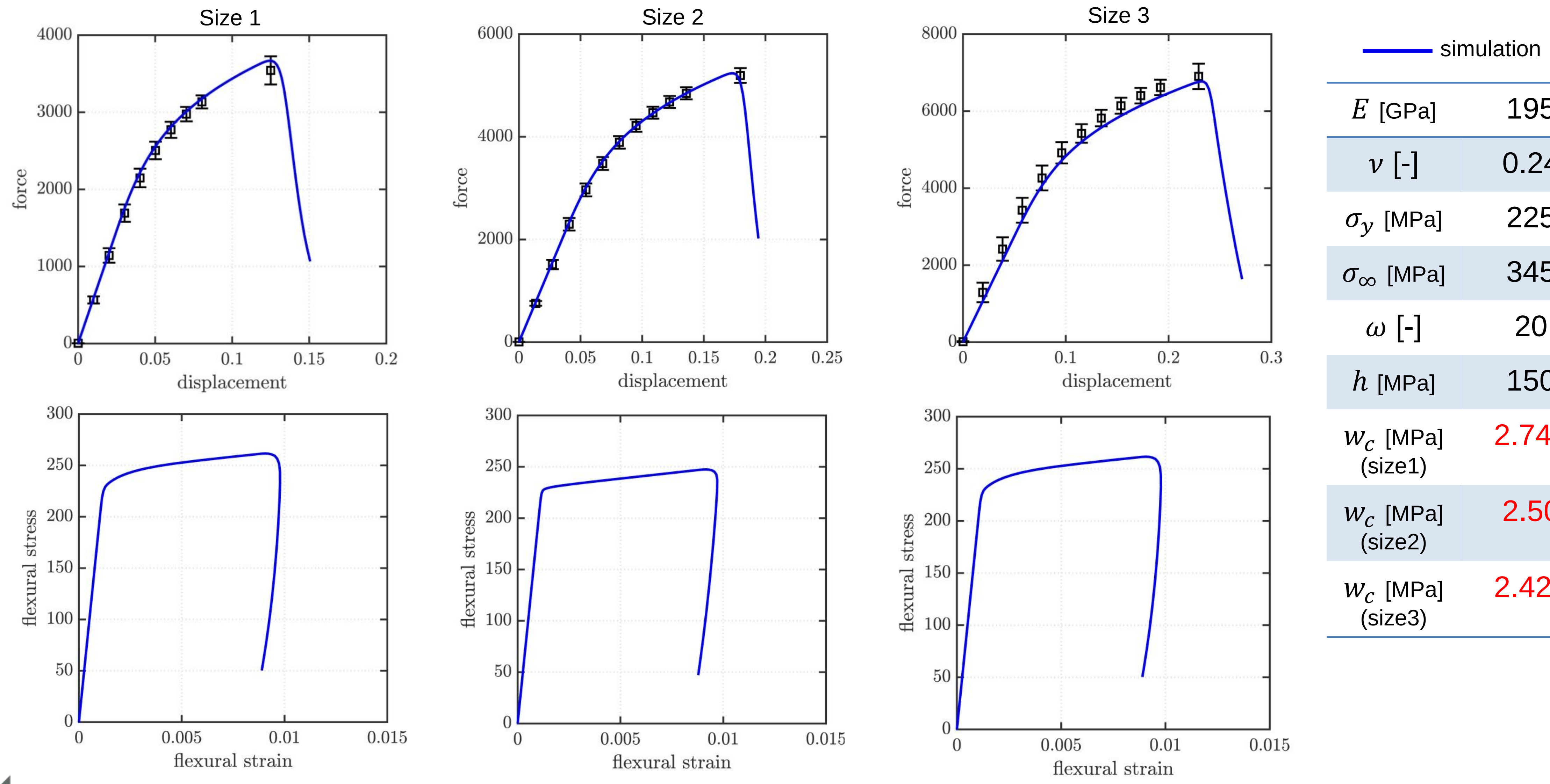
$$\mathfrak{P} = \left\langle \frac{w_e(\boldsymbol{\varepsilon}^e) + w_p(\alpha, \nabla\alpha)}{w_c} - 1 \right\rangle$$

[1] C. Miehe, F. Aldakheel, A. Raina (2016)

DLR

Contents

Simulations of average 3PB response

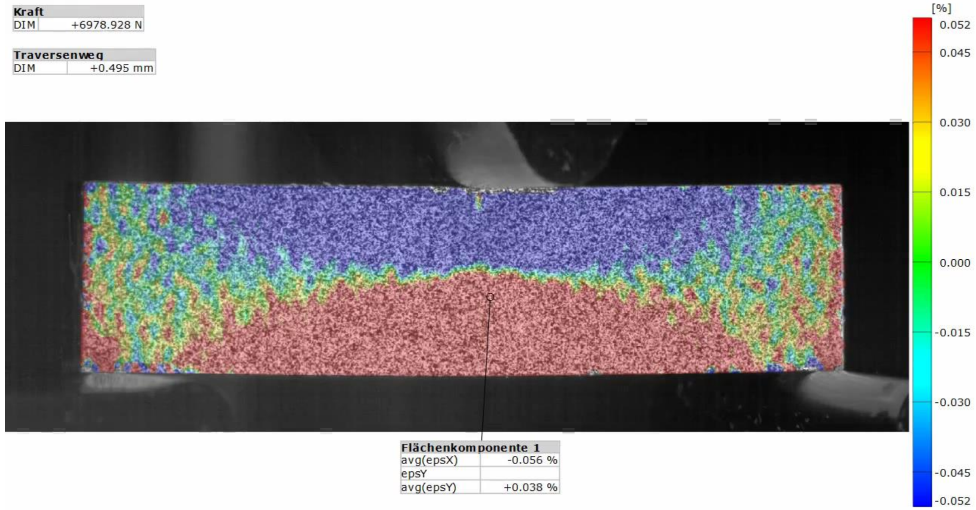


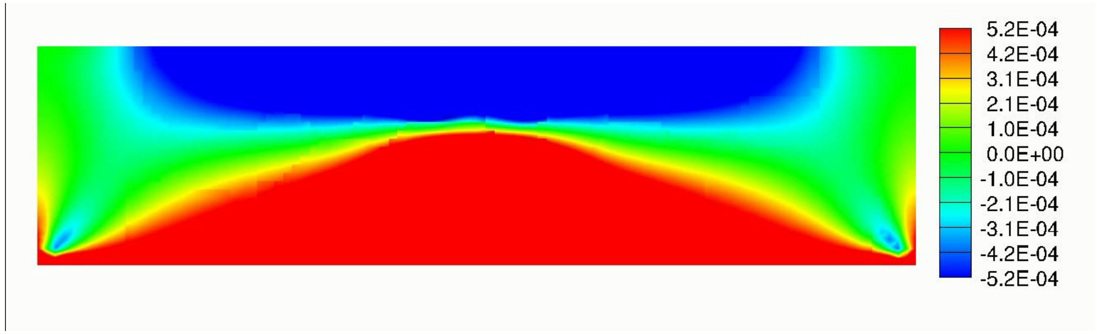
E [GPa]	195
ν [-]	0.24
σ_y [MPa]	225
σ_∞ [MPa]	345
ω [-]	20
h [MPa]	150
w_c [MPa] (size1)	2.749
w_c [MPa] (size2)	2.50
w_c [MPa] (size3)	2.425

DLR

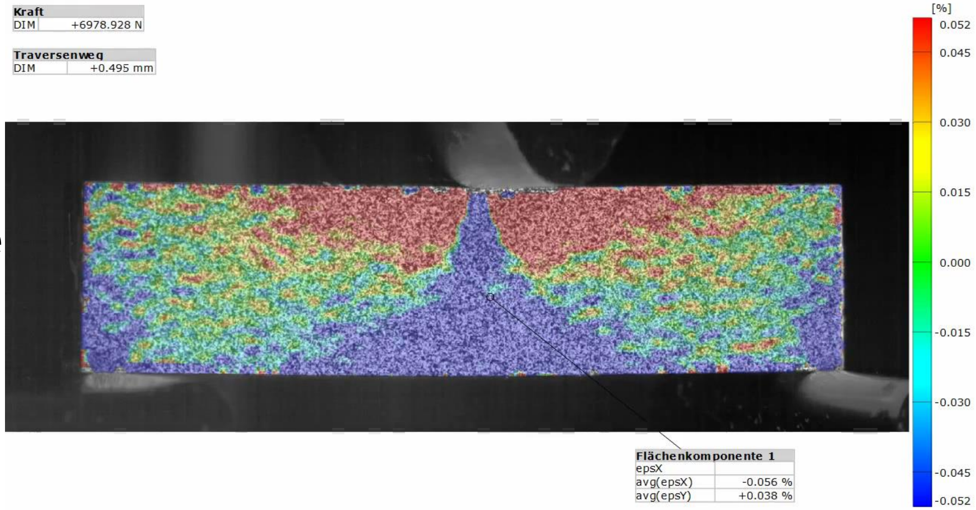
Validation with DIC data

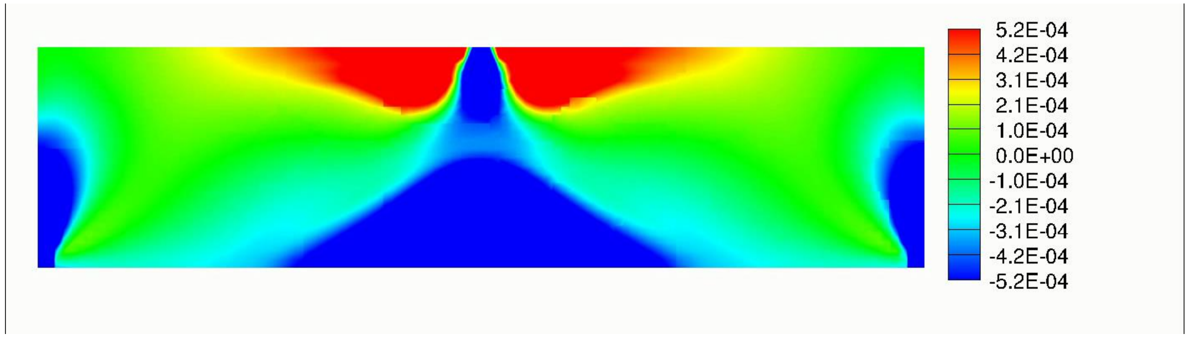
Flexural strain



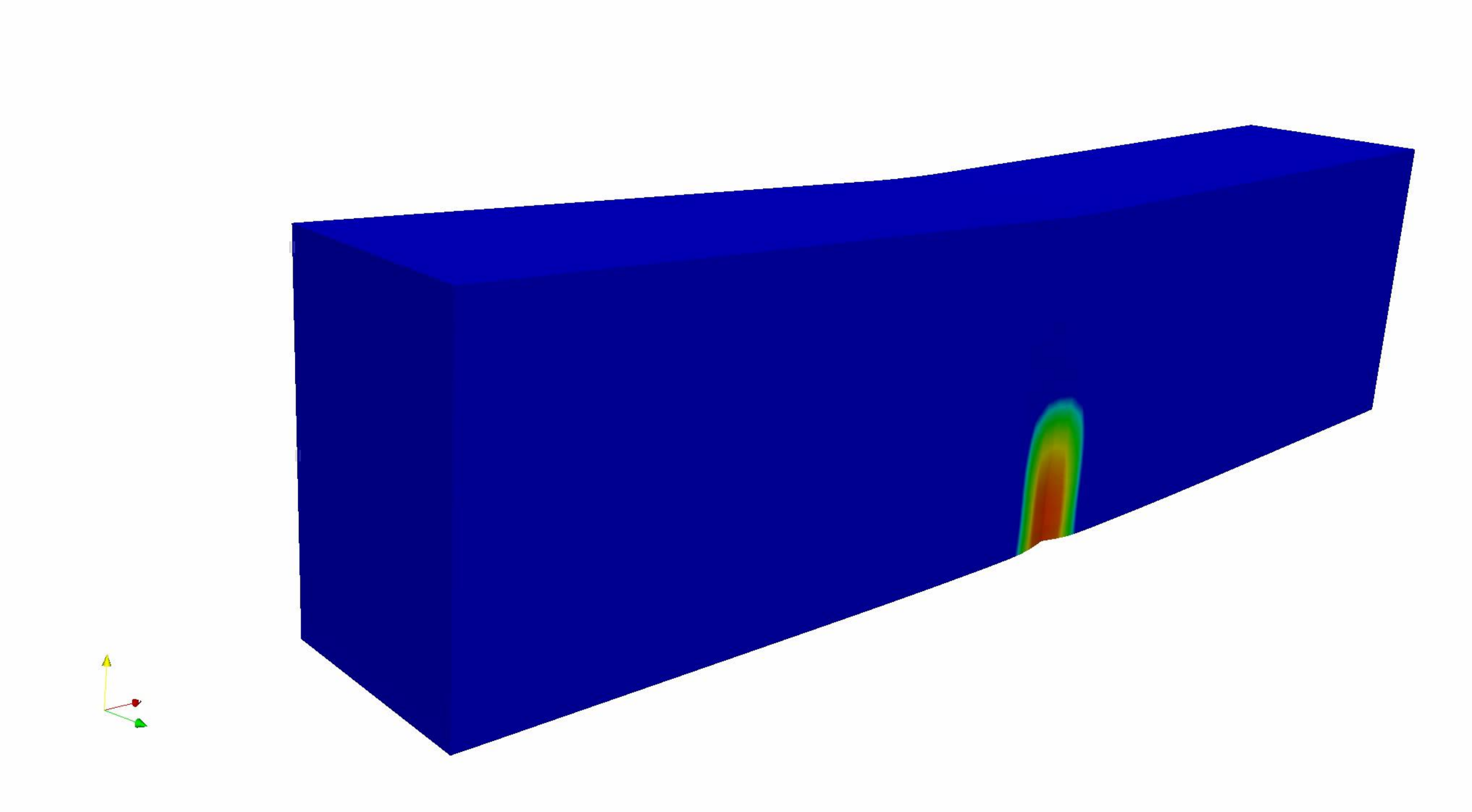


Transverse strain





Fracture with crack phase field



We propose an empirical relation for the size effect

- Volume dependent critical fracture energy is proposed as

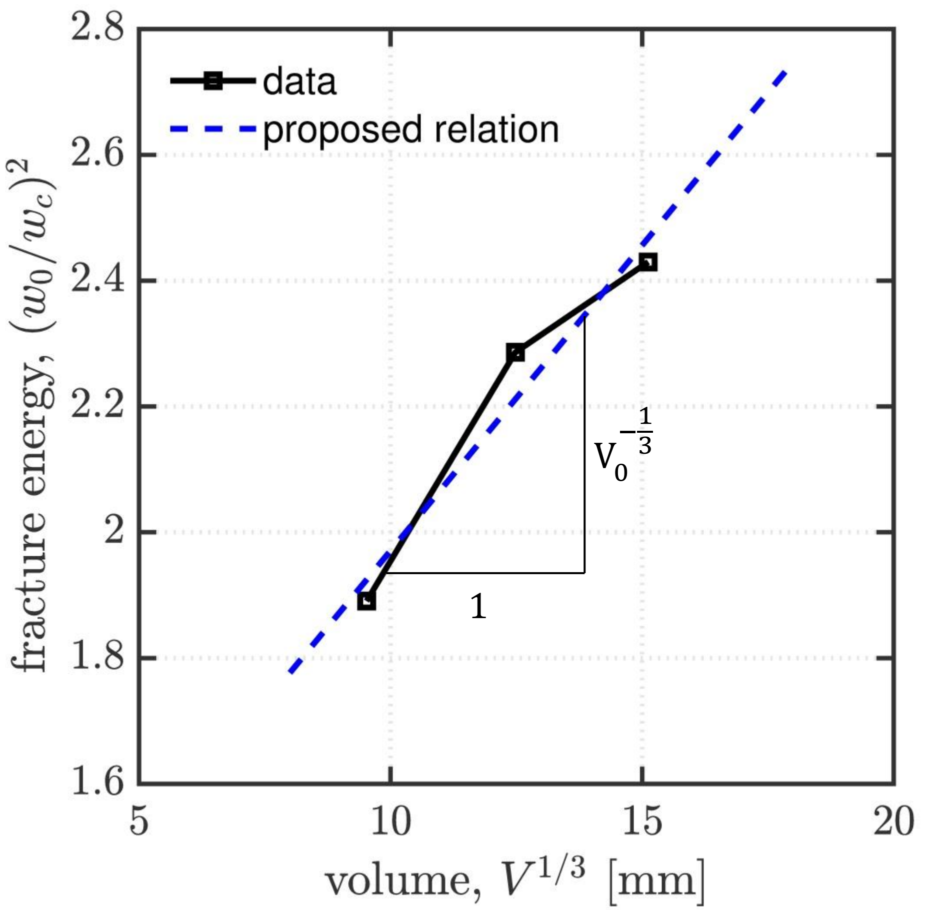
$$w_c = \frac{w_0}{\sqrt{\left(1 + \left(\frac{V}{V_0}\right)^{\frac{1}{3}}\right)}}$$

- Rearranging the terms, we get

$$\left(\frac{w_0}{\mathrm{w_c}}\right)^2 = \mathrm{V}_0^{-\frac{1}{3}} \cdot \left(V^{\frac{1}{3}}\right) + 1$$

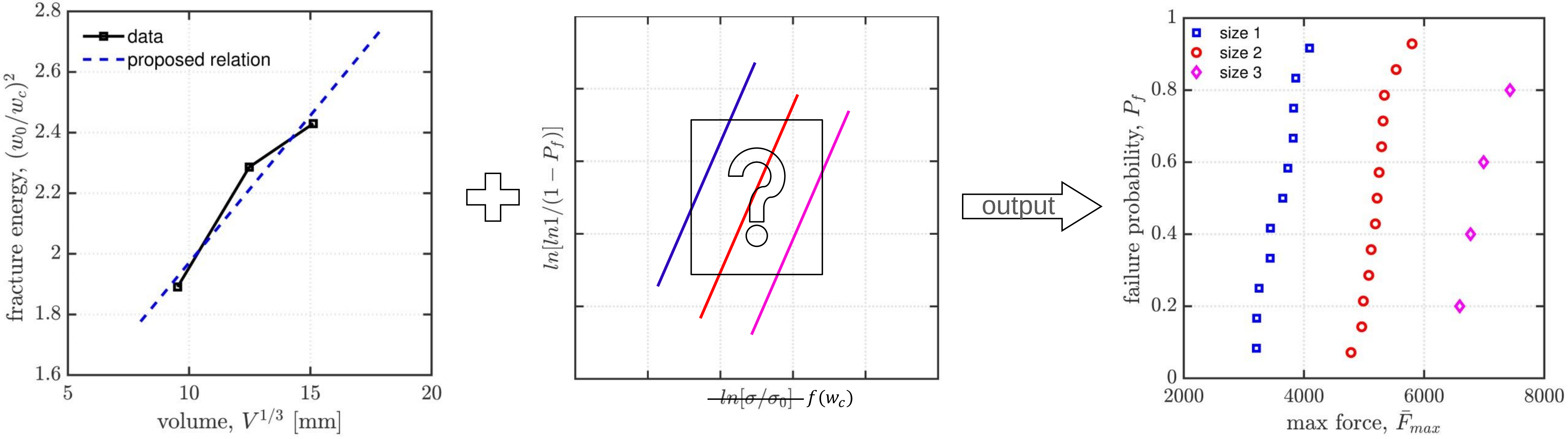
$$V_0 = 1092.7\ \mathrm{mm}^3$$
$$w_0 = 3.78\ \mathrm{Mpa}$$

- See Bažant and Kazemi (1990).



Contents

To be done …



- Can we simulate the stochastic nature of observed properties during tests to make the design and analysis of components more efficient?
- We start with finding an alternative to the weakest link Weibull model.

Contents

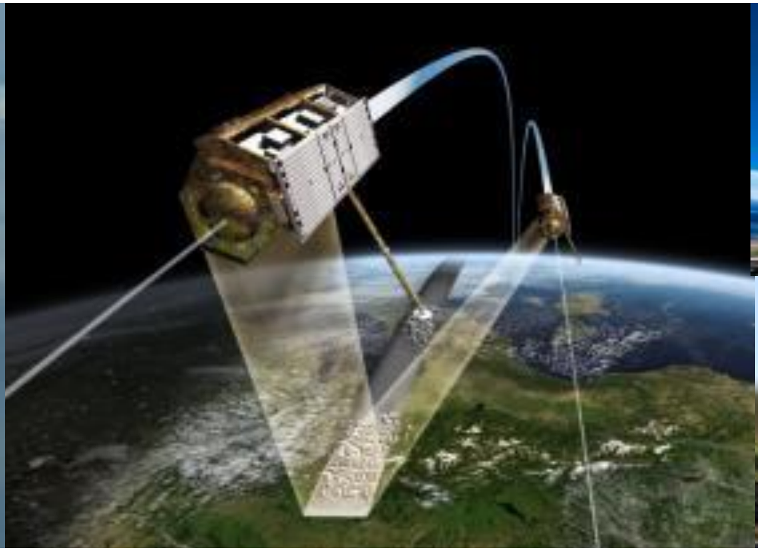
Conclusion & Outlook

Conclusion

- Titanium Aluminide alloys present a potential alternative to traditional Ni-basis super alloys.
- An empirical relation for size dependent fracture energy density is proposed.
- Crack initiation to final fracture accompanied by SSY is accurately captured by gradient-extended plasticity damage theory.

Outlook

- A multiscale model accounting for statistical descriptors of duplex microstructure in a SRUC.
- A crystal-plasticity coupled phase-field fracture theory for micromechanical motivation of size effect.
- An alternative to the weakest link Weibull model to account for failure in presence of SSY.



Thank you for your attention!

DLR Deutsches Zentrum für Luft- und Raumfahrt

German Aerospace Center

DLR