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Size Effect in Intermetallics: Experiments and Numerics

Dr.-Ing. Arun Raina
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1. Motivation, background and overview
2. Experimental studies
3. Gradient-extended plasticity damage theory
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5. Stochastic size effect
6. Conclusion & outlook
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Motivation

- Aviation accounts for $\approx 2.1\%$ 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 $[3]$.

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# Background

## Why Intermetallics?

![Rolls-Royce engine](image)

### Intermetallics Table

<table>
<thead>
<tr>
<th></th>
<th>$\sigma_{UTS}$ [MPa]</th>
<th>$\sigma_Y$ [MPa]</th>
<th>$\rho$ [g/cm$^3$]</th>
<th>$\sigma_{UTS}/\rho$ [°]</th>
<th>$E$ [GPa]</th>
<th>$\varepsilon_f$ [%]</th>
<th>$T_{oxid}$ [°C]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stainless Steel AISI 304 [3]</td>
<td>505</td>
<td>215</td>
<td>8</td>
<td>63</td>
<td>200</td>
<td>70</td>
<td>850</td>
</tr>
<tr>
<td>Ni-based super alloy [4]</td>
<td>1500</td>
<td>1200</td>
<td>8.5</td>
<td>176</td>
<td>210</td>
<td>35</td>
<td>900</td>
</tr>
<tr>
<td>Titanium Aluminide [5]</td>
<td>600</td>
<td>450</td>
<td>3.8</td>
<td>158</td>
<td>170</td>
<td>&lt;1</td>
<td>1000</td>
</tr>
</tbody>
</table>


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[1] Rolls-Royce

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Single-crystal superalloys

- Ti
- TiAl

Specific strength $*$ [MPa$\cdot$Mg$^{-1}$.m$^3$]

- Mg
- Al
- Super-alloys

![Diagram showing specific strength vs. temperature](image)
Weakest link Weibull model

- Failure probability\(^\text{\cite{1}}\) is written as

\[
P = 1 - \exp\left(- \int s(\sigma) dV\right)
\]

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

- 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.

\[\text{[1] Weibull (1951)}\]
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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:

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fracture toughness</td>
<td>15 – 18 MPa√m</td>
</tr>
<tr>
<td>Fracture strength</td>
<td>450 – 500 MPa</td>
</tr>
<tr>
<td>Density</td>
<td>3.97 g/cm³</td>
</tr>
<tr>
<td>Hardness</td>
<td>285 HV10</td>
</tr>
<tr>
<td>Young’s Modulus</td>
<td>160 GPa</td>
</tr>
<tr>
<td>Yield strength</td>
<td>430 MPa</td>
</tr>
</tbody>
</table>

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.

<table>
<thead>
<tr>
<th>Size</th>
<th>Length (L)</th>
<th>Height (H)</th>
<th>Width (B)</th>
<th>Count (n)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Size 1</td>
<td>25.2</td>
<td>6.0</td>
<td>6.0</td>
<td>11</td>
</tr>
<tr>
<td>Size 2</td>
<td>37.8</td>
<td>9.0</td>
<td>6.0</td>
<td>14</td>
</tr>
<tr>
<td>Size 3</td>
<td>50.4</td>
<td>12.0</td>
<td>6.0</td>
<td>4</td>
</tr>
</tbody>
</table>

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)
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Phase field modeling of elastic-plastic fracture \[\text{[1]}\]

- Define the space-time accumulated work density as

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

where \(C = \{\varepsilon, \varepsilon^p, \alpha, \nabla \alpha, d, \nabla d\}\) is the constitutive set.

- Make the energetic-dissipative split

\[
\hat{W} = \psi^e(\varepsilon - \varepsilon^p, d) + \mathcal{D}^{pf}(\alpha, \nabla \alpha, d, \nabla d)
\]

- Stored energy takes the form

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

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

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

\[\text{[1]}\ C. Miehe, F. Aldakheel, A. Raina (2016)\]
Phase field modeling of elastic-plastic fracture [1] ...

- Define a dissipation potential function
  \[
  \hat{V}(\mathcal{C}) = \sup_{f^p, r^p, f^f, r^r} \sup_{\lambda_p, \lambda_f} \left[ f^p : \dot{\varepsilon}^p - r^p \dot{\alpha} + (f^f - r^r) \dot{\lambda} - \lambda_p \phi_p - \lambda_f \phi_f \right]
  \]

- Define the global rate potential of coupled gradient-plasticity-gradient damage
  \[
  \Pi = \int_V \left( \int_0^t \left( \dot{\mathcal{W}}(\mathcal{C}) + \hat{V}(\mathcal{C}) \right) - \mathcal{P}_{ext}(\dot{\mathbf{u}}) \right) dt
  \]

- The global minimization of the multi-field problem yields the primary unknowns
  \[
  \{ \dot{\mathbf{u}}, \dot{\alpha}, \dot{d}, \dot{\varepsilon}^p \} = \text{Arg} \{ \inf \Pi \}
  \]

- Of particular interest is the Euler equation derived for the evolution of phase field fracture
  \[
  \dot{d} = (1 - d) \mathcal{H} - [d - l_f^2 \Delta d]
  \]

- The dimensionless crack driving state function is
  \[
  \Psi = \frac{w_e(\varepsilon^e) + w_p(\alpha, \nabla \alpha)}{w_C} - 1
  \]

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Simulations of average 3PB response

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$ [GPa]</td>
<td>195</td>
</tr>
<tr>
<td>$\nu$ [-]</td>
<td>0.24</td>
</tr>
<tr>
<td>$\sigma_y$ [MPa]</td>
<td>225</td>
</tr>
<tr>
<td>$\sigma_\infty$ [MPa]</td>
<td>345</td>
</tr>
<tr>
<td>$\omega$ [-]</td>
<td>20</td>
</tr>
<tr>
<td>$h$ [MPa]</td>
<td>150</td>
</tr>
<tr>
<td>$w_c$ [MPa] (size1)</td>
<td>2.749</td>
</tr>
<tr>
<td>$w_c$ [MPa] (size2)</td>
<td>2.50</td>
</tr>
<tr>
<td>$w_c$ [MPa] (size3)</td>
<td>2.425</td>
</tr>
</tbody>
</table>
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
  \[ \left(\frac{w_0}{w_c}\right)^2 = V_0^{-\frac{1}{3}} \cdot \left(V_0^{\frac{1}{3}}\right) + 1 \]

- \( V_0 = 1092.7 \text{ mm}^3 \)
- \( w_0 = 3.78 \text{ Mpa} \)

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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.
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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!