Microstructure-sensitive modelling of deformation and fracture of TiAl alloys

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TiAl for turbine blade: Requirement and goal

- Need for improvements in mechanical properties:
  - Strength at high temperature
  - Creep resistance
  - Ductility
  - Fatigue strength
  - Fracture toughness

Can be improved by

Modelling for microstructure-property correlations

Simulation Assisted Material Engineering

Microstructure optimization
Outline:
Modelling of TiAl alloy behaviour considering microstructure sensitivity

Three problem areas will be demonstrated

- Modelling of deformation behaviour
- Modelling of crack initiation and propagation
- Modelling of dynamic fracture
Micromechanical modelling: Deformation of multi-phase structure


Small domain aspect ratio

Equal-strain (Voigt) model

Large domain aspect ratio

Equal-stress (Reuss) model

Homogenized domain

Homogeneous lamellae

Matrix orientations of domains: 0°-120°-240°

Twin orientations of domains: 180°-300°-60°

Wenwer et al., Int J Plast 22 (2006) 1683
Micromechanical modelling: Deformation of multi-phase structure

**Major Phases**

- $\alpha_2$ Ti$_3$Al
- $\gamma$TiAl

### Deformation of lamellar phases

- Prismatic $\langle 1120 \rangle \{1100\}$
- Basal $\langle 1120 \rangle \{0001\}$
- Pyramidal $\langle 1126 \rangle \{1121\}$

### Deformation modes for lamellar grains

- Longitudinal
- Mixed
- Transverse

**Slip systems in $\gamma$-TiAl**

<table>
<thead>
<tr>
<th>Slip type</th>
<th>Slip system</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ordinary</td>
<td>$\frac{1}{2}\langle 110 \rangle {111}$</td>
</tr>
<tr>
<td>Super</td>
<td>$\langle 011 \rangle {111}$</td>
</tr>
<tr>
<td>Twinning</td>
<td>$\frac{1}{6}\langle 112 \rangle {111}$</td>
</tr>
</tbody>
</table>

**Slip systems in $\alpha_2$ (Ti$_3$Al)**

<table>
<thead>
<tr>
<th>Slip type</th>
<th>Slip system</th>
</tr>
</thead>
<tbody>
<tr>
<td>Prismatic</td>
<td>$\langle 1120 \rangle {1\overline{1}00}$</td>
</tr>
<tr>
<td>Basal</td>
<td>$\langle 11\overline{2}0 \rangle {0001}$</td>
</tr>
<tr>
<td>Pyramidal</td>
<td>$\langle 1\overline{1}26 \rangle {1\overline{1}21}$</td>
</tr>
</tbody>
</table>

References:
- Lebensohn et al., Acta mater 46 (1998) 4701
- Werwer et al., Int J Plast 22 (2006) 1683
Polycrystal models for FE analysis

- Voxel based polycrystal model
- Voronoi based polycrystal model
- Idealization of the microstructure
- FE Model
- Globular grains
- Lamellar microstructure
- Globular microstructure
Global-local coupling for average mechanical behaviour

FE Model

FE Element (Continuum)

64 PUCs

Deformation with 9 DOF
1 integration point
stretch shear rotation

 deformation

reaction force

Unit Cell

Constitutive behaviour of TiAl phases
Crystal plasticity model

Classical (Huang et al)
Gradient enhanced (Kabir, Shahid)
Temperature sensitive (Kabir, Ilyas)

Model validation and parameter estimation

- PST lamellar alloy
- Fully lamellar alloy
- Duplex alloy

References:
- Lebensohn et al., Acta mat 46, 1998
- Werwer et al., Int J Plast 22, 2006
- Corne, Kabir, Mat Sci Engg A620, 2014
Prediction: Microstructural influence on mechanical properties

Microstructural influence on Yield

Localized strain for lamellar orientation

Change of Vol% Unit cell with fine microstructure

Influence of phase volume%

Orientation distribution of grains/lamellae
Micromechanical modelling of crack initiation and propagation


- Two basic mechanisms:
  - Interlamellar fracture, grain boundary fracture
    - Interface failure/debonding
  - Translamellar fracture, Transgranular fracture
    - Splitting of material
Micromechanical modelling of crack initiation and propagation

Single crystal PST alloy: Ti-49.8 Al (at.%)  
K.-F. YAO, H. INUI, K. KISHIDA and M. YAMAGUCHI  

Yield stress, MPa
- Orientation, φ
- Tensile stress, MPa
- Orientation, φ

Tensile loading, F
- LE, Max. Principal (Avg. 75%)
- Vertical drop (failure)
Prediction of component failure using stochastic data

Material Model for deformation and fracture

Deformation

Fracture

Analysis of maximum allowable RPM for compressor blade
Component failure: Demonstration on a model-compressor blade

Test case with simple boundary condition

Analysis of maximum allowable RPM for compressor blade

16350 rpm

22050 rpm

30600 rpm

FE-Model

Cohesive Box

Cohesive layer

Full thickness

Crack initiation spot

Lower Cohesive Box

Radial Stresses (MPa)

+520.0
+751.7
+683.3
+615.0
+546.7
+478.3
+410.0
+341.7
+273.3
+205.0
+136.7
+68.3
0
Dynamic fracture: High velocity particle Impact on TiAl alloy


Goal:
To understand domestic object damage (DOD) on turbine blade

High velocity particle Impact experiment
Institute of Structures and Design, DLR, Stuttgart

As Cast microstructure
Globular grains
β-phases at boundaries

As forged microstructure
Elongated grains
β-phases at boundaries
High velocity particle impact: Microstructure influence on backside crack-network

As Cast microstructure

Crack profile: Star shape

Fracture along grain boundaries in presence of β-phases

As forged microstructure

Crack profile: elongated

Forged

Crack length vs microstructure

- Analysis of residual strength
- Calculation of fatigue life

Modelling of impact fracture: Synthetic (virtual) microstructures and FE model

- As Cast microstructure
- As forged microstructure

- Tapered edge specimen (idealized turbine blade component)
- Explicit grain and grain boundary modelling
- Graded microstructure with graded mesh

- Voronoi based synthetic microstructure
  - Grain statistics are incorporated

- Microstructure simplification
  - Grains with ideal grain boundary
  - Grain boundary contains $\beta$-phases

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Model generated with Neper[1]

Modelling of impact fracture: prediction of crack profile

Constitutive behaviour: Combined damage and fracture approach

For grain damage (tensile damage model):
Pressure stress > Hydrostatic cut-off stress
(Diagonastic component remains zero)

For interface damage (cohesive model):
Interface strength > critical strength at interface
Crack initiates at critical material separation

Microstructural sensitivity on back side crack network (Exp. and Sim.)

Cast
T0=675, d0=0.1

Forged
T0=300, d=0.001

Cast
T0=600, d=0.001

Forged

Parameter study: crack profile for different damage parameters
Summary: Microstructure-sensitive modelling of TiAl alloy

**Deformation**
- Local heterogeneity

**Crack Propagation**
- Micro-meso fracture

**Fracture**
- STATIC
- DYNAMIC
- High velocity particle impact
Thank you for your attention

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