Microstructure-sensitive modelling of deformation and fracture of TiAl alloys

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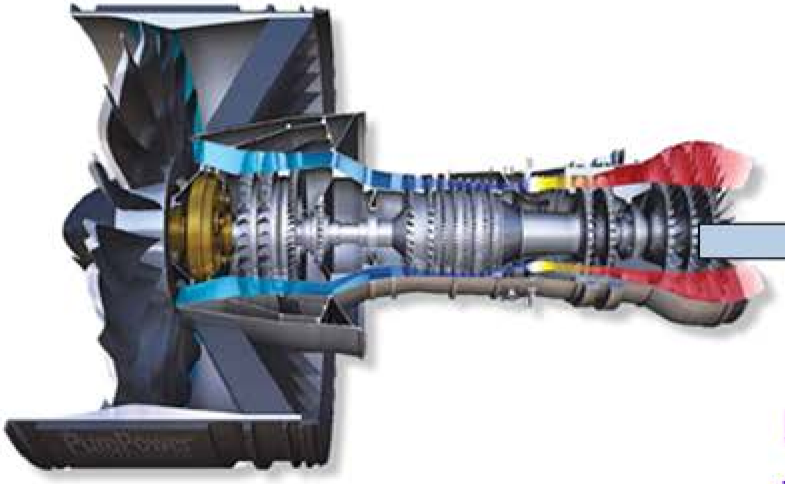
Werkstoff-Kolloquium
DLR Köln
05.12.2017

Citation:
MR Kabir, Werkstoff-Kolloquium 2017, Institute of Materials Research, German Aerospace Center, Cologne, Germany.

TiAl for turbine blade: Requirement and goal



Low pressure turbine blade

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

Can be improved by

Microstructure optimization → Simulation Assisted Material Engineering → Modelling for microstructure-property correlations → Simulation Assisted Material Engineering → Microstructure optimization

Outline:
Modelling of TiAl alloy behaviour considering microstructure sensitivity

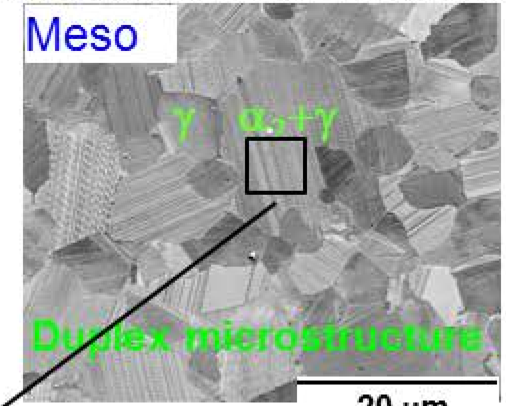
Three problem areas will be demonstrated

- Modelling of deformation behaviour
- Modelling of crack initiation and propagation
- Modelling of dynamic fracture

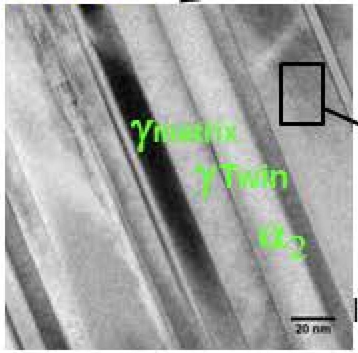
DLR

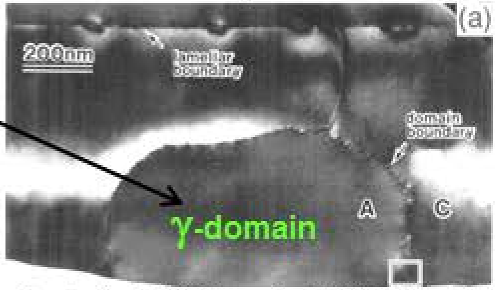
Micromechanical modelling: Deformation of multi-phase structure

Kabir et al., Mat Sci Eng A 635(2015)13-22



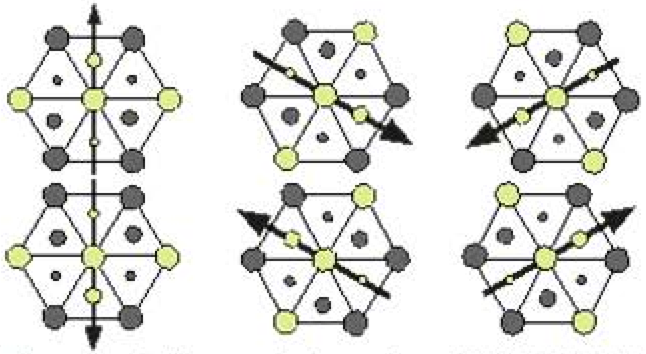
Micro





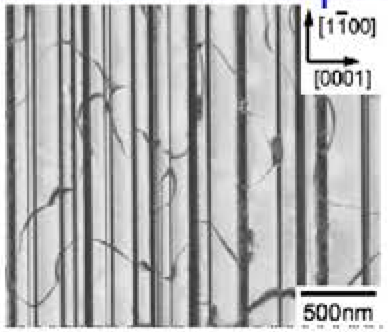
Inui et al., Phil Mag A, 66(1992) 539

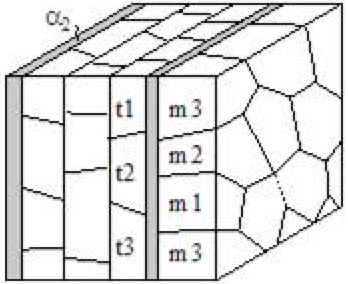
Matrix orientations of domains: 0°-120°-240°

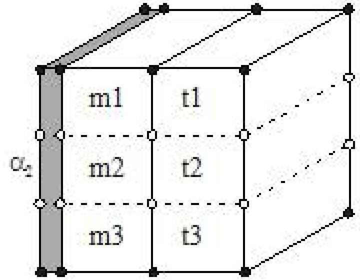


Twin orientations of domains: 180°-300°-60°

Small domain aspect ratio

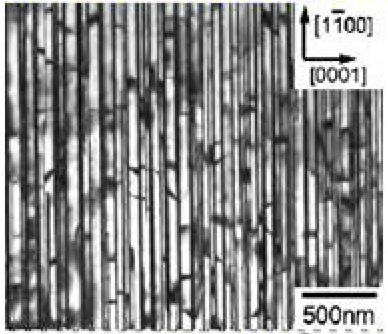


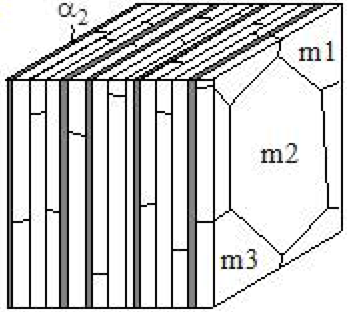


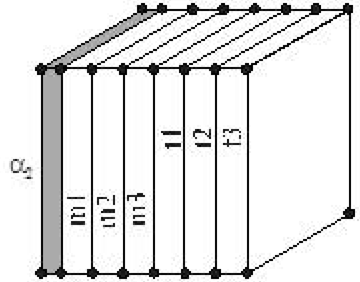


Equal-strain (Voigt) model

Large domain aspect ratio

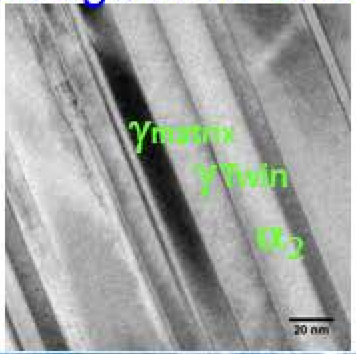


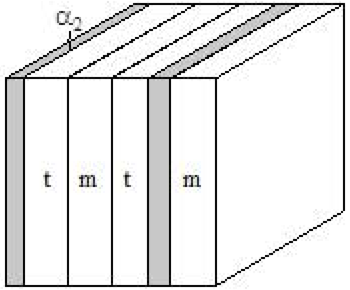


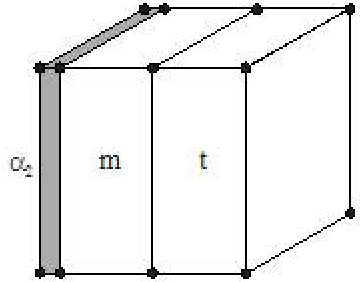


Equal- stress (Reuss) model

Homogenized domain





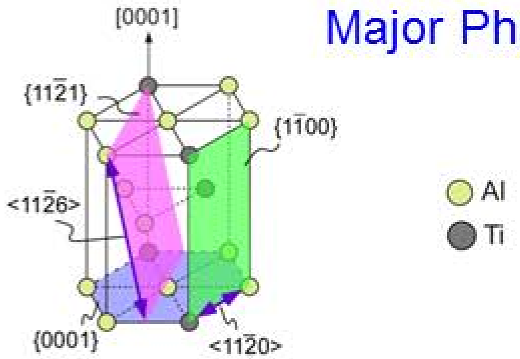


Homogeneous lamellae

Werwer et al., Int J Plast 22 (2006) 1683

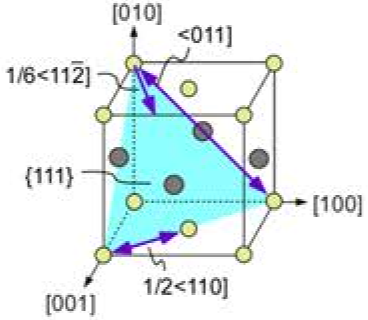
Micromechanical modelling: Deformation of multi-phase structure

Major Phases



α_2 Ti_3Al

Prismatic <1120>{1100}
Basal <1120>{0001}
Pyramidal <1126>{1121}



γTiAl

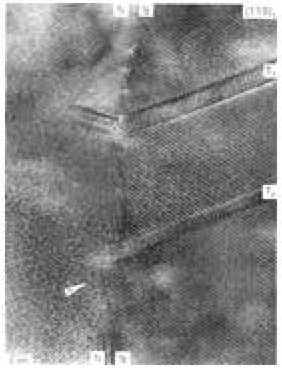
Ordinary 1/2<110]{111}
Twinning 1/6<112]{111}
Super <110]{111}

Slip systems in γ-TiAl			
Slip type			
Ordinary	$1/2[1\bar{1}0]\{111\}$	$1/2[1\bar{1}0]\{11\bar{1}\}$	$1/2[110]\{1\bar{1}1\}$ $1/2[110]\{\bar{1}\bar{1}1\}$
Super	$[01\bar{1}]\{111\}$ $[10\bar{1}]\{111\}$	$[01\bar{1}]\{\bar{1}1\bar{1}\}$ $[10\bar{1}]\{1\bar{1}1\}$	$[0\bar{1}\bar{1}]\{11\bar{1}\}$ $[0\bar{1}\bar{1}]\{1\bar{1}1\}$ $[\bar{1}0\bar{1}]\{11\bar{1}\}$ $[\bar{1}0\bar{1}]\{\bar{1}\bar{1}1\}$
Twinning	$1/6[11\bar{2}]\{111\}$	---	$1/6[\bar{1}\bar{1}\bar{2}]\{11\bar{1}\}$ $1/6[\bar{1}1\bar{2}]\{\bar{1}1\bar{1}\}$ $1/6[\bar{1}1\bar{2}]\{1\bar{1}\bar{1}\}$

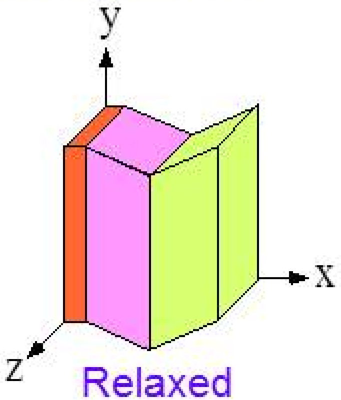
Slip systems in α_2 (Ti_3Al)			
Slip type			
Prismatic	---	$<11\bar{2}0>\{\bar{1}100\}$	---
Basal	$<11\bar{2}0>(0001)$	---	---
Pyramidal	---	---	$<\bar{1}\bar{1}26>(11\bar{2}1)$

Lebensohn et al., Acta mater 46 (1998)4701

Deformation of lamellar phases

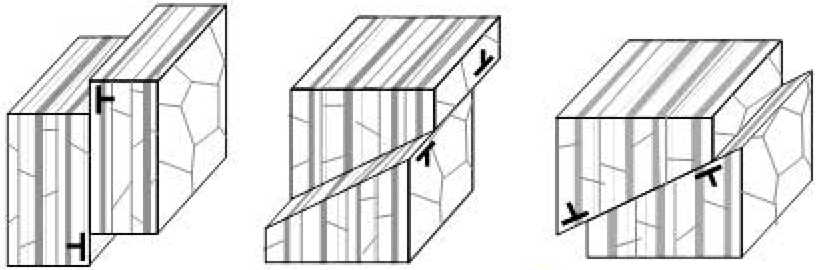


Appel , F. (2005)
Philos. Mag. , **85** , 205



Relaxed constraint BC

Deformation modes for lamellar grains

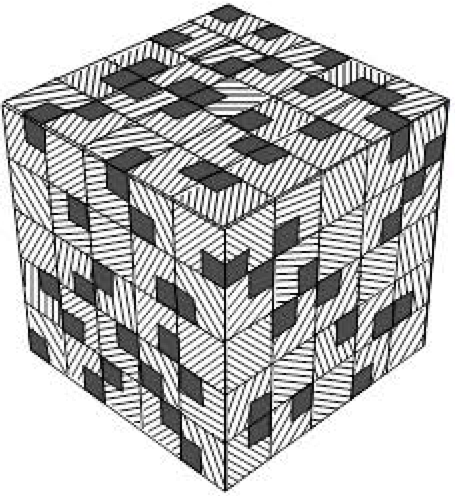


Longitudinal Mixed Transverse

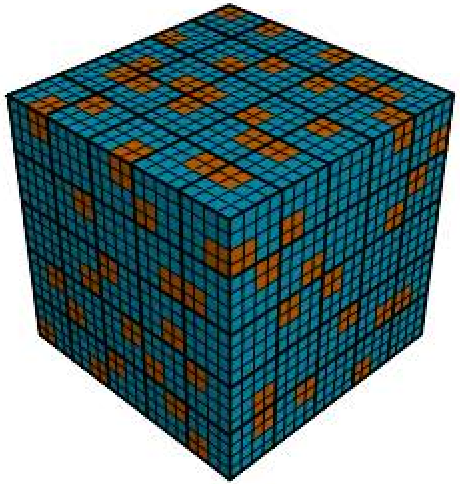
Werwer et al., Int J Plast 22 (2006) 1683

Polycrystal models for FE analysis

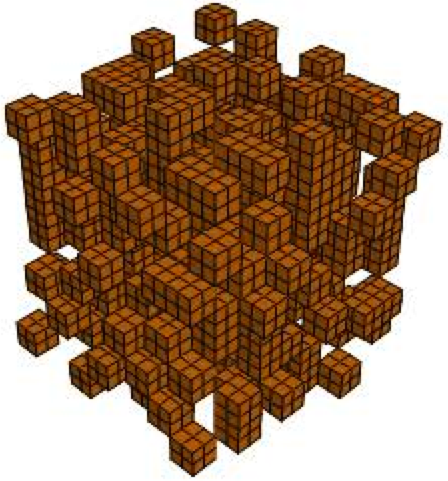
Voxel based polycrystal model



Idealization of the microstructure

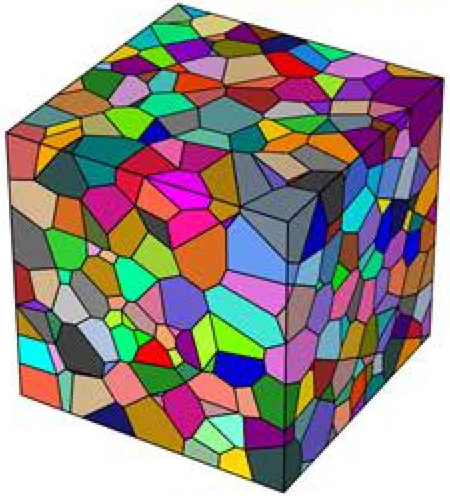


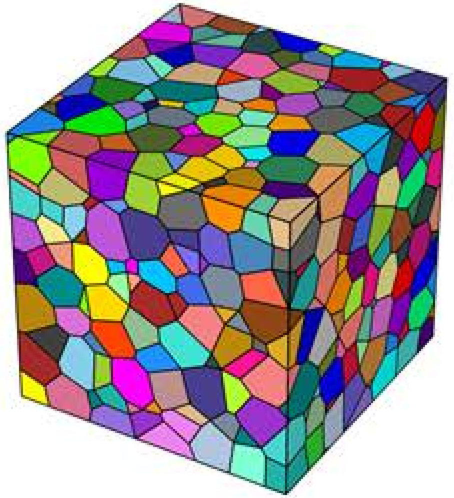
FE Model

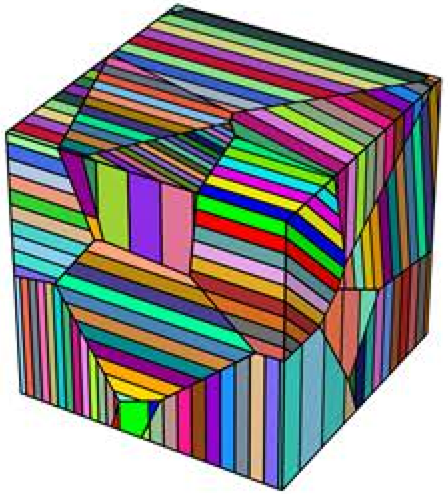


Globular grains

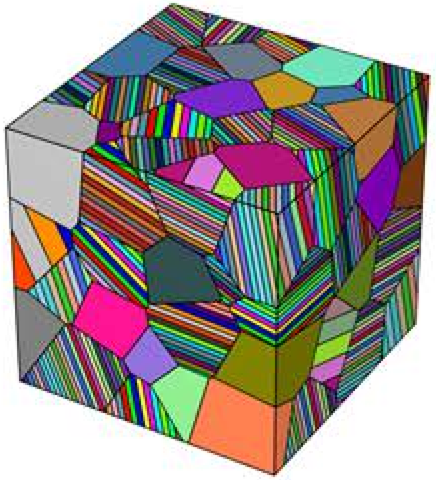
Voronoi based polycrystal model





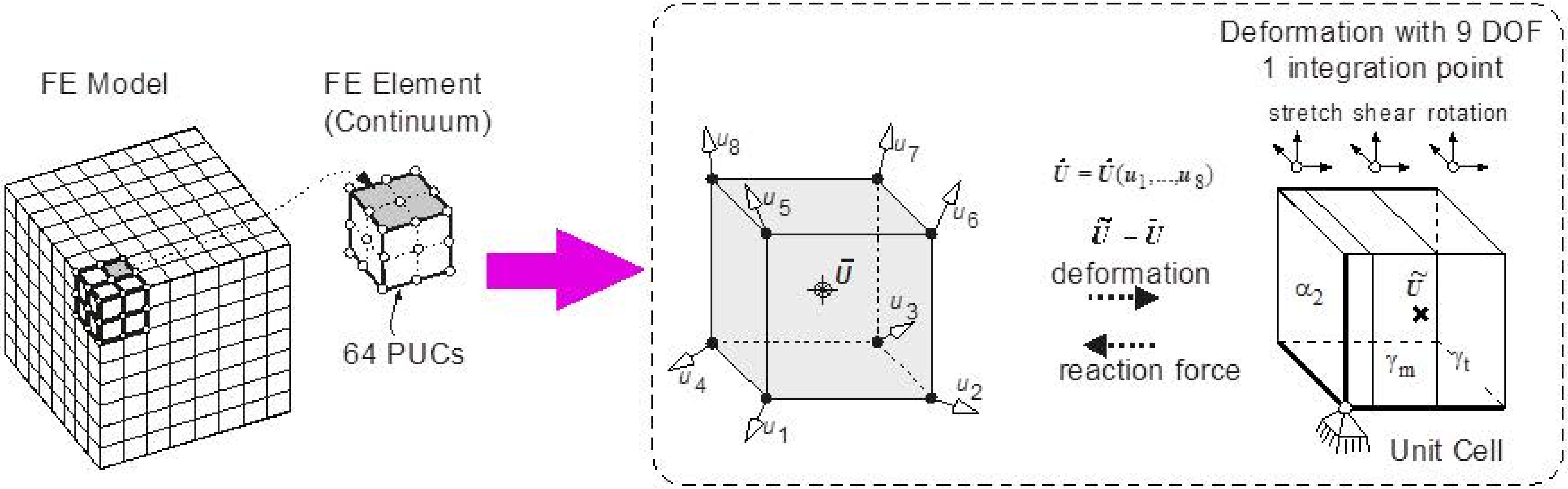


Lamellar microstructure



Globular microstructure

Global-local coupling for average mechanical behaviour



Werwer et. al. Comp. Mat. Sci. 19, 2000

Model validation and parameter estimation

- ❑ PST lamellar alloy
- ❑ Fully lamellar alloy
- ❑ Duplex alloy

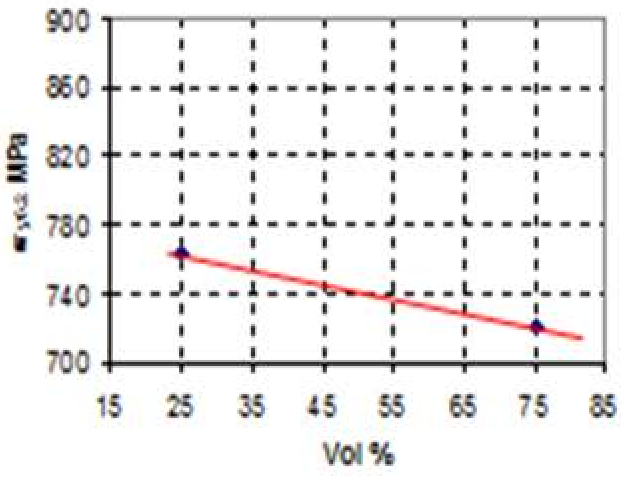
References:
- Lebensohn et al., Acta mat 46, 1998
- Werwer et al., Int J Plast 22, 2006
- Kabir et al. Acta Mat 58, 2010
- Cornec, Kabir, Mat Sci Engg A620, 2014

Constitutive behaviour of TiAl phases
Crystal plasticity model

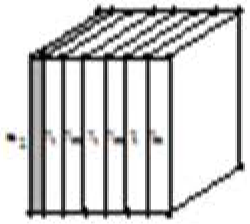
Classical (Huang et al)	Gradient enhanced (Kabir, Shahid)	Temperature sensitive (Kabir, Ilyas)

Prediction: Microstructural influence on mechanical properties

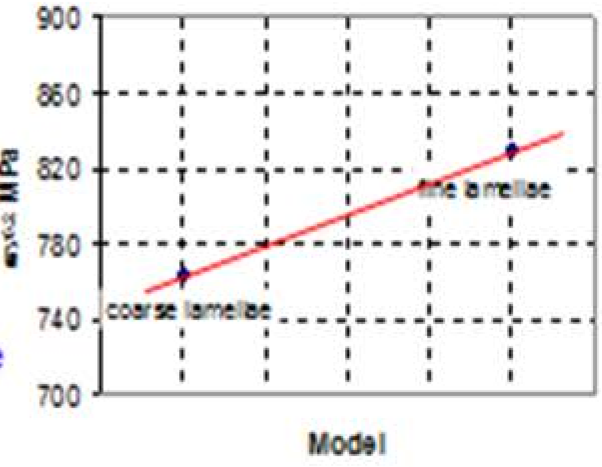
Microstructural influence on Yield



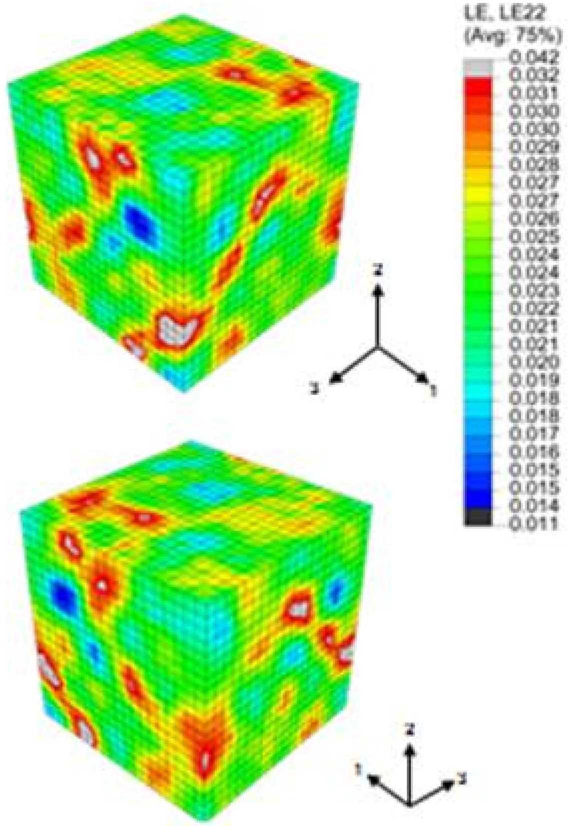
Change of Vol %

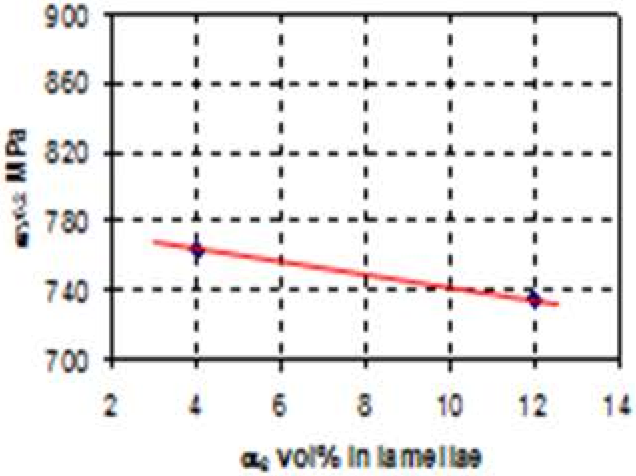


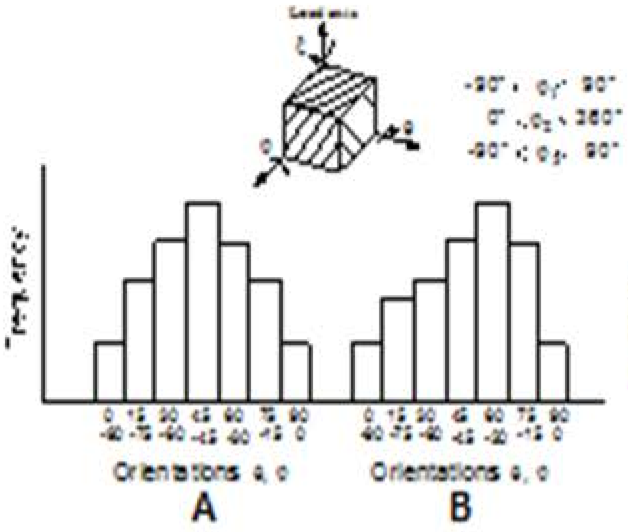
Unit cell with fine microstructure



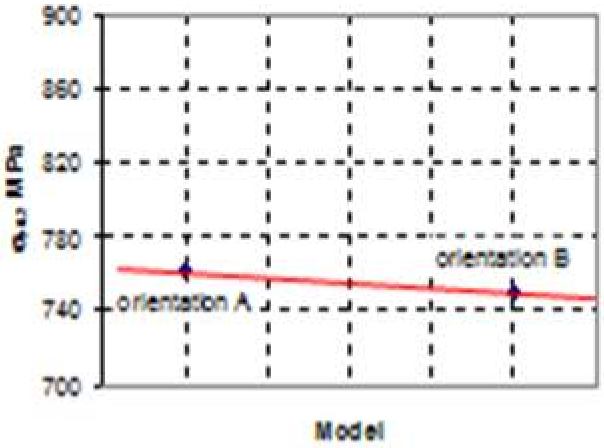
Localized strain for lamellar orientation





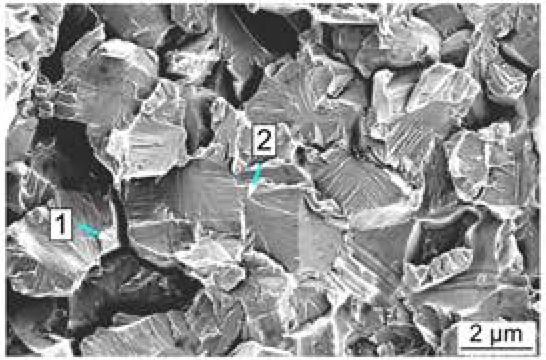


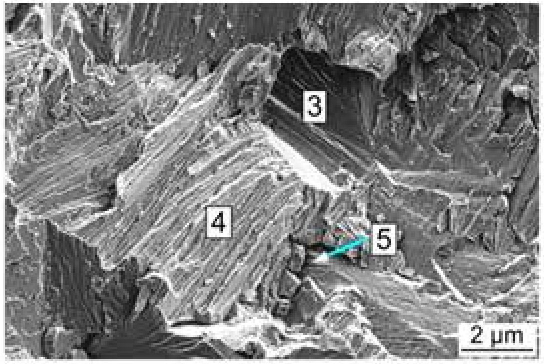
Orientation distribution of grains/lamellae



Micromechanical modelling of crack initiation and propagation

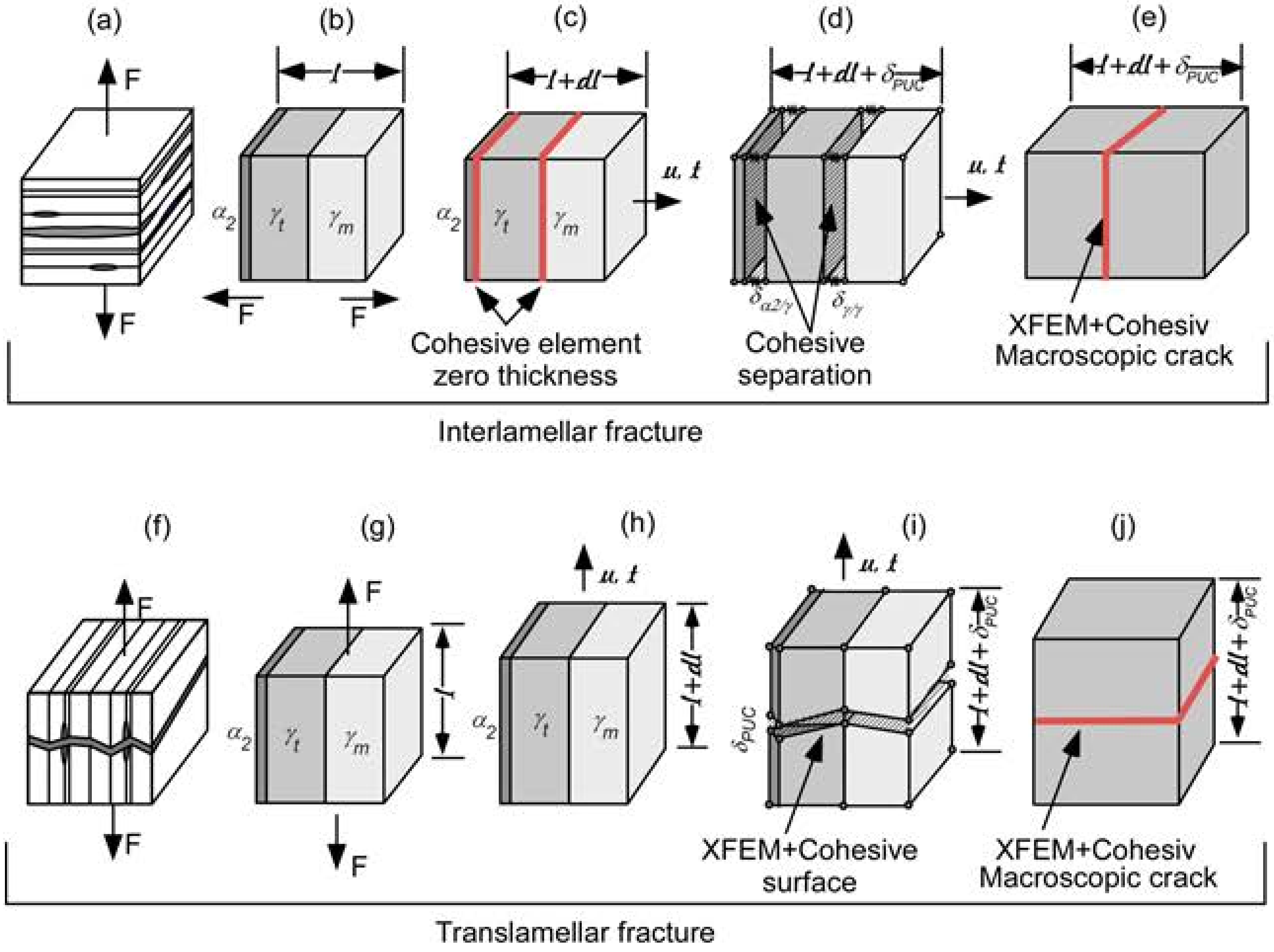
Kabir et al., Mat Sci Eng A 635(2015)13-22





Q1 (annealed at 1230°C)
1 Inter-granular cracks
2 Trans-granular fracture

Q7 (annealed at 1290°C)
3 Trans-granular fracture
4 Trans-lamellar fracture
5 Cracking at colony boundary

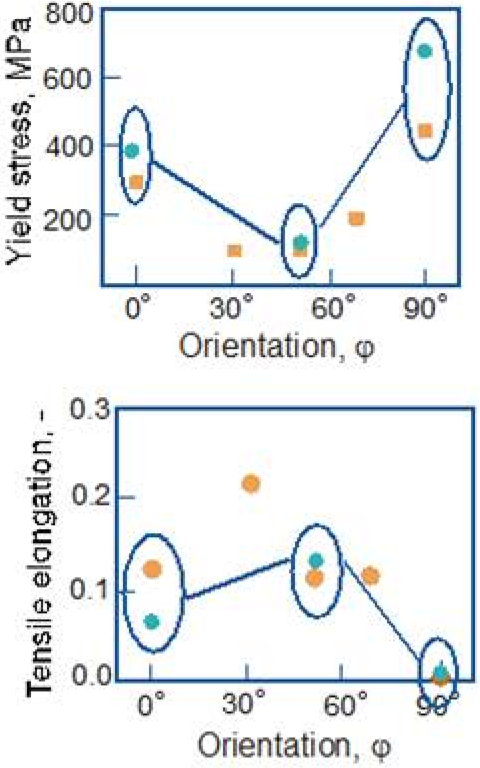


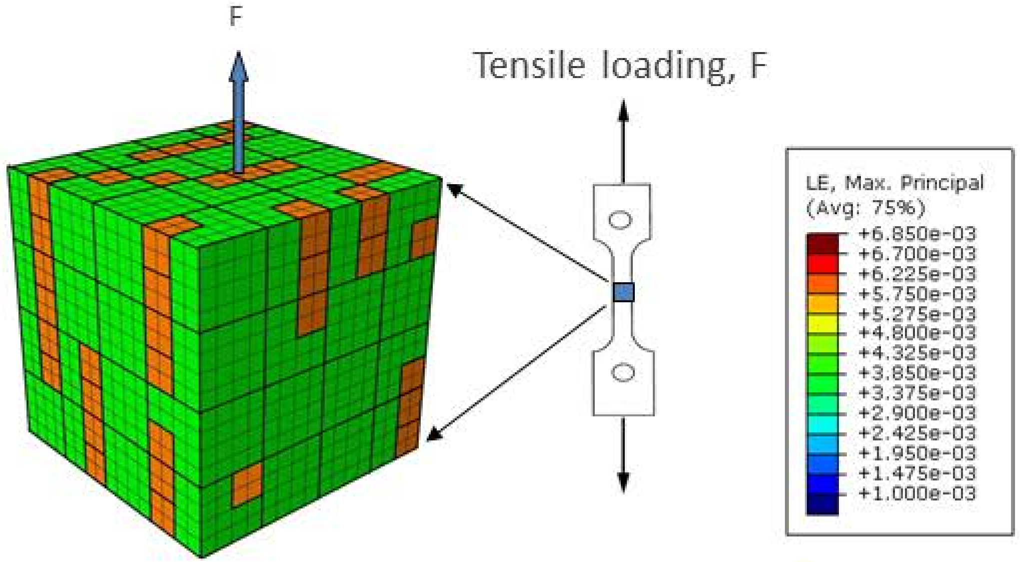
- Two basic mechanisms:
- Interlamellar fracture, grain boundary fracture
  - Interface failure/debonding
- Translamellar fracture, Transgranular fracture
  - Splitting of material

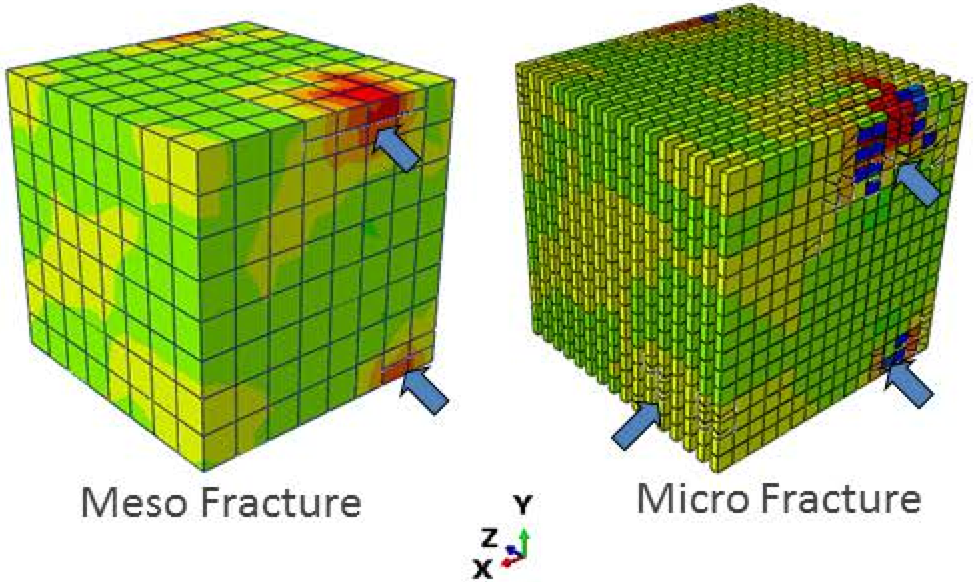
DLR

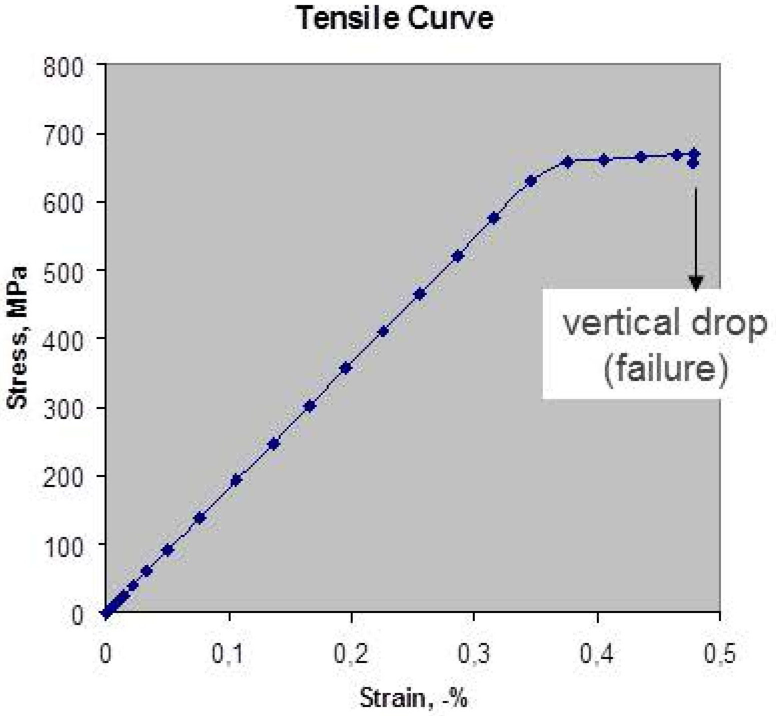
Micromechanical modelling of crack initiation and propagation

Single crystal PST alloy: **Ti-49.8 Al (at.%)**
K.-F. YAO, H. INUI, K. KISHIDA and M. YAMAGUCHI
Acta metall, mater. 43 (1995) pp. 1075

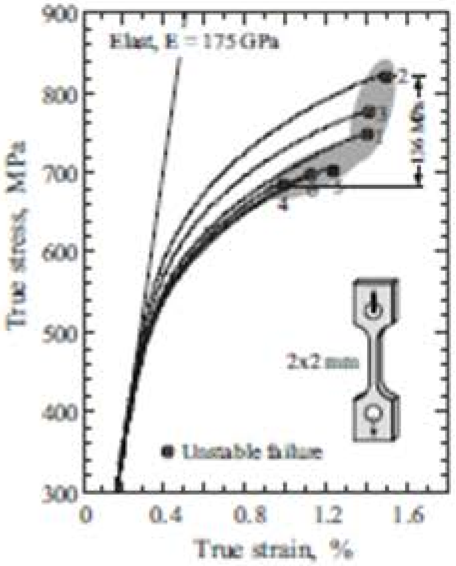


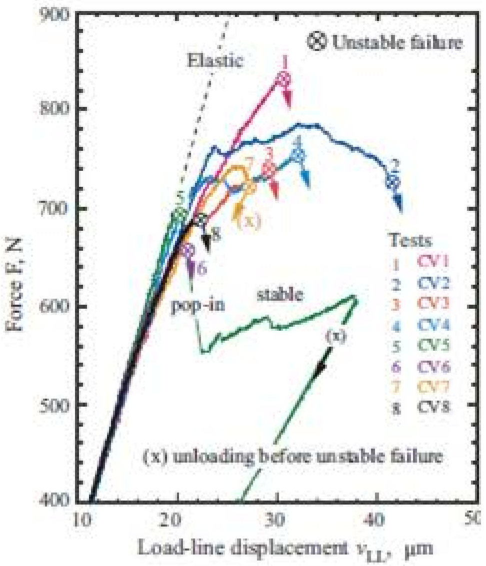




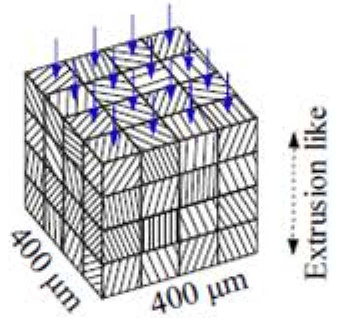


Prediction of component failure using stochastic data



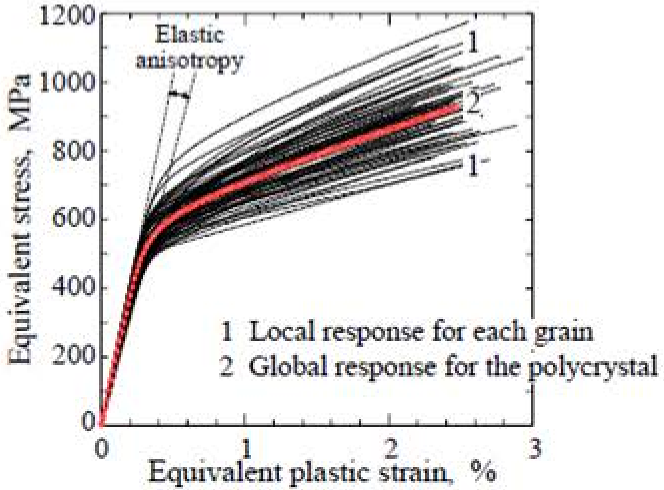


Polycrystal FE Cube

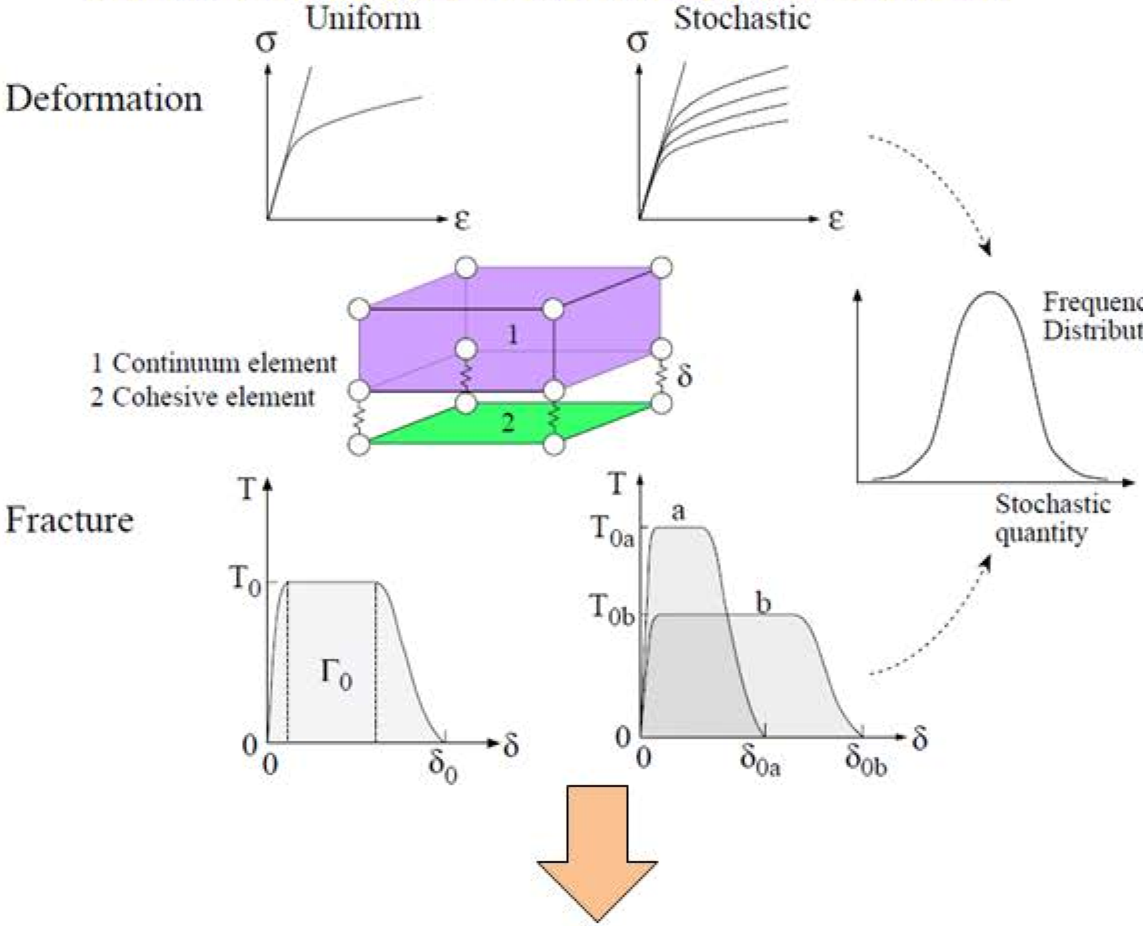


Polycrystal cube with with 64 lamellar grains

Simulation Response



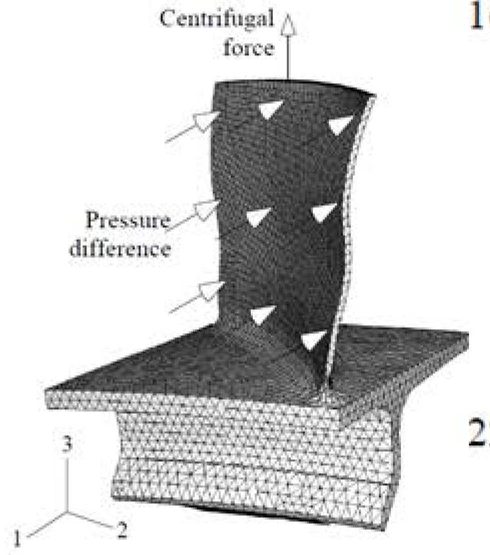
Material Model for deformation and fracture



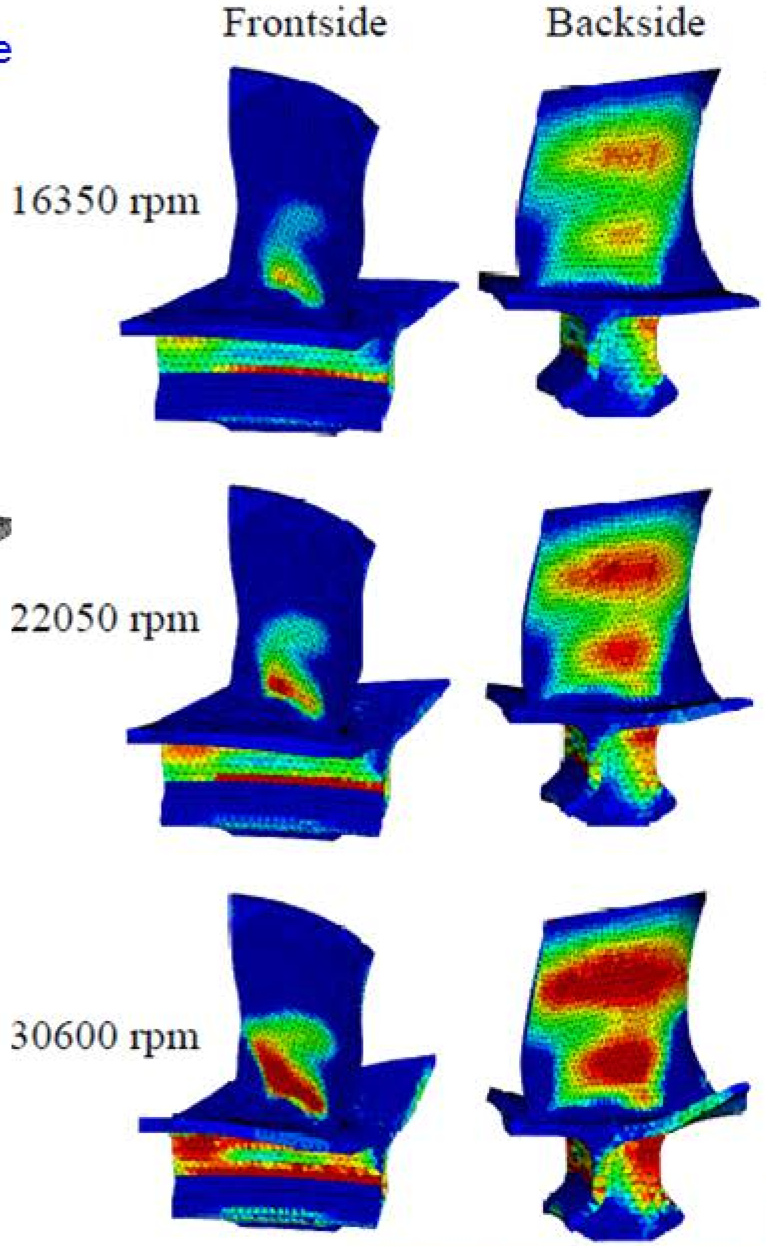
Analysis of maximum allowable RPM for compressor blade

Component failure: Demonstration on a model-compressor blade

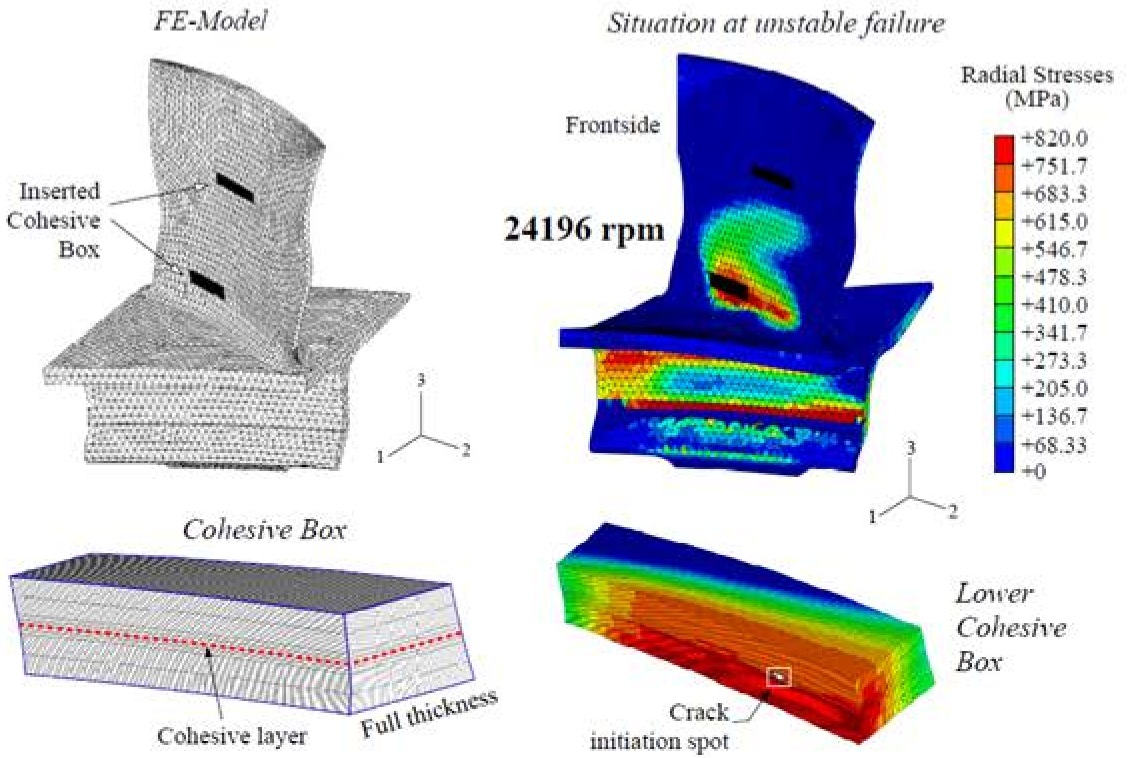
Test case with simple boundary condition



40003 tetra. elements



Analysis of maximum allowable RPM for compressor blade



DLR

Dynamic fracture: High velocity particle Impact on TiAl alloy

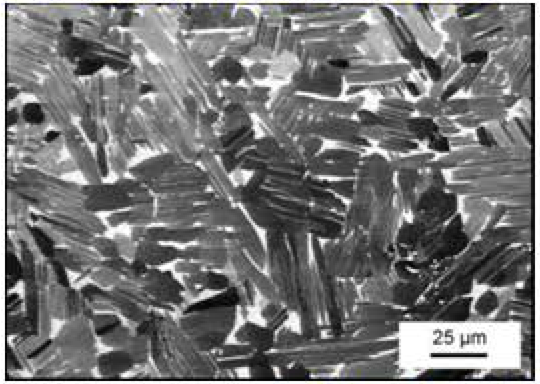
References: 1) Susanne Gebhard, PhD Thesis, University of Stuttgart, 2011
2) Gebhard et al, Materials Science and Engineering A 527 (2010) 5883–5891

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

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

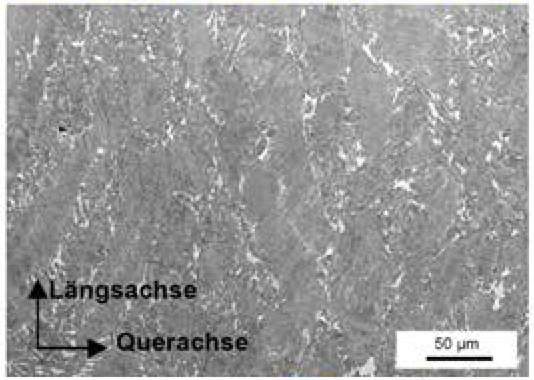
Tapered edge specimen
(turbine blade edge)

As Cast microstructure



Globular grains
β-phases at boundaries

As forged microstructure

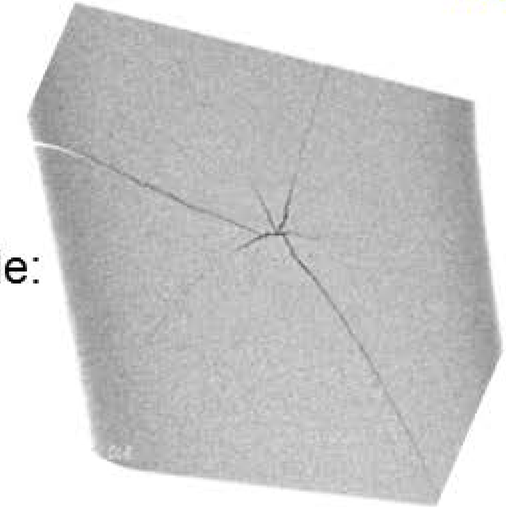


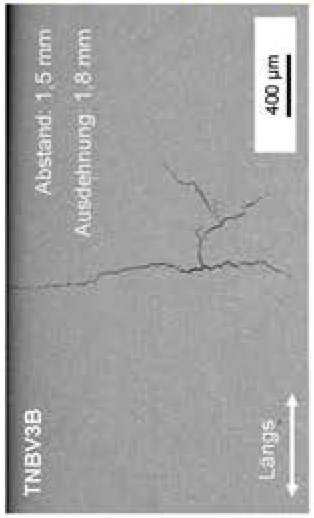
Elongated grains
β-phases at boundaries

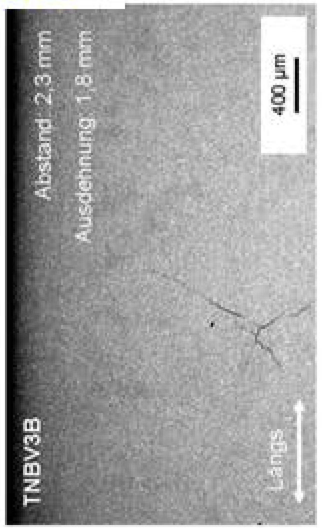
High velocity particle Impact: Microstructure influence on backside crack-network

As Cast microstructure

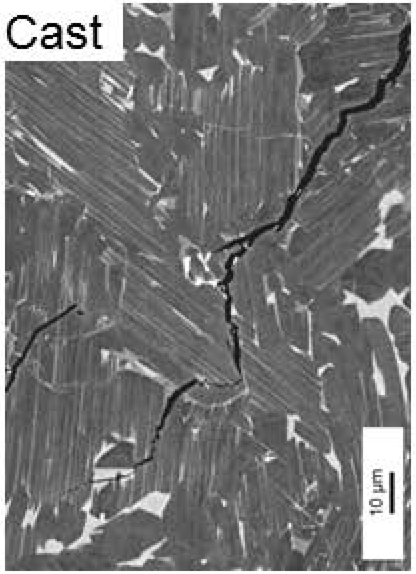
Crack profile:
Star shape







Cast

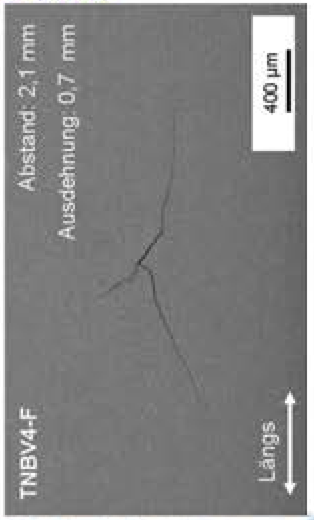


Fracture along grain boundaries in presence of β-phases

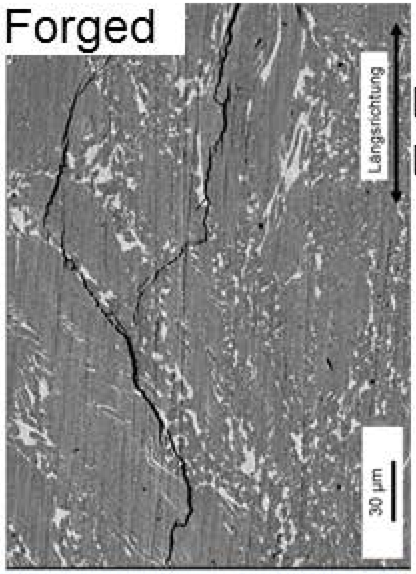
Crack length vs microstructure

As forged microstructure

Crack profile:
elongated



Forged



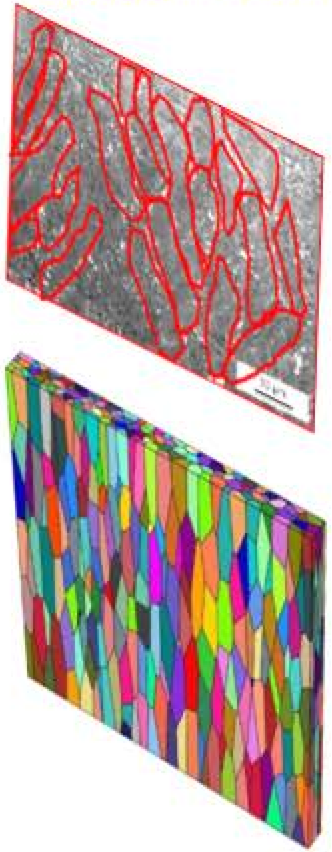
- ❑ Analysis of residual strength
- ❑ Calculation of fatigue life

Ref 1) S Gebhard, PhD Thesis, 2011

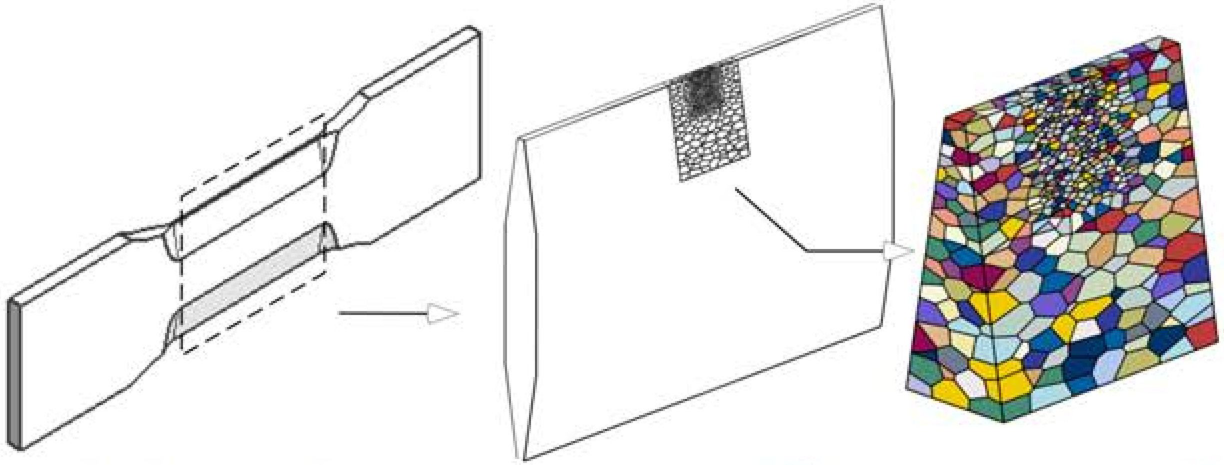
Modelling of impact fracture: Synthetic (virtual) microstructures and FE model

As Cast microstructure

As forged microstructure



- ❑ Voronoi based synthetic microstructure
  - ❑ Grain statistics are incorporated
- ❑ Microstructure simplification
  - ❑ Grains with ideal grain boundary
  - ❑ Grain boundary contains β-phases



Tapered edge specimen (idealized turbine blade component)

Explicit grain and grain boundary modelling

Graded microstructure with graded mesh

Model generated with Neper[1]

[1] R. Quey, et al., Comp Methods in App Mech Eng, 2011 (200)1729

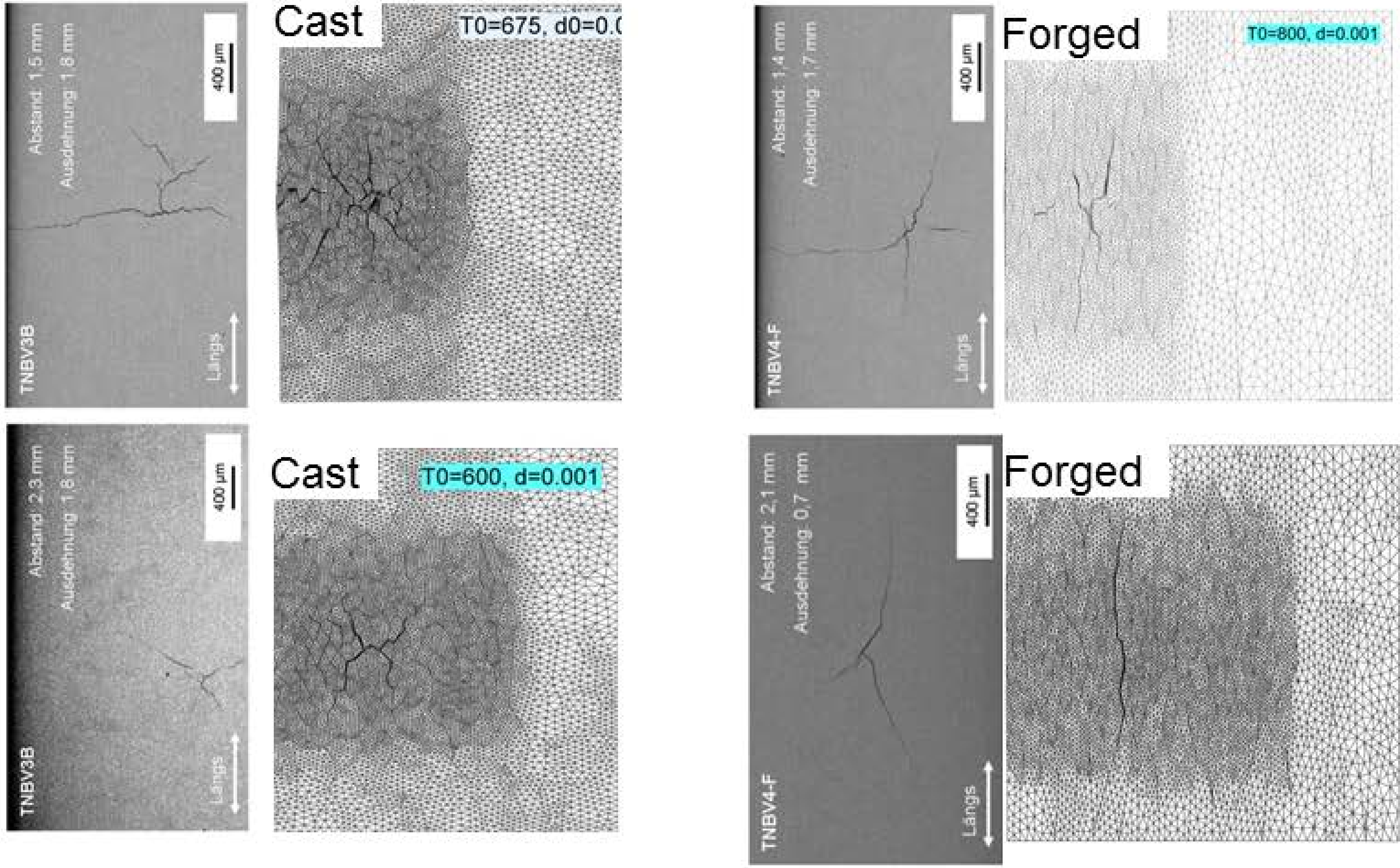
Modelling of impact fracture: prediction of crack profile

Constitutive behaviour:
Combined damage and fracture approach

For grain damage (tensile damage model)
pressure stress > Hydrostatic cut-off stress
(Deviatoric component remains zero)

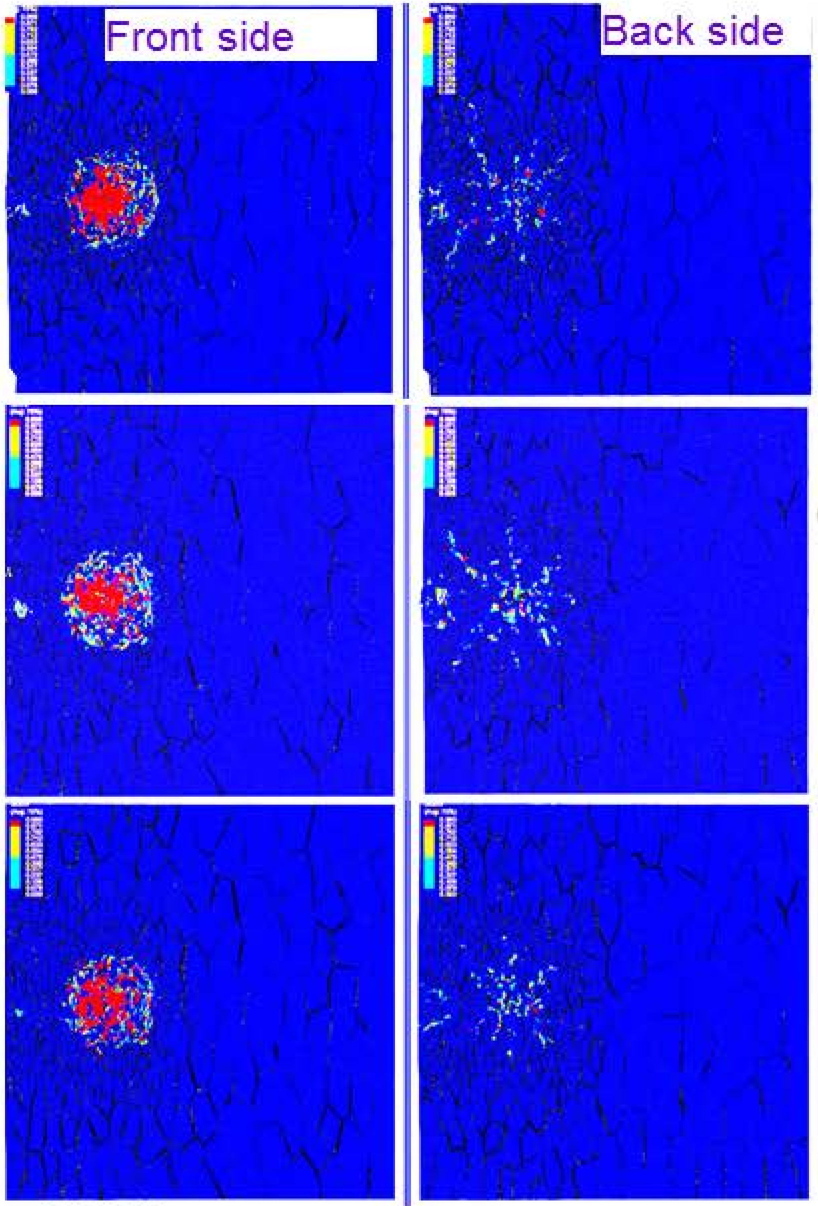
For interface damage (cohesive model):
Interface strength > critical strength at interface
Crack initiates at critical material separation

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

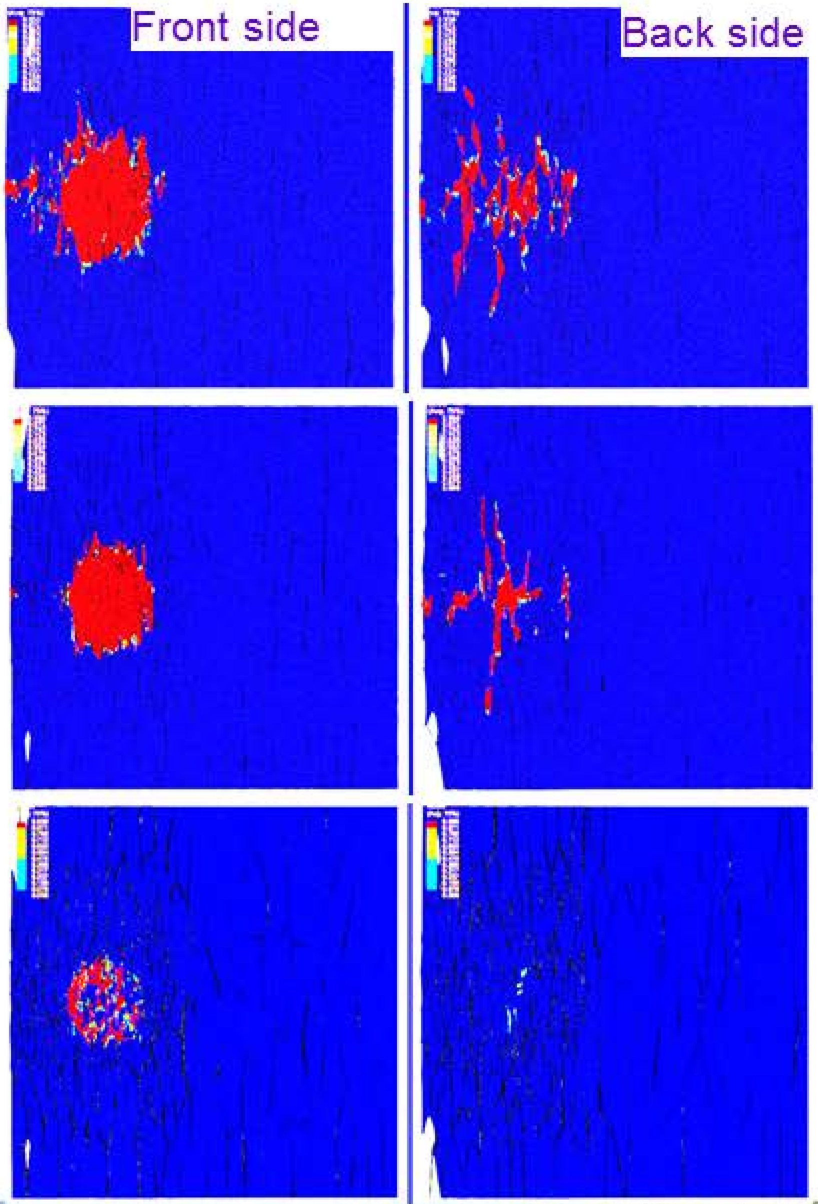


DLR

Parameter study: crack profile for different damage parameters



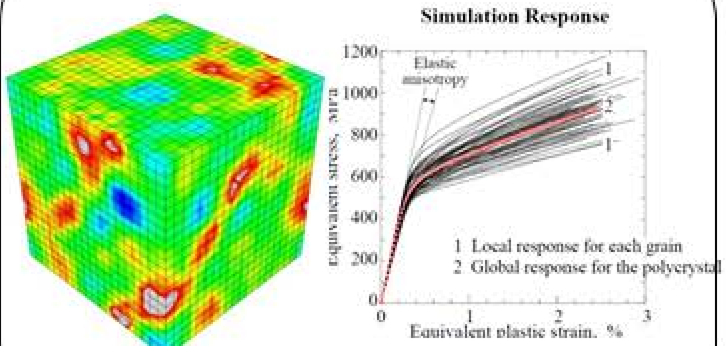
Cast



Forged

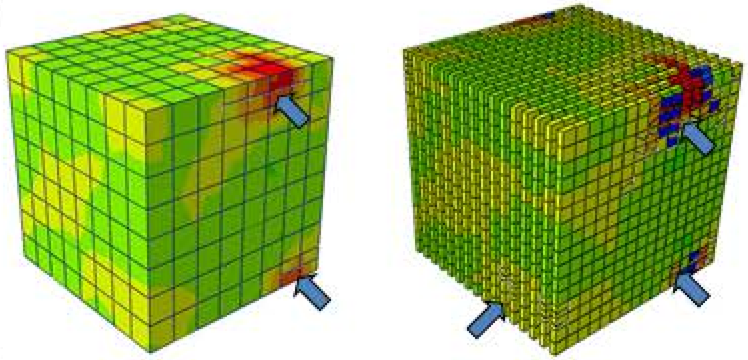
Summary: Microstructure-sensitive modelling of TiAl alloy

Deformation



Local heterogeneity

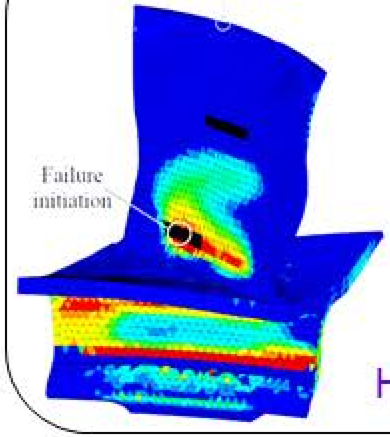
Crack Propagation



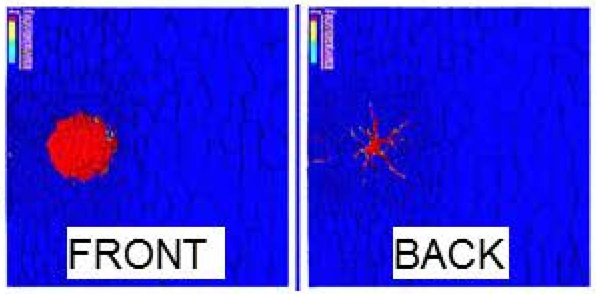
Micro-meso fracture

Fracture

STATIC



DYNAMIC



High velocity particle impact

Thank you for your attention

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