

Microstructure Modelling and Simulation of TiAl Alloy

Project Meeting

Date: 17.05.2017

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Wissen für Morgen



Outlook

Microstructure
Modelling

Fracture/Failure
Prediction

Constitutive
behaviour

Material/Model
Parameter

Experimental validation
Double shear test



(A) Microstructure Modelling

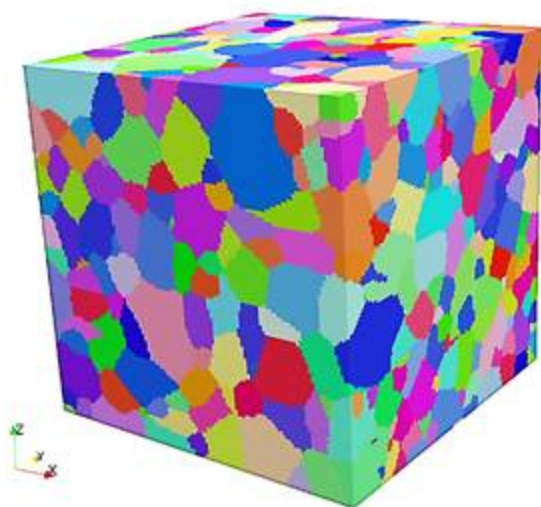


Synthetic/Virtual Microstructure

- Using mathematical algorithms: Voronoi tessellations

OPEN SOURCE SOFTWARE

DREAM3D



Air Force Research Laboratory (AFRL)
BlueQuartz Software
Ohio State University/Johns Hopkins University
Carnegie Mellon University

NEPER



R. Quey, CNRS France
Quey et al, Comput Methods Appl Mech Eng, 2011



Voronoi Tessellation – Centroidal Voronoi

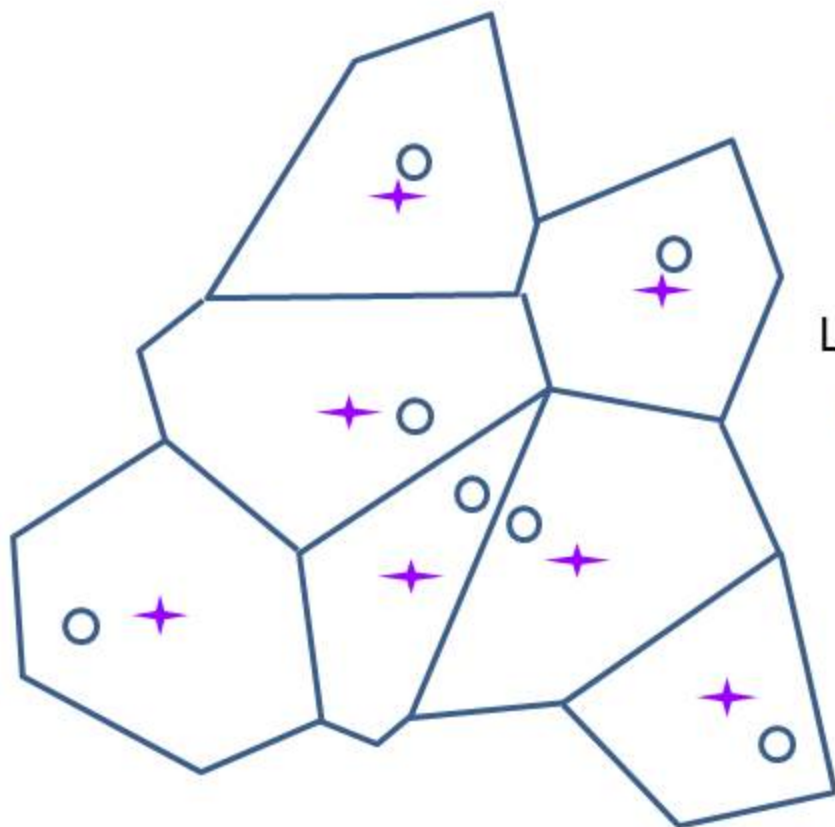
○ Seed Points

✦ Centroids

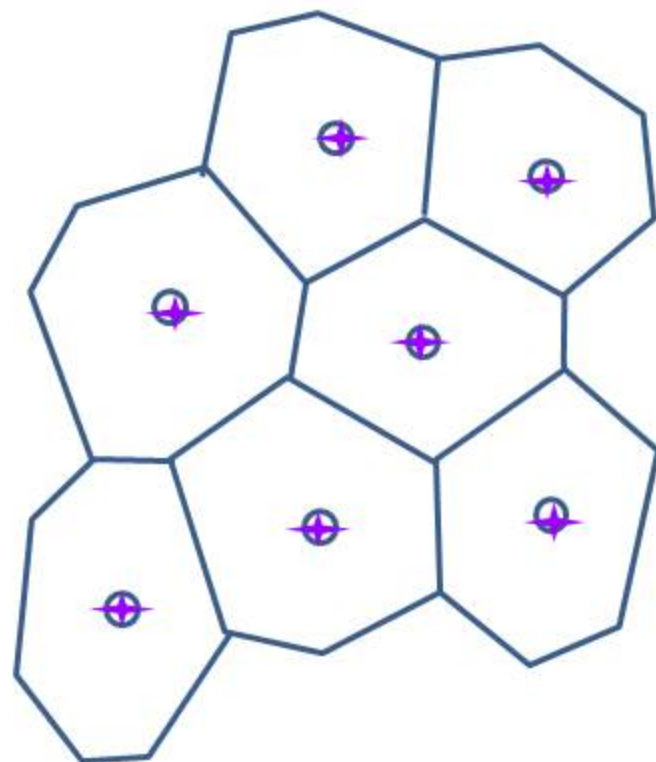
Lloyd's Algorithm



Iteration



Voronoi



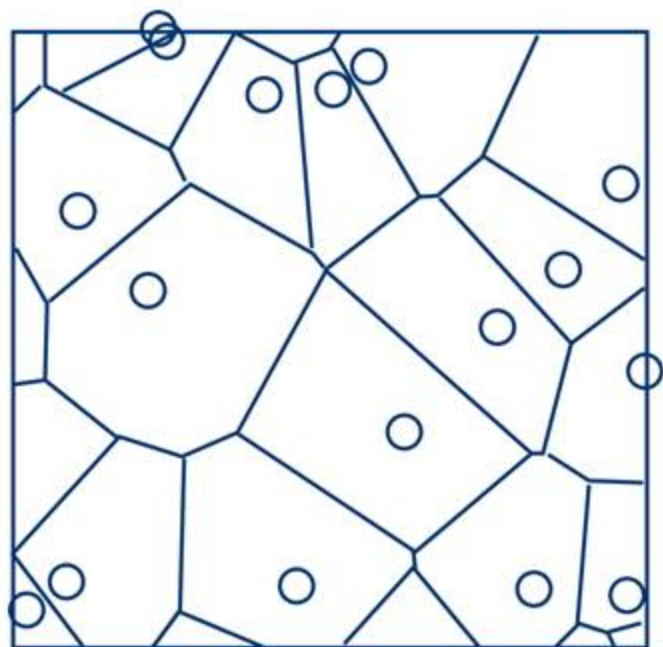
Centroidal voronoi



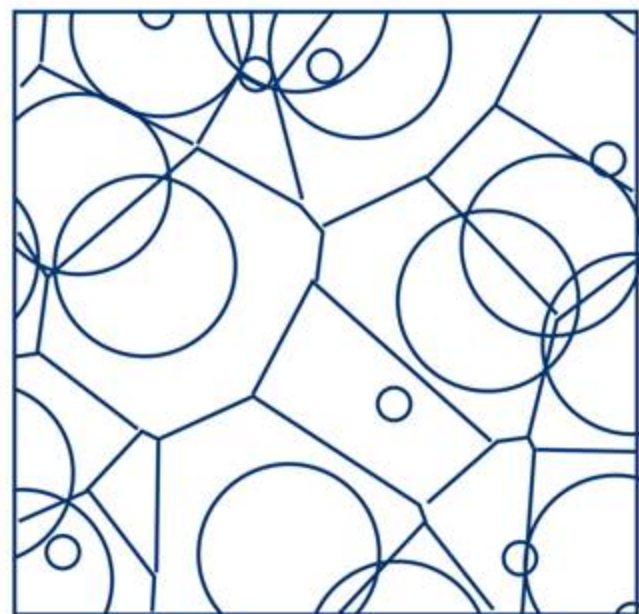
Voronoi Tessellation – Laguerre Tessellation

○ Seed Points

- Assign weight to the Seed
- Calculate power-distance of the seeds
(Radius of circle at that seed)
- Cut through circle intersections



Voronoi



Laguerre



Microstructure Parameters

Statistics from Microstructure analysis
(user input in a Text/ASCII file)

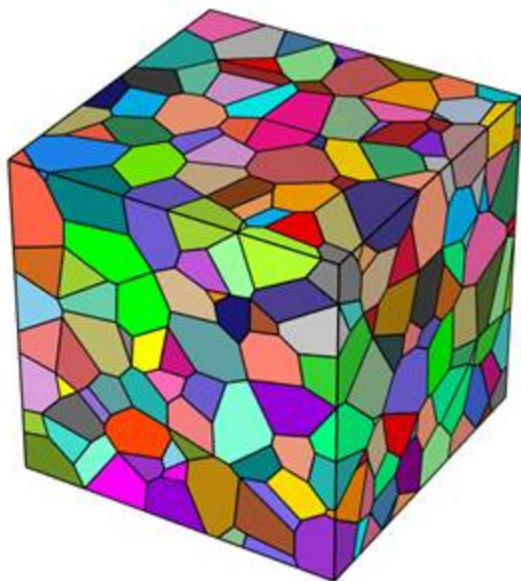
- Grain size distribution (area in 2D, volume in 3D, equivalent diameter)
- Sphericity (grain shape parameter)
- Grain centroid position (x,y,z-coordinate)
- Distribution function (gauss, log normal, etc)

- Lamellar width
- Lamellar normal
- Crystal direction

User Script to manipulate the data

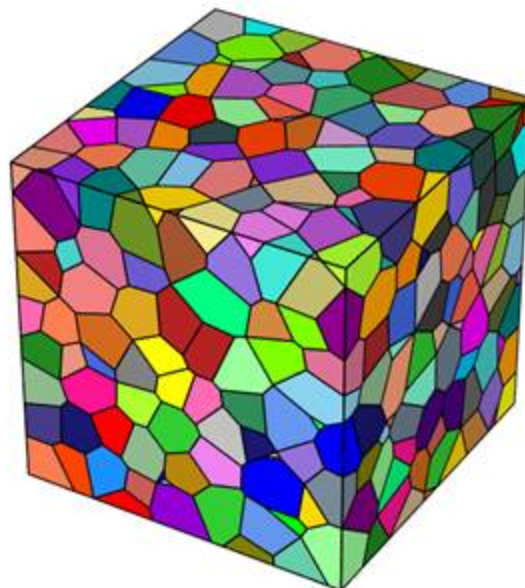


Voronoi Seeds from Mathematical Algorithms



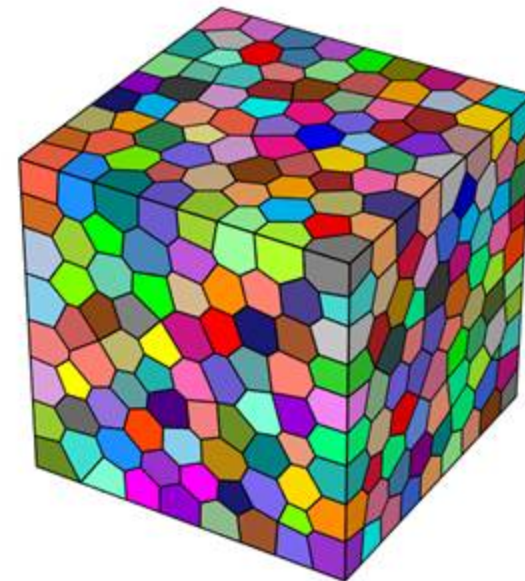
Poisson Voronoi

Seed positions
are random



Hardcore Voronoi

Exists a non-zero minimum
distance between the
seeds.

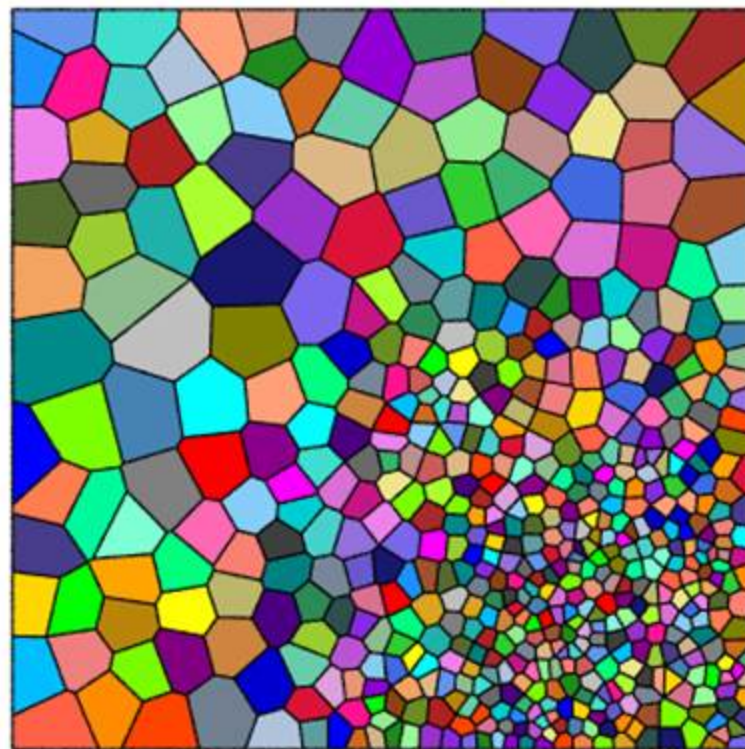
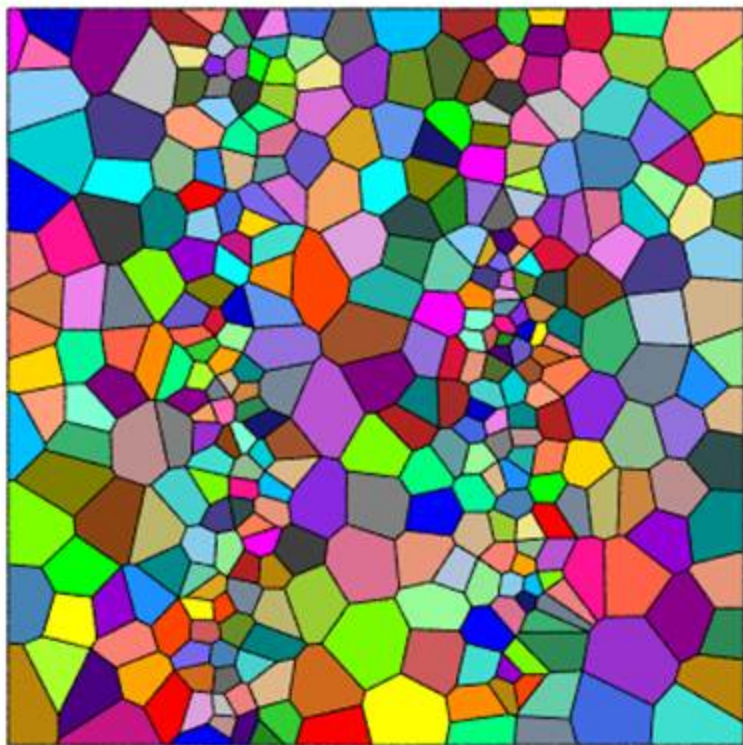


Centroidal Voronoi

Seeds and centroids
coincide



Voronoi Seeds: user specific manipulation

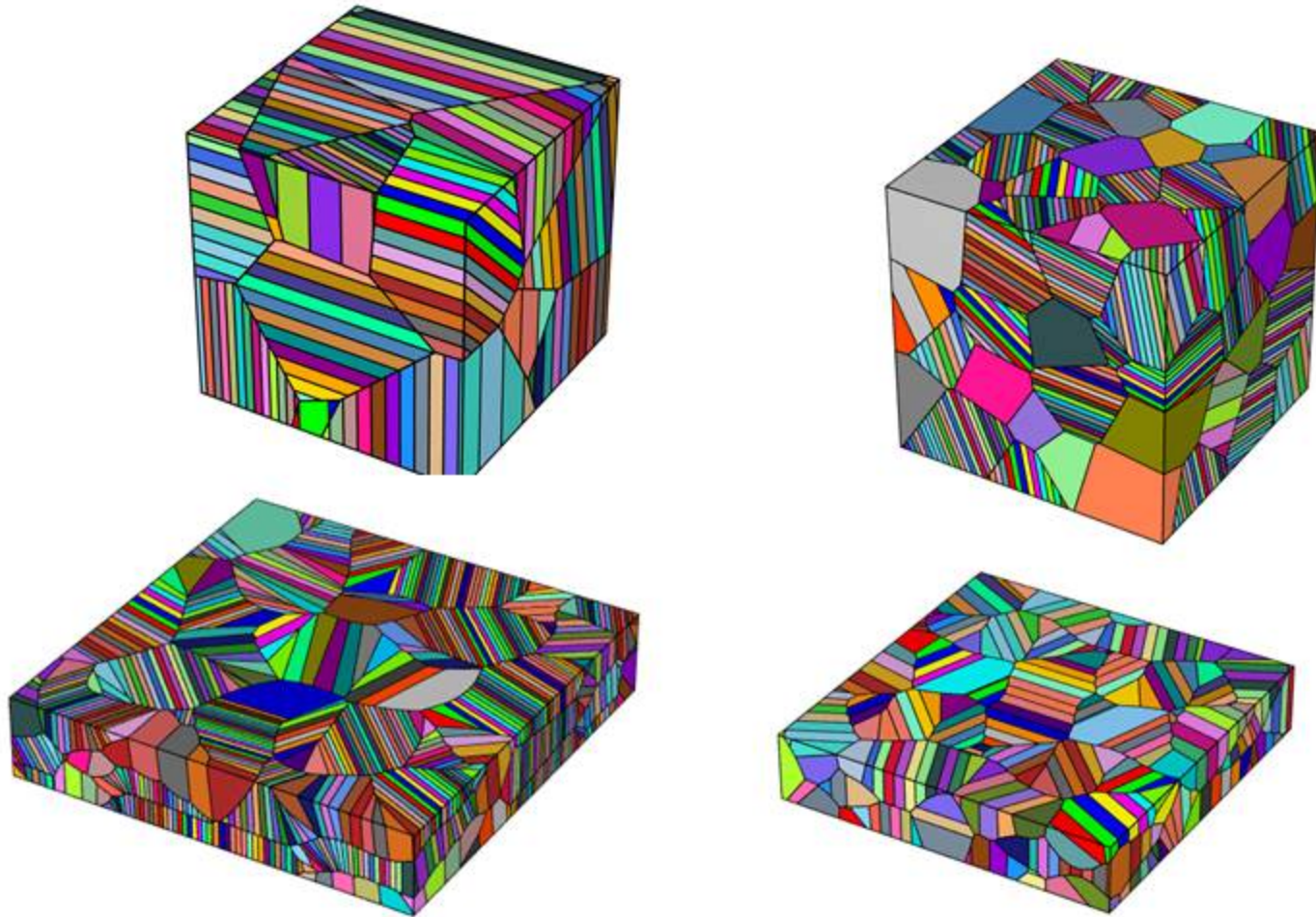


Procedure followed:

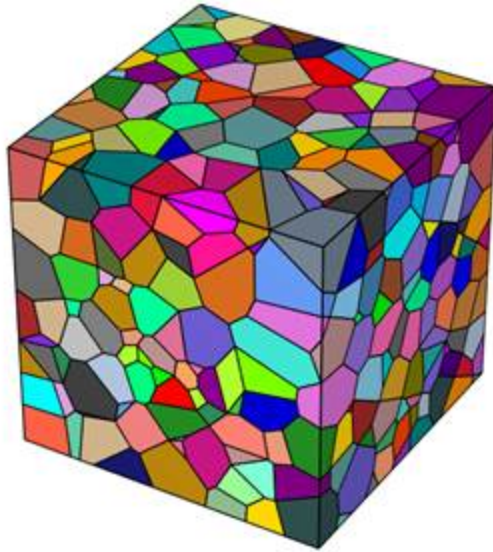
- Manipulate seed density
- Mix hardcore and centroidal voronoi



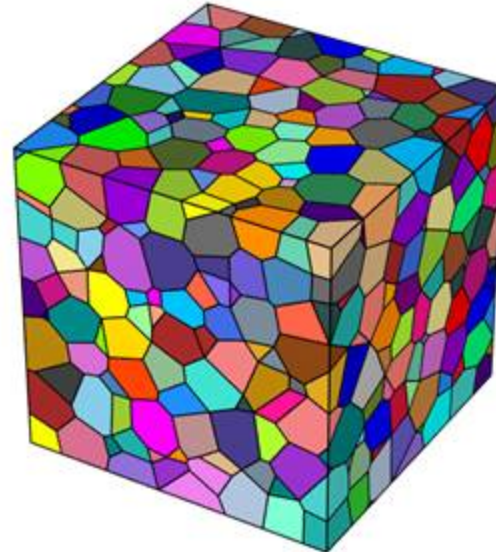
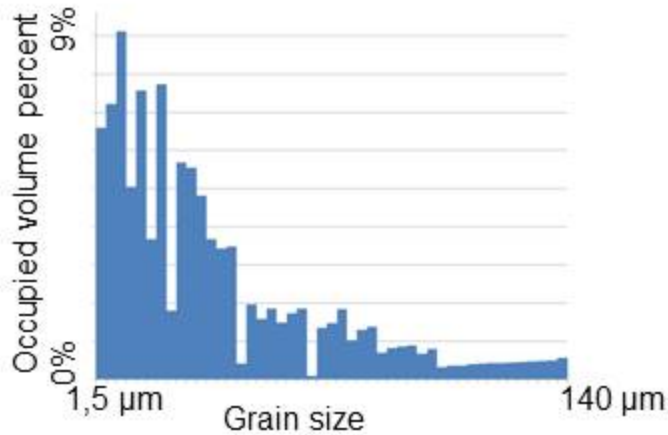
Two-Phase Microstructure



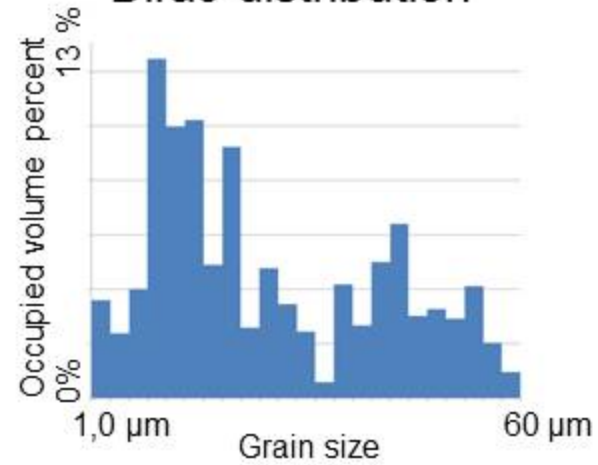
Use of Statistics from Microstructure analysis



Gaussian distribution



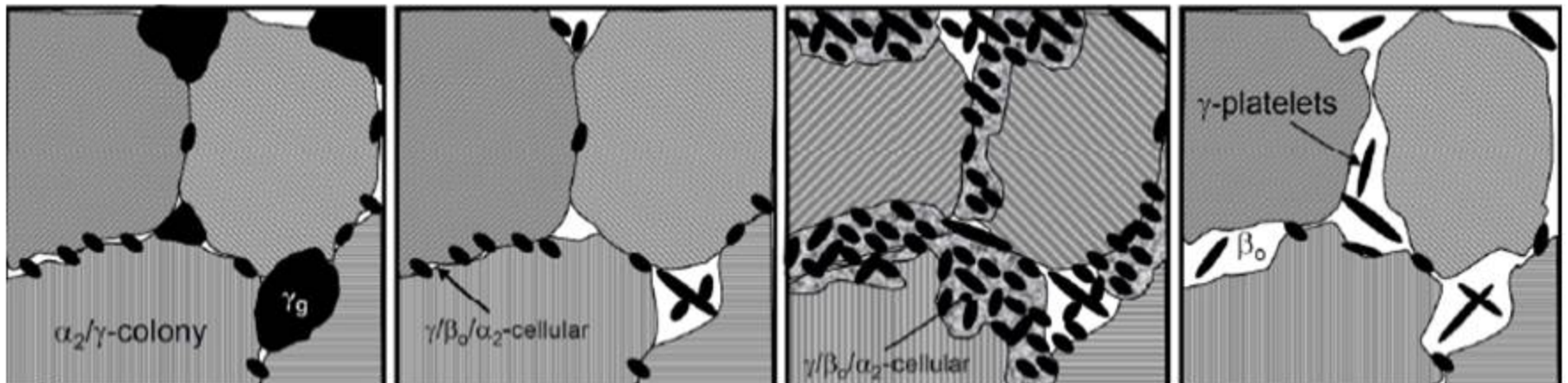
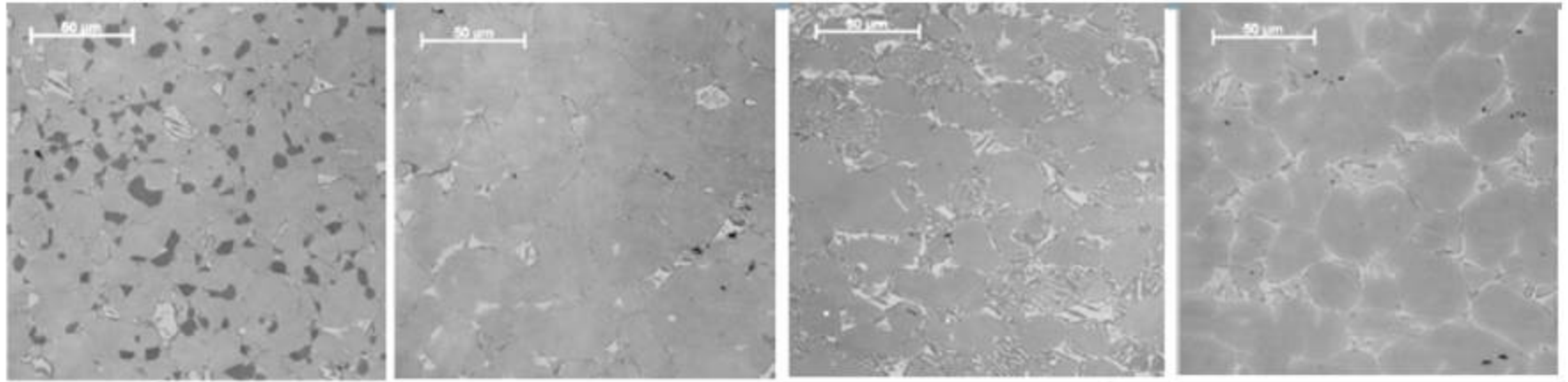
Dirac distribution



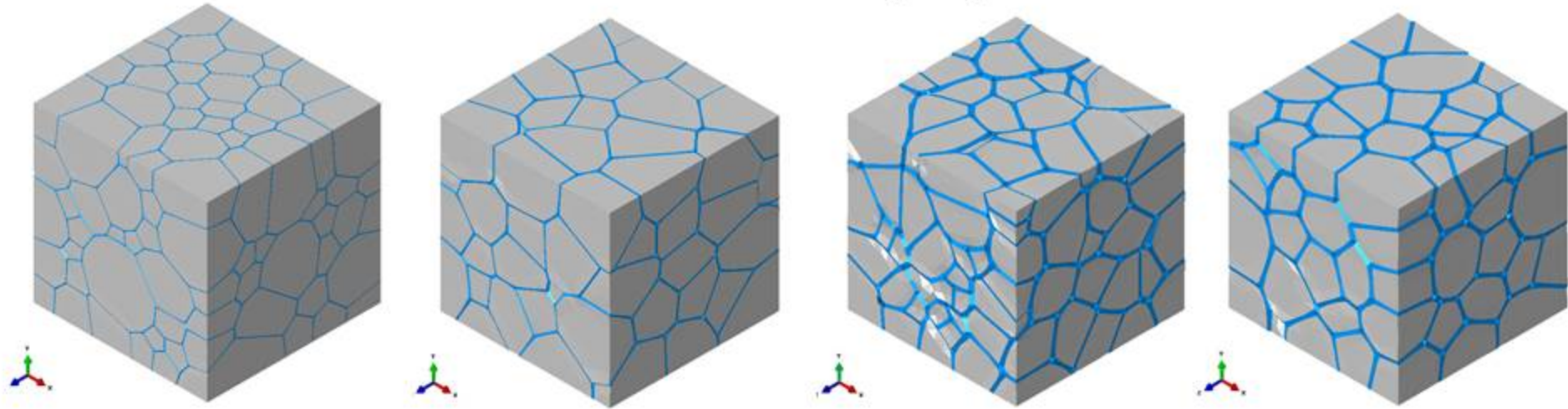
Microstructure TiAl (TNM)

Reference:

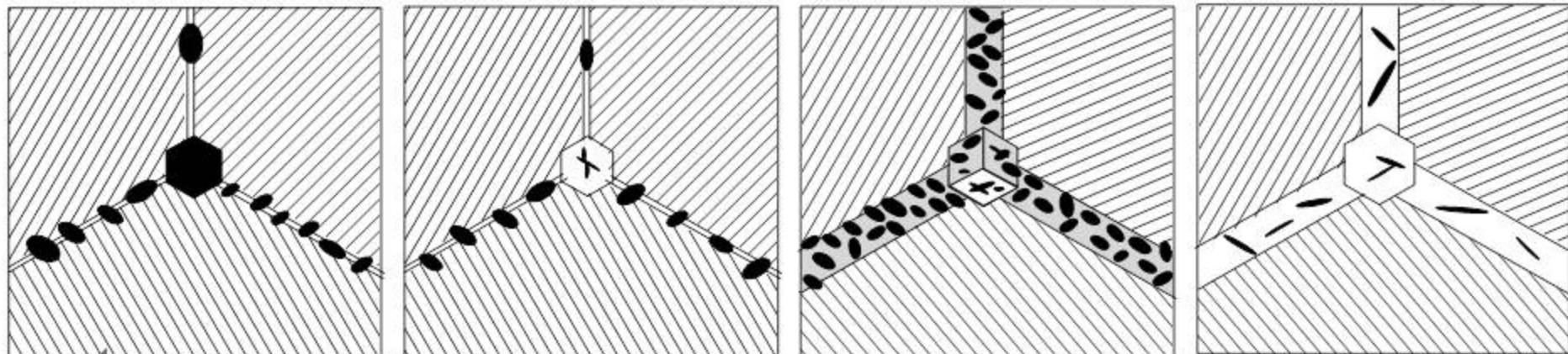
Schloffer et al, R-curve behaviour of different nearly lamellar microstructures in Ti-43.5Al-4Nb-1Mo-0.1B alloy, 146th Annual Meeting & Exhibition TMS 2017 Februar 26 – March 2, 2017, San Diego, California, USA



Virtual TiAl (TNM) Microstructure Mesoscale Polycrystal



Microscale Grain Boundary



(B) Constitutive Material Model

Temperature sensitive Crystal Plasticity model



Constitutive Behaviour of Phases: Crystal Plasticity Model

Open code for ABAQUS UMAT, Prof. Y Huang, Harvard University, 1991

Crystalline slip is assumed to obey Schmid's law:

$$\tau = n^{*(\alpha)} \frac{\rho_0}{\rho} \sigma \cdot m^{*(\alpha)}$$

Yield condition: $|\tau^{(\alpha)}| = g^{(\alpha)}$

Flow rule for slip:

- a viscoplastic power-type law
- a CRSS-based activation

$$\frac{\dot{\gamma}^{(\alpha)}}{\dot{\gamma}_0} = \left| \frac{\tau^{(\alpha)}}{g^{(\alpha)}} \right|^{n-1} \text{sign} \left(\frac{\tau^{(\alpha)}}{g^{(\alpha)}} \right)$$

Shear strain rate: $\dot{\gamma}^{(\alpha)}$

Reference strain rate: $\dot{\gamma}_0$

Current strength: $g^{(\alpha)}$

Physically motivated kinetic equation proposed by Kothari and Anand (1998).

$$\dot{\gamma}_\alpha = \dot{\gamma}_0 \exp \left\{ -\frac{\Delta F}{k_B T} \left[1 - \left(\frac{\tau_t^\alpha}{g_t^\alpha} \right)^p \right]^q \right\} \text{sign}(\tau^\alpha)$$

$$\text{where } \tau_t^\alpha = \left[1 - \left(\frac{T}{T_C} \right)^{1/q} \right]^{1/p} \text{ and } T_C = \frac{\Delta F}{k \ln \left(\frac{\dot{\gamma}_0}{\dot{\gamma}_0^\alpha} \right)}$$

ΔF = Activation free energy required to overcome the obstacles to slip without the aid of an applied shear stress

k_B = Boltzmann Constant

p, q = Glide resistance profile for short range dislocation ($0 \leq p \leq 1$ and $1 \leq q \leq 2$)

T = Temperature

T_C = Temperature above which there is enough thermal energy to overcome the barriers only by thermal activation



Constitutive Behaviour of Phases: Crystal Plasticity Model

Rate sensitivity m from Kothari and Anand (1998)

$$m = \frac{\partial \ln|\tau|}{\partial \ln|\dot{\gamma}|} = \frac{k_B T}{\Delta F} \frac{1}{pq} \left(\frac{\left(\frac{T}{T_c}\right)^{\frac{1}{q}-1}}{1 - \left(\frac{T}{T_c}\right)^{\frac{1}{q}}} \right)$$

Implemented by:
R. Kabir, U. Ilyas

Modified CPFEM for temperature sensitivity

$$\dot{\gamma} = \dot{\gamma}_0 \frac{\tau}{g} \left| \frac{\tau}{g} \right|^{\frac{1}{m}-1} \quad \dot{\gamma} = f(\dot{\gamma}_0, \tau, g, T, \Delta F)$$

Flow rule for twin (Kalidindi 2001):

- a power-type law
- a unidirectional, CRSS-based activation

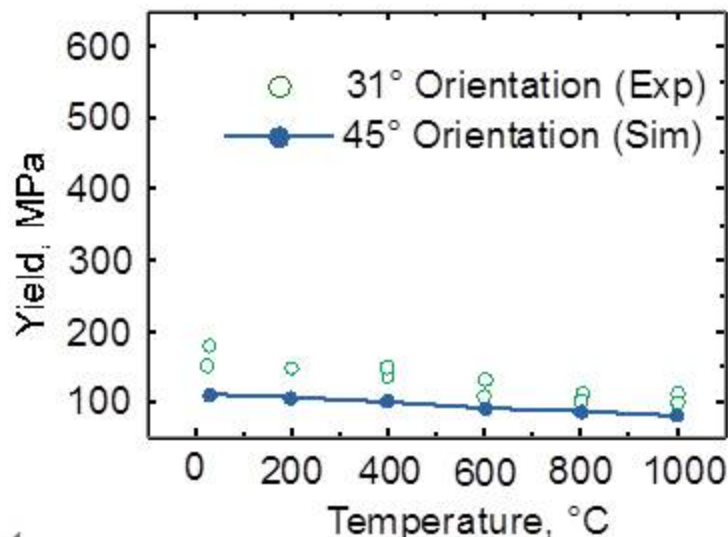
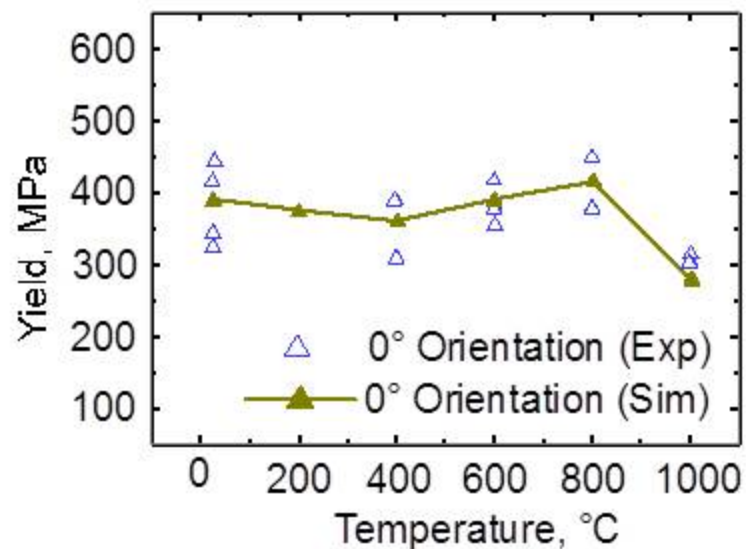
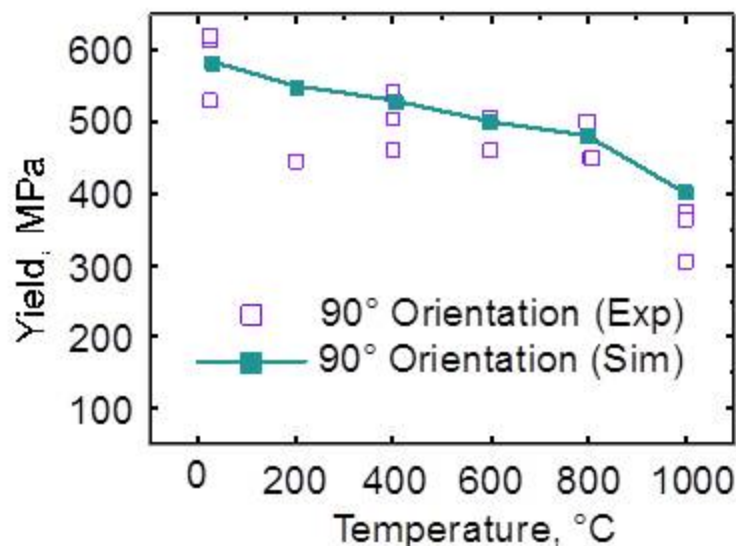
$$\frac{\dot{f}^{(\beta)}}{\dot{f}_0} = \left| \frac{\tau_{twin}^{(\beta)}}{g^{(\beta)}} \right|^{n-1} \quad \text{if} \quad \frac{\tau^{(\beta)}}{g^{(\beta)}} > 0$$

Evolution of slip system hardening (Linear type):

$$\dot{g}^{(\alpha)} = \sum_{\beta} h_{\alpha\beta} \dot{\gamma}^{(\beta)} \quad \text{Where,} \quad h_{(\alpha\beta)} = q_{(\alpha\beta)} h_{\beta}$$



Validation: Simulation for High temperature behaviour



Experiment: Inui et al., Philosophical Magazine A, 78, 1-28, 1998.



(C) Double Shear Test simulation



Double Shear Test: Experiment from Uni Bochum

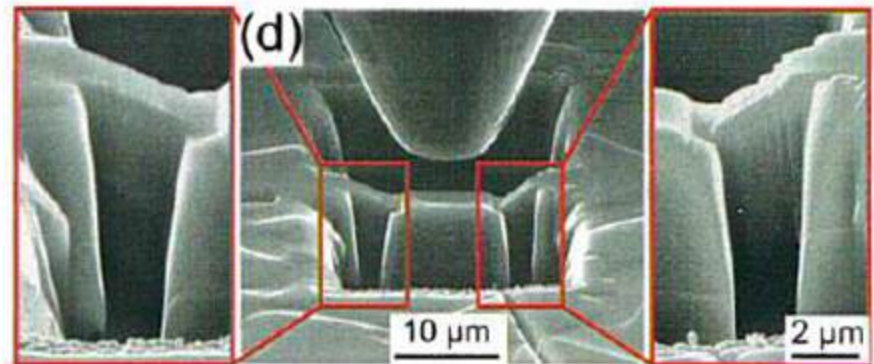
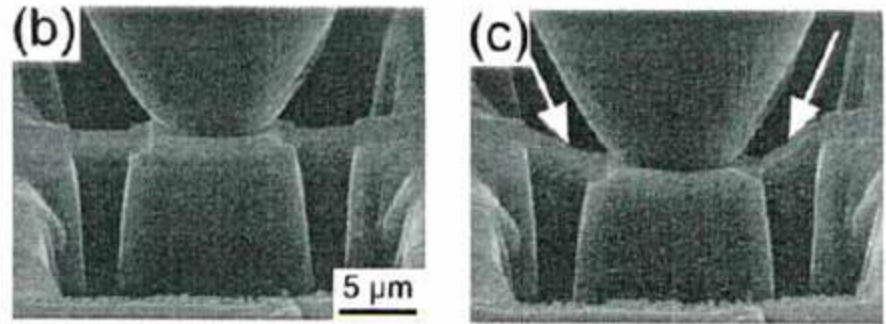
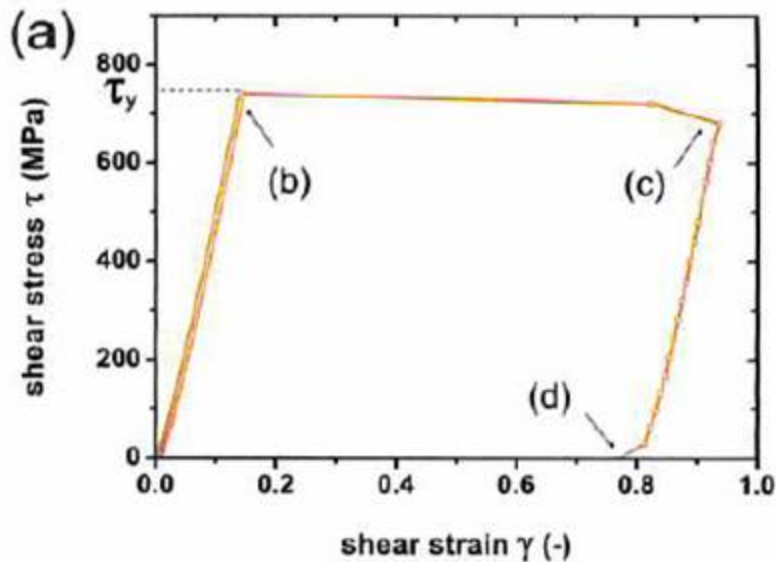


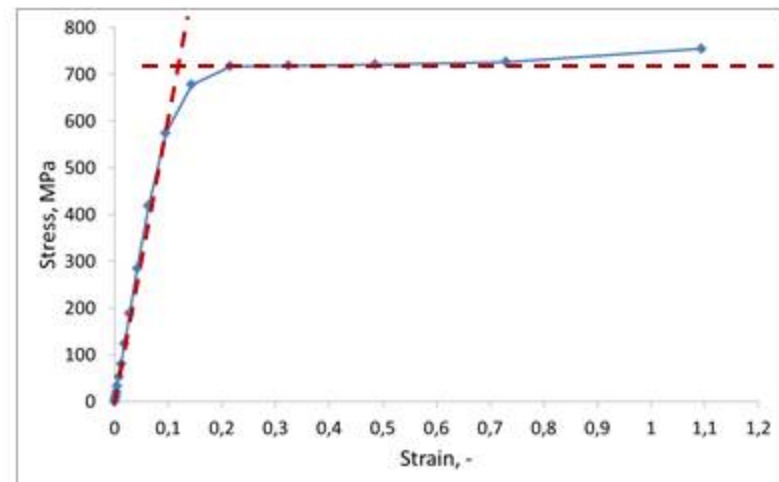
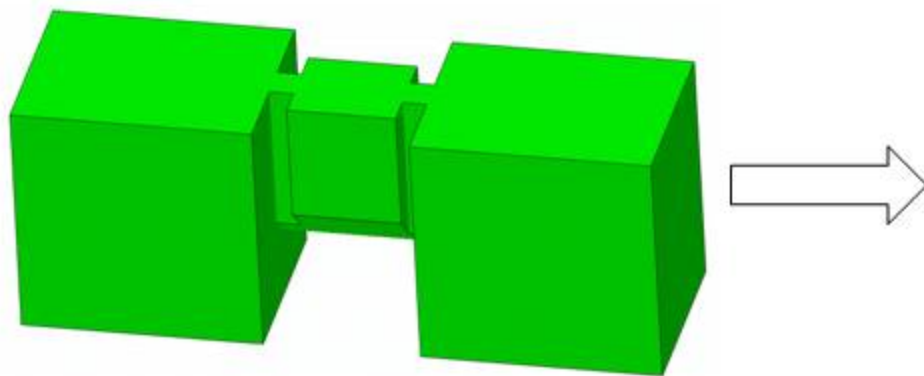
Fig. 5: In situ SEM microshear experiment. (a) Shear stress-shear strain curve. (b-d) SEM images, which show the shear specimen after different amounts of shear strain.

- Activation of a specific slip system.
- Localized plastic deformation.

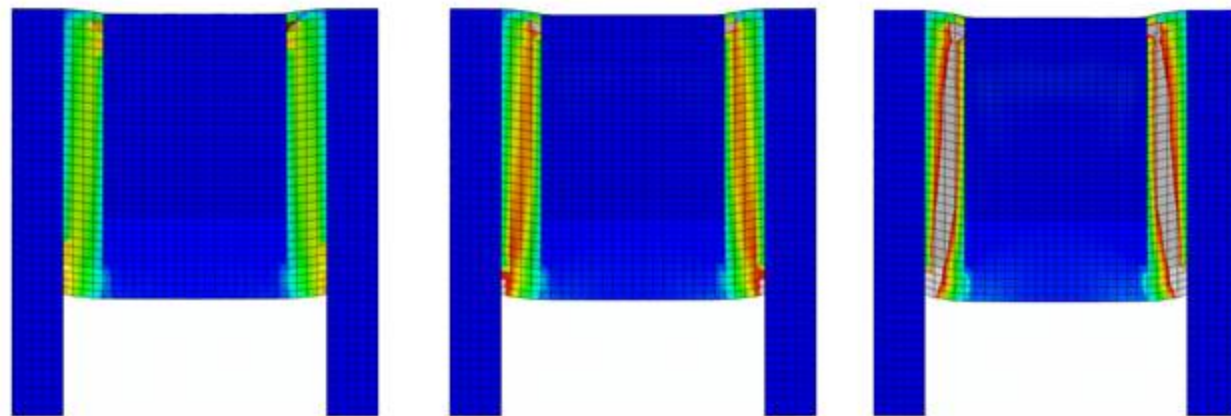
Wieczorek et. al, 2016,
Poster, TiAl workshop Tokyo



Simulation: Double Shear Test



SDV145 (Total Shear Strain)



Key Interest:

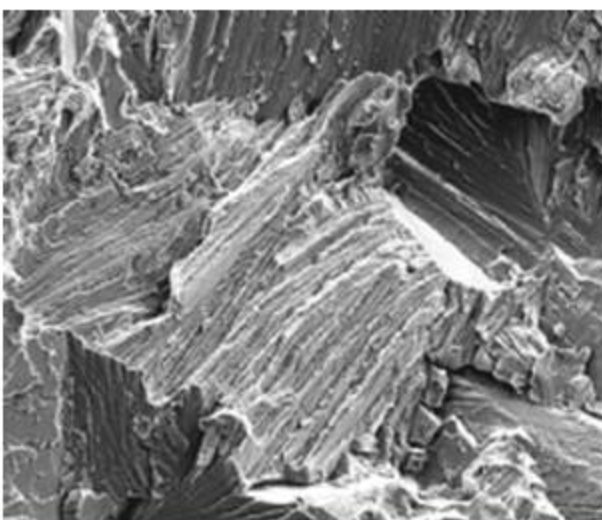
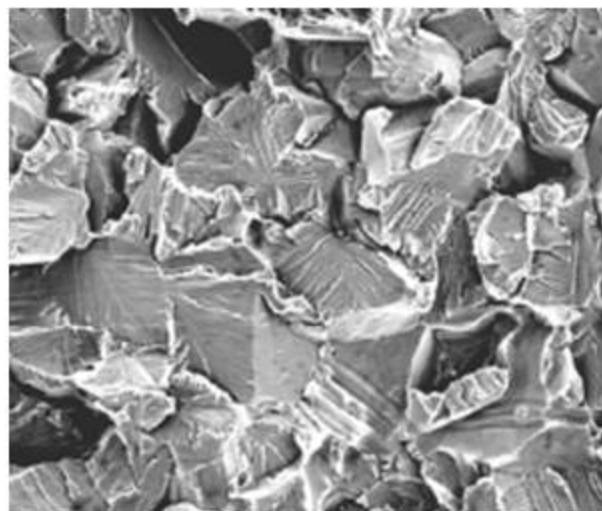
- Strength of material at a particular slip plane
- Damage parameter for a particular slip plane



(D) Modelling of Fracture of TiAl using Unit cells



Fracture surfaces of TiAl



- Trans granular fracture
- Trans-lamellar fracture
- Inter-lamellar separation
- Grain boundary fracture

Two basic mechanisms:

- Interlamellar fracture, grain boundary fracture
 - **Interface failure/debonding**
- Translamellar fracture, Intergranular fracture
 - **splitting of material**



Focus on Lamellar fracture
(capture both interface failure and splitting)

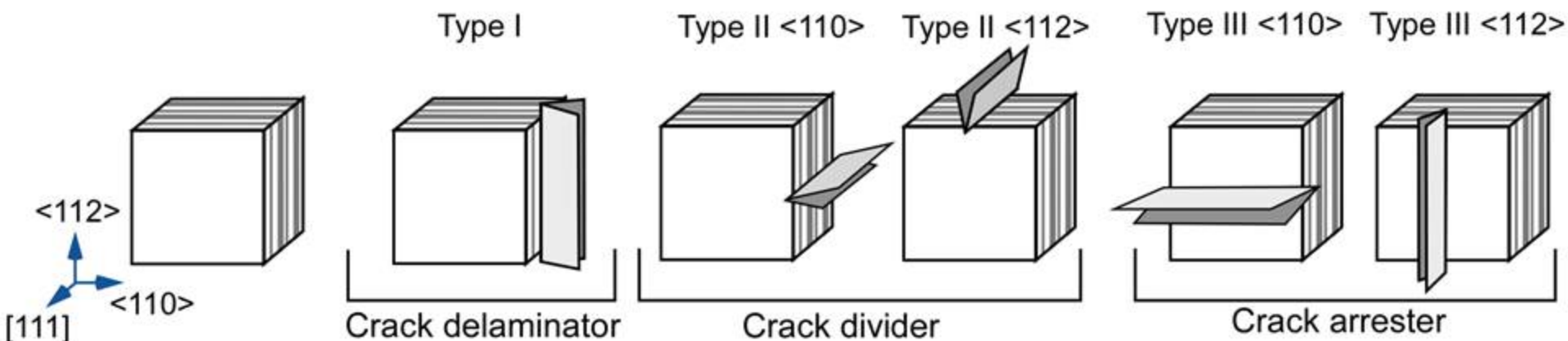
Study of PST-TiAl

Kabir et al, Mat Sci Engg, 2015



Understanding fracture from PST-TiAl alloy

Notch-tip orientation with respect to lamellar plane



H Inui, MH Oh, A Nakamuar, M Yamaguchi, 1992

M Yamaguchi, H Inui, J Mater Sci Technol, 1994

S. Yokoshima, M. Yamaguchi, Acta mater 1996

R. Lebensohn, H. Uhlenhut, C. Hartig, H. Mecking, Acta Mater. 1998



Experiment of PST single crystal

3-point bending test:
Poly synthetically twinned (PST) crystal

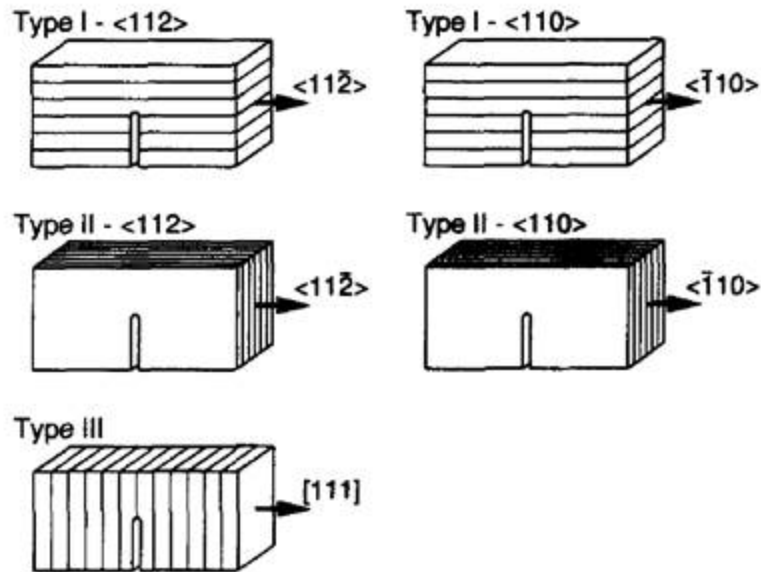


Fig. 5. Notch orientations of three-point bend specimens cut from PST crystals.

Kishida et al, Intermetallics 6 (1998) 679-683

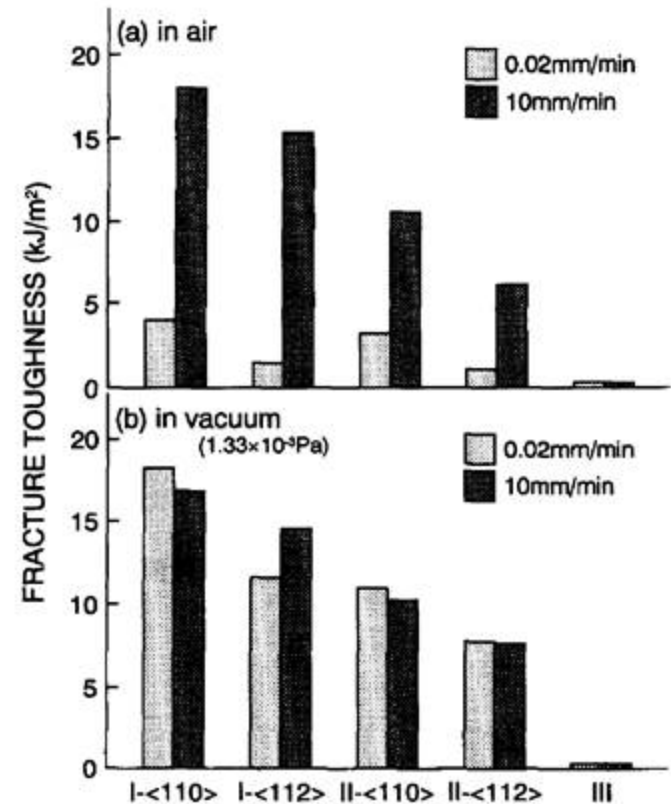
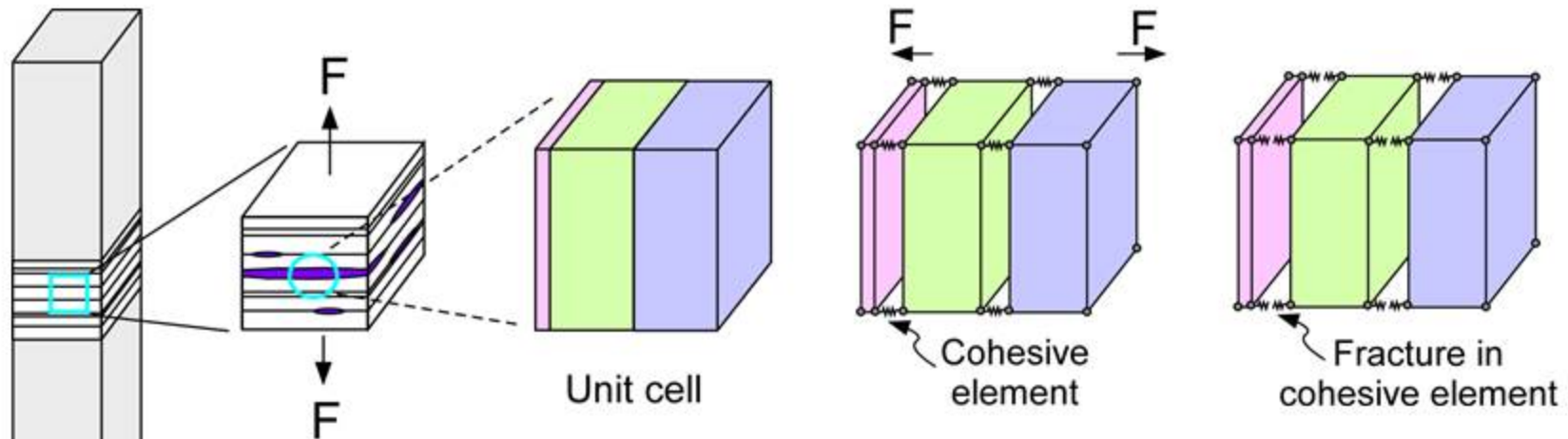


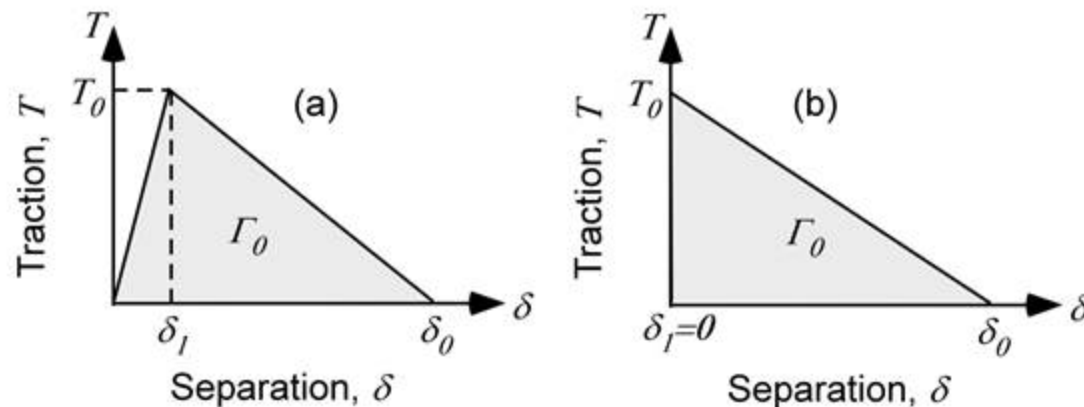
Fig. 6. Fracture toughness values for five notch orientations of Ti-49.3Al (at %) PST crystals at load-line displacement rates of 0.02 and 20 mm min⁻¹ in air and in vacuum.



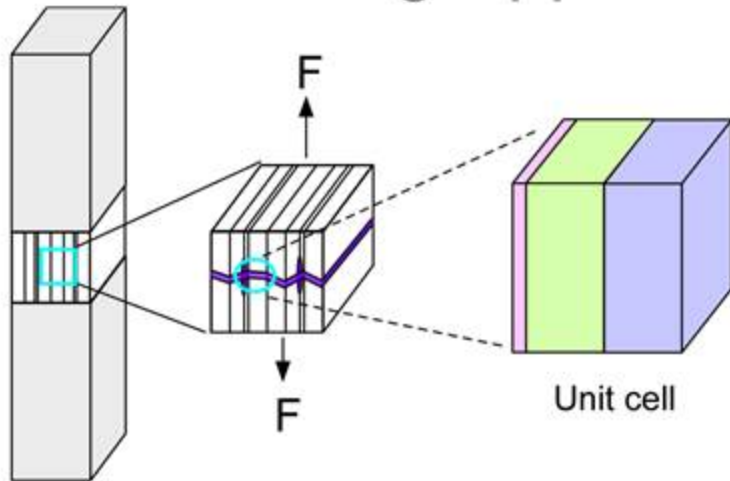
Modelling approach for interlamellar fracture



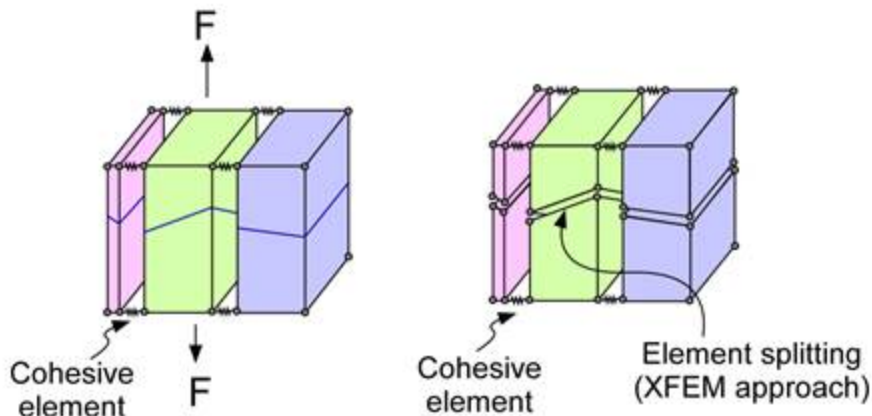
Decohesion between two phases are modeled by a **traction-separation law** using cohesive model (local approach)



Modelling approach for translamellar fracture



- At lamellar interface - the crack path is known
- Inside the lamellae - crack may develop at any place, any angle



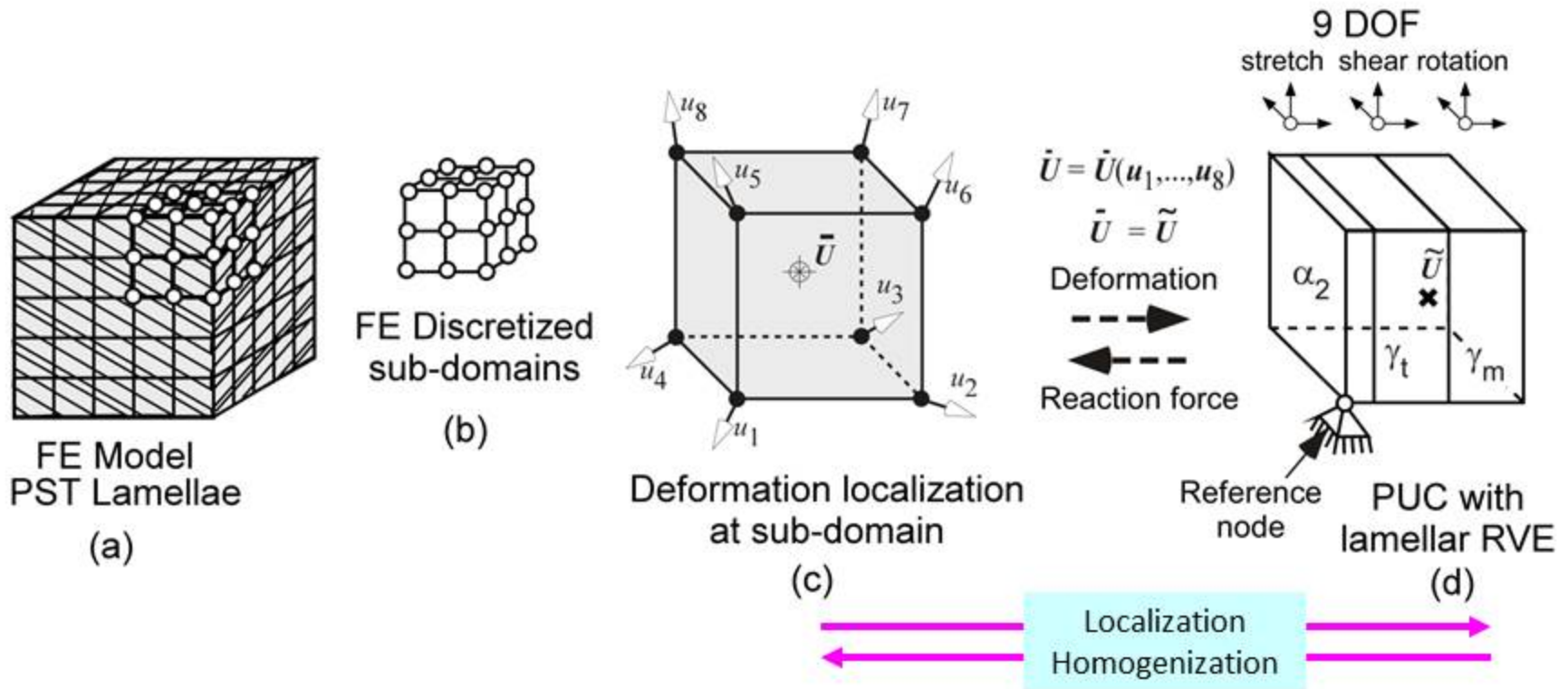
- For the numerical implementation of **material splitting** two actions need to be incorporated:
- Splitting the geometry (here, element)
 - Numerical approach
- Criteria for splitting
 - Material models for damage (Cohesive Model)



- Can be handled by using eXtended Finite Element Method (XFEM)
- Method for modelling discontinuity
- No predefined crack path is required (Position of crack is a part of the solution)



Two-scale linking (based on FE2 approach)



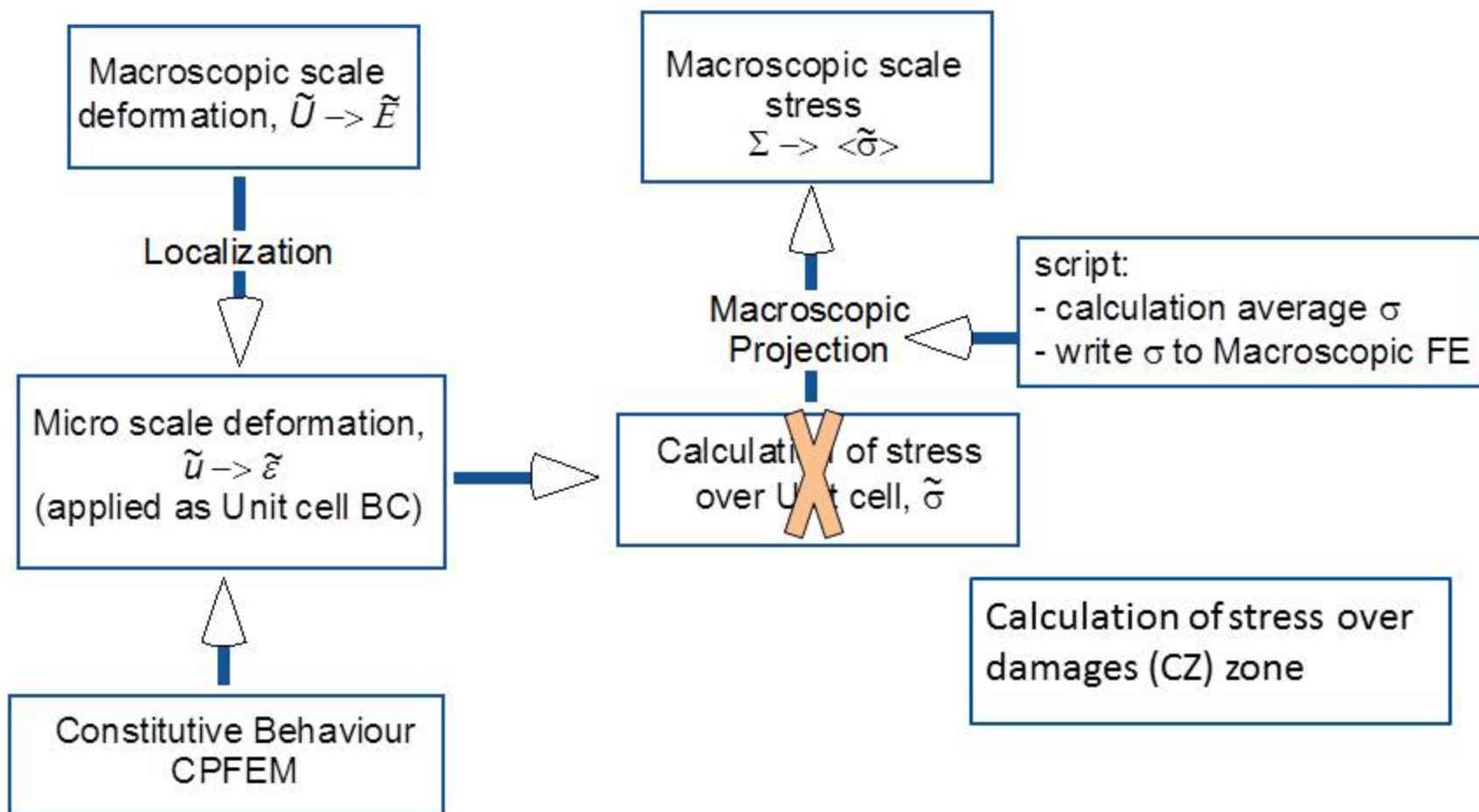
Implemented in ABAQUS through script files

- Relaxed constraint BC for matrix and twin deformation
- Anisotropic elasticity
- Crystal plasticity constitutive model

Werwer et. al. *Comp. Mat. Sci.* 19, (2000) 97
 Kabir et. al, *Acta Mat* 58 (2010), 5834



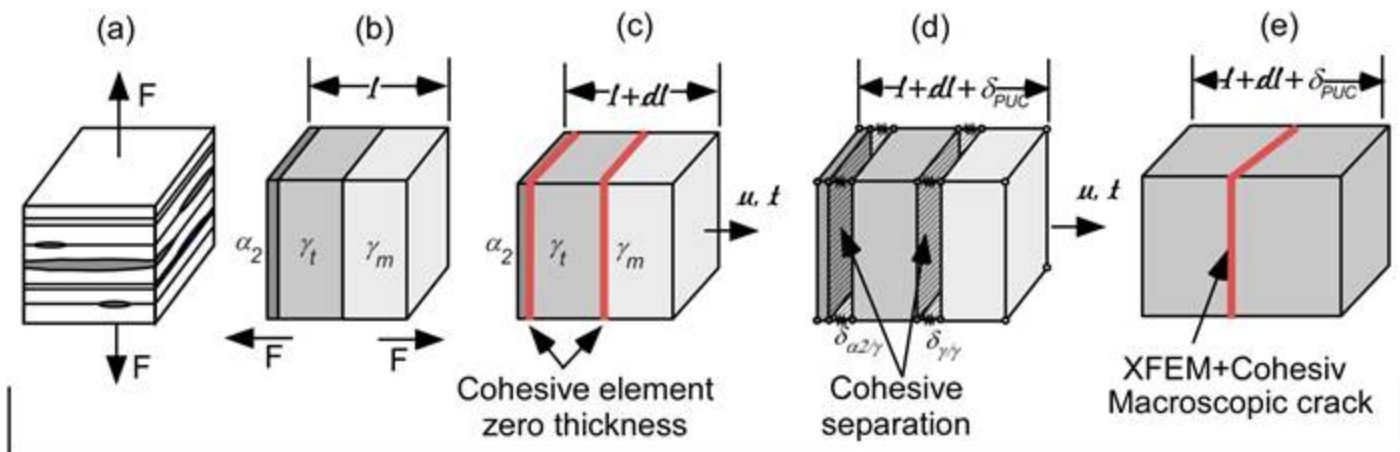
Calculation Flowchart



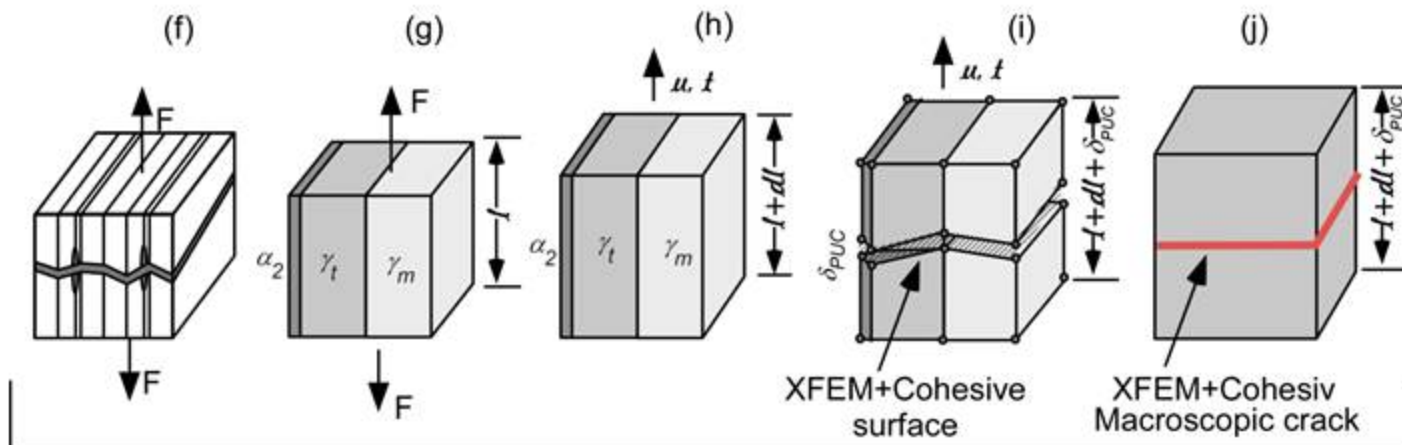
Verhoosel et al, Int. J. Numer. Meth. Engng, 2010



Fracture modelling approach



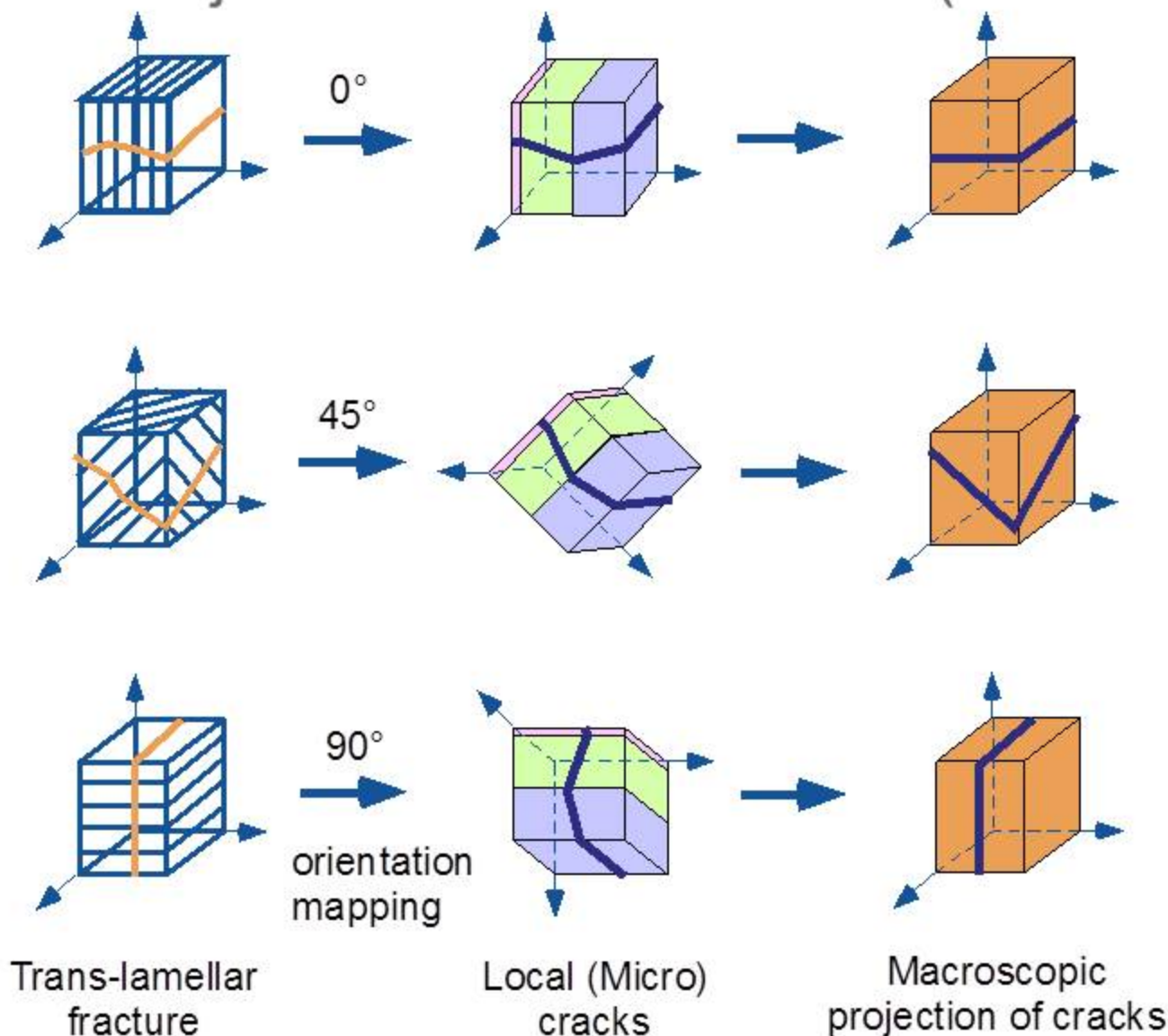
Interlamellar fracture



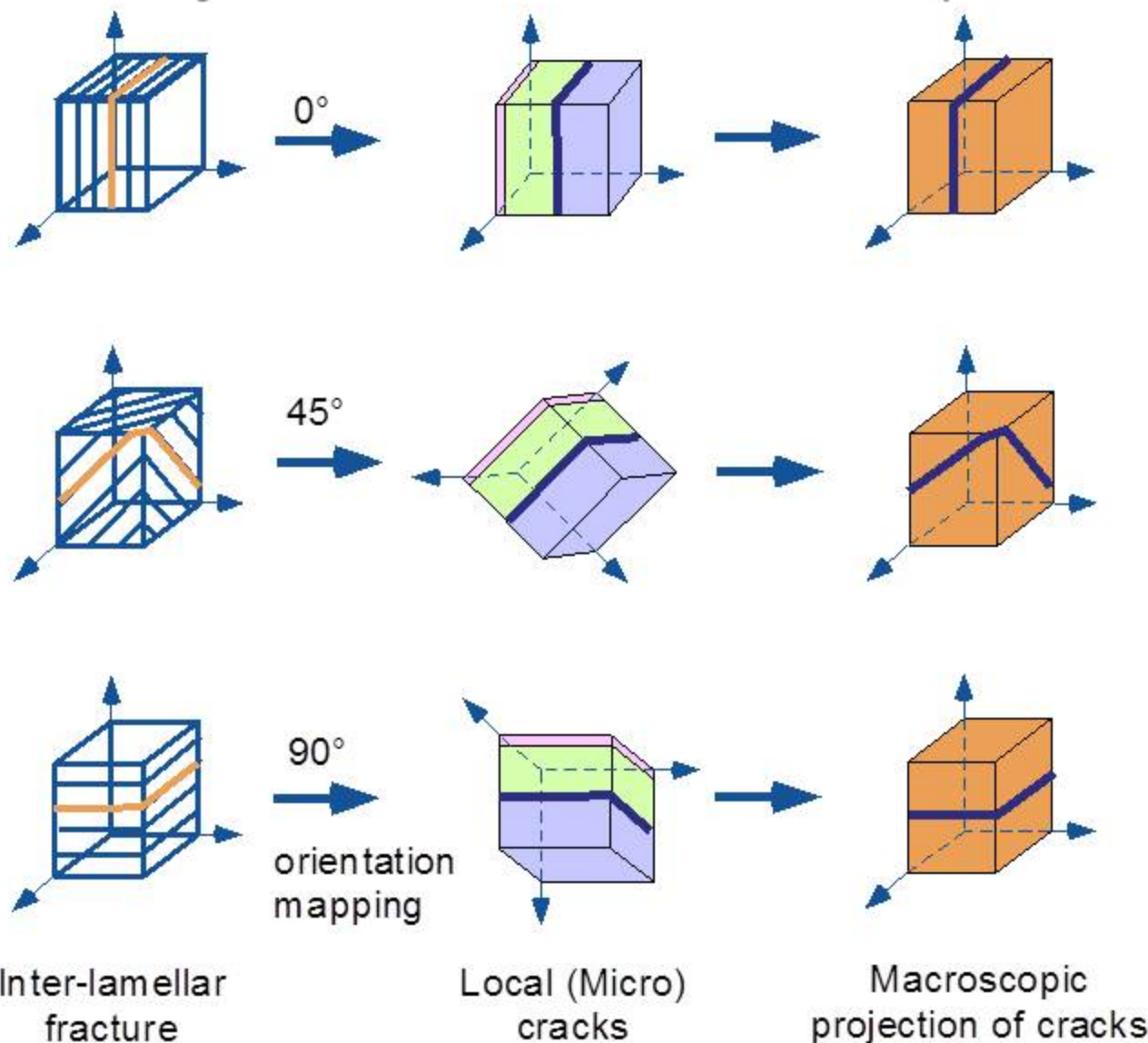
Translamellar fracture



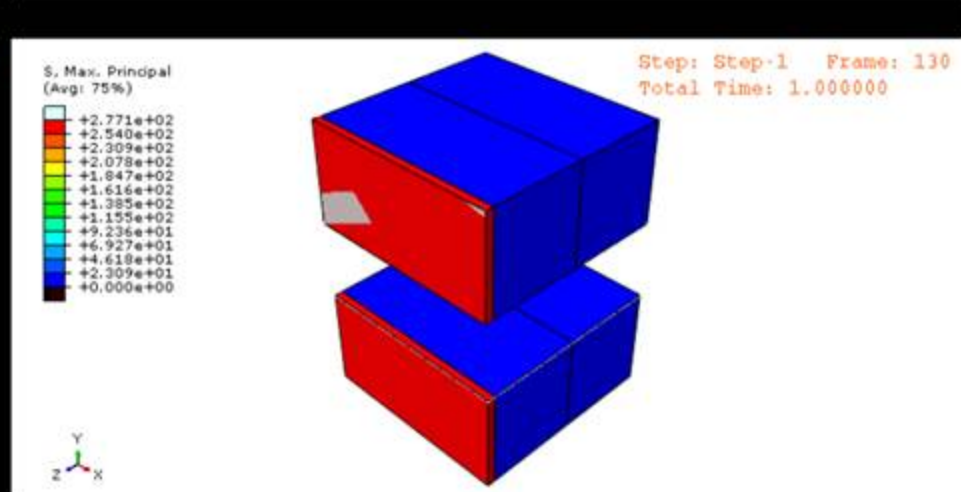
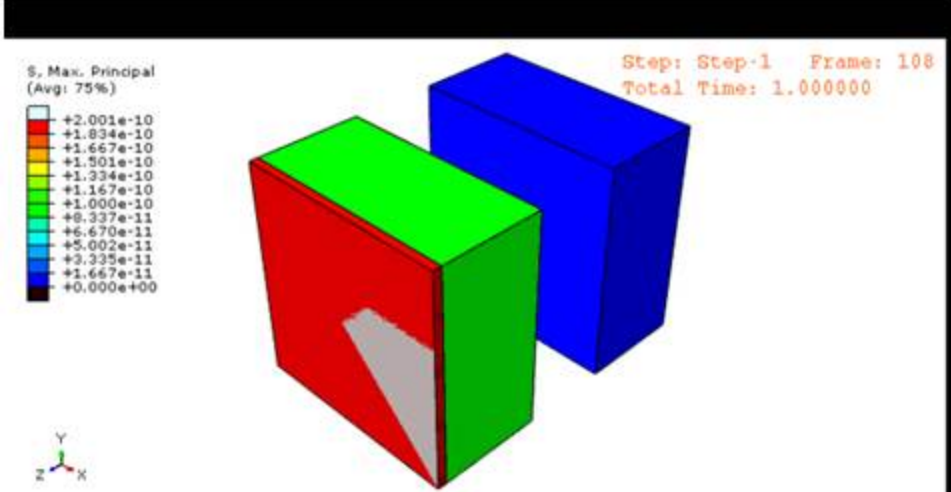
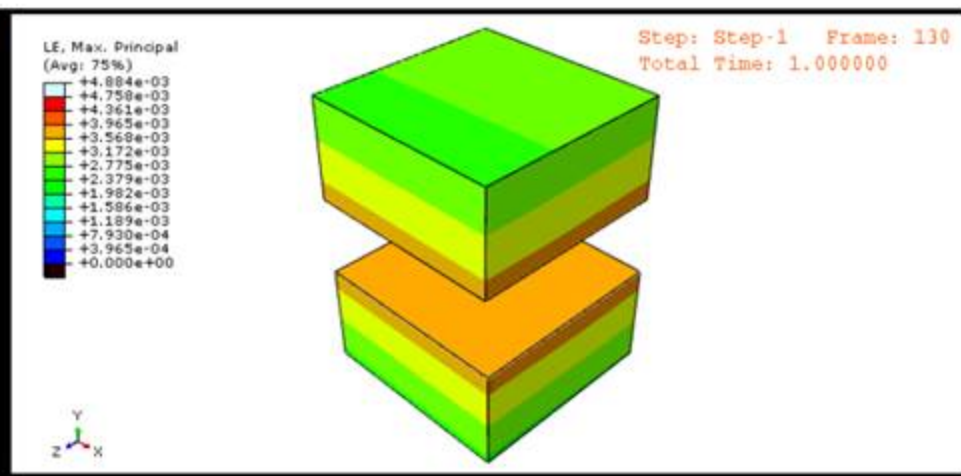
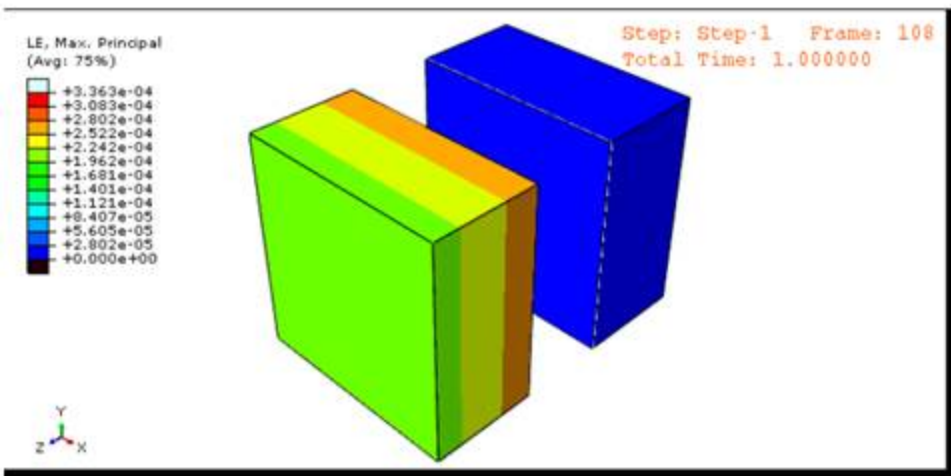
Micro-Macro Projection: Oriented cracks (Trans-lamellar)



Micro-Macro Projection: Oriented cracks (Inter-lamellar)



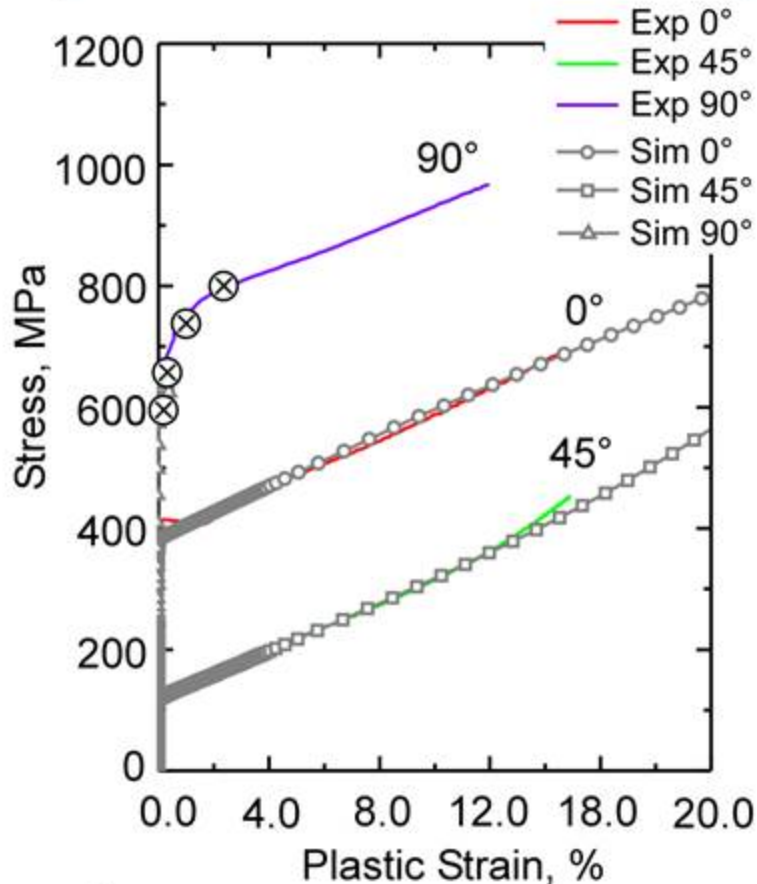
Single element test: Interlamellar & Translamellar fracture



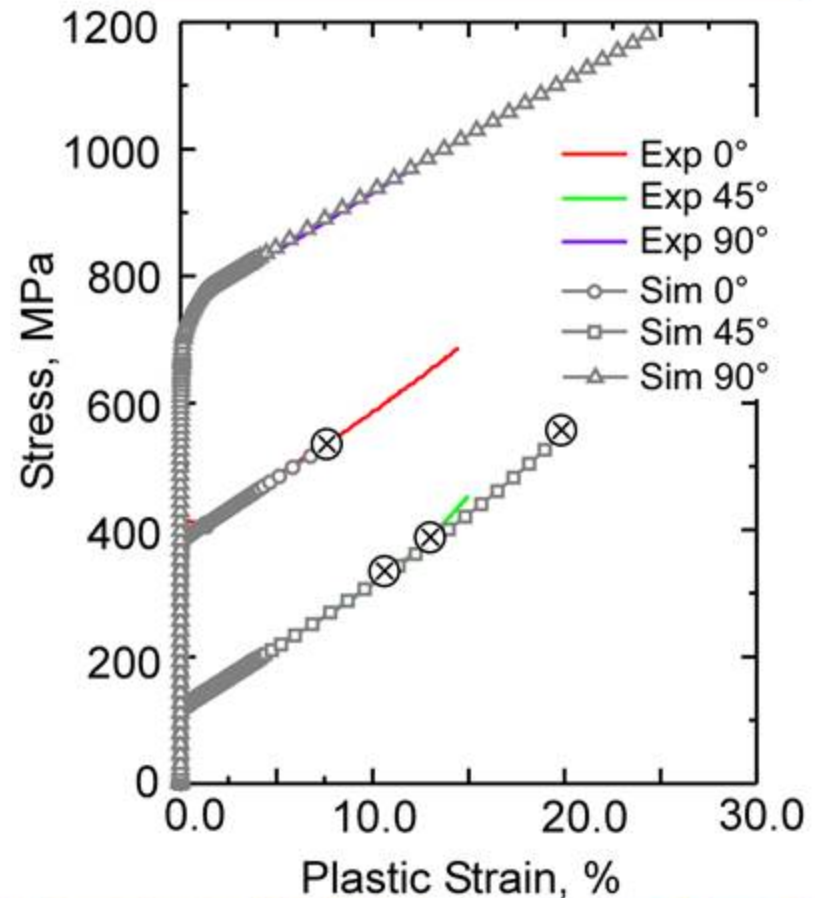
Simulations: Parameter Study

Single crystal: Ti-49Al (two-phase lamellar PST alloy), Experiments: H. Uhlenhut, TUHH, 1999

Estimation of Interlamellar fracture strength, $T_{\alpha/2/\gamma}$



Estimation of Translamellar fracture strength, $T_{\alpha 2}, T_{\gamma}$



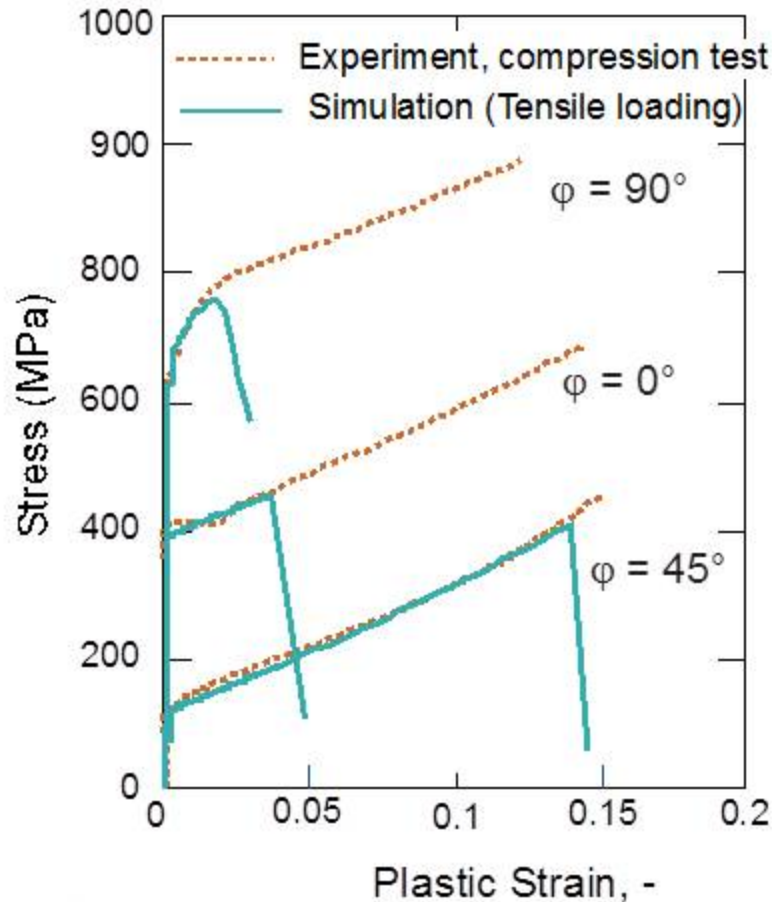
Experiment vs simulation: Single lamellar crystal

Single crystal PST alloy: **Ti-49Al (at.%)**

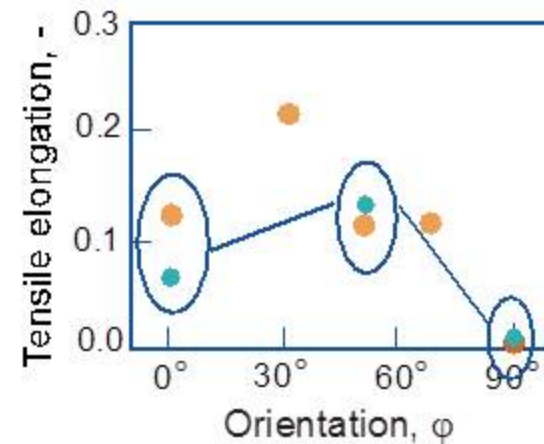
H. Uhlenhut, PhD Thesis, TUHH, 1999

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*



Results: Fracture strength
properties $T_{\alpha 2} > T_{\gamma} > T_{\alpha 2/\gamma}$



Thank you for your attention

Email: mohammad-rizviul.kabir@dlr.de

