



# **Influence of microstructural heterogeneity on the micro-meso deformation of a two-phase TiAl alloy investigated by nanoindentation and a numerical two scale model**

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# Outline

- Material and microstructure
- Investigation of material behavior
  - Nanoindentation testing
  - Influence of heterogeneity: scatter in Young's modulus
- Modeling approach
  - FE model
  - Model parameters
- Simulation of nanoindentation
  - Simulation results
- Summary and conclusion

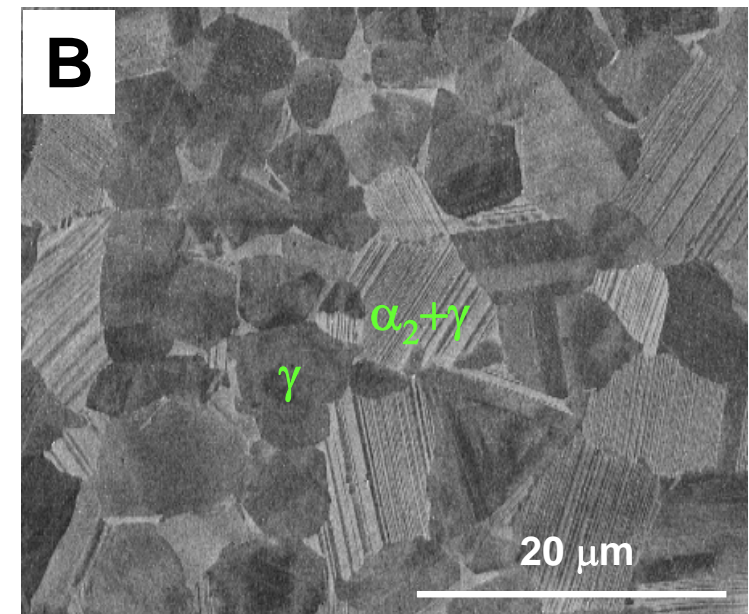
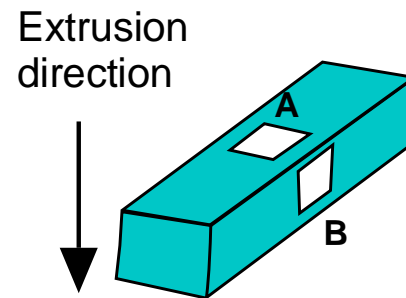
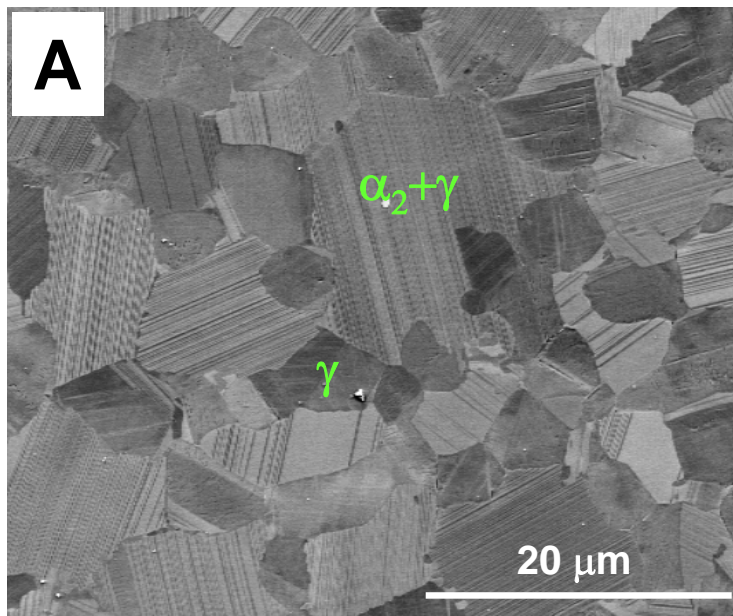
# Material and microstructure

## TNB alloy: Ti -45Al -5Nb-0.2B (at%)

- Extruded and forged
- HT: 1260°C, 1h, AC + 850°C, 6h, FC in calm air
- Microstructure: Duplex type
- 20-30% vol. of globular grains

## Microstructural heterogeneity

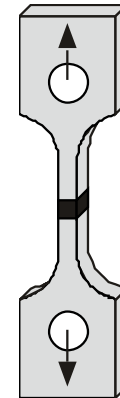
- Presence of different phases
- Distribution of grain/colony size and orientations
- Variable lamellae thickness
- Clusterization of grains/colonies



# Influence of heterogeneity on material and structural behavior on different length scales

## ➤ Macro scale (specimen, component)

- Scatter in E-modulus
- Variable plastic strain limit
- Scatter in fracture strength

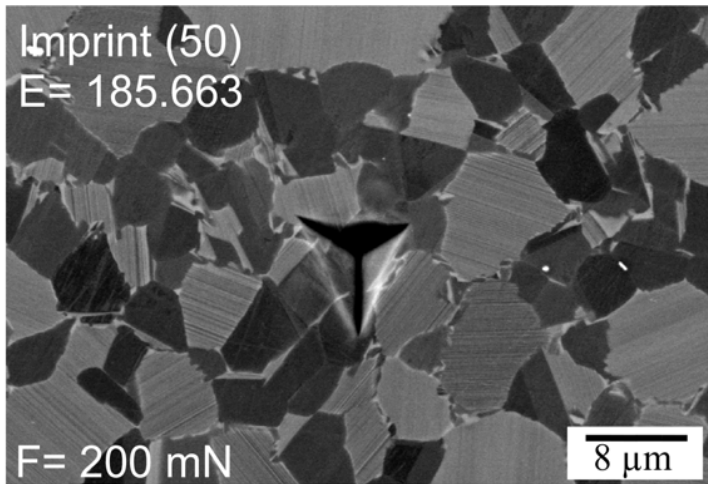
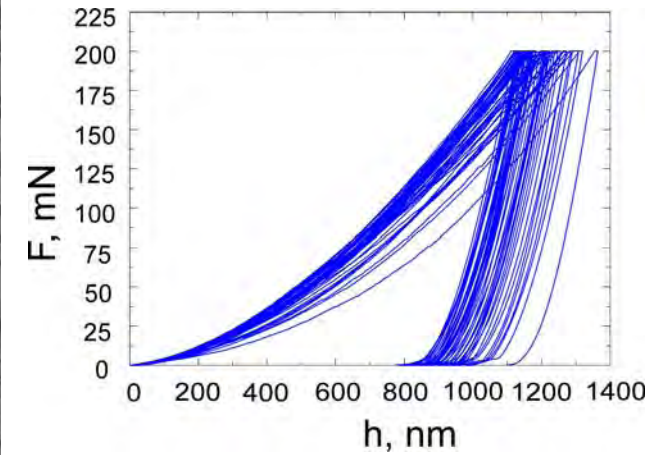
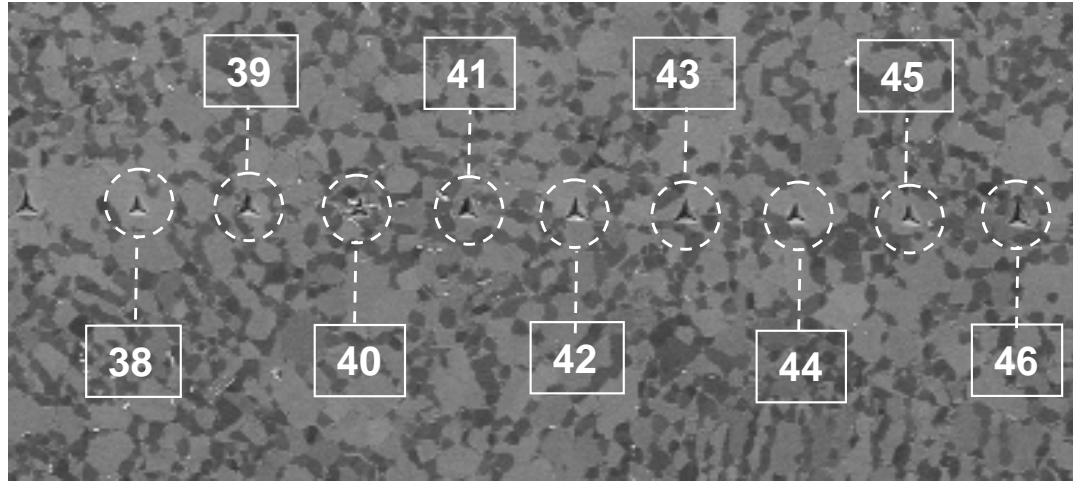
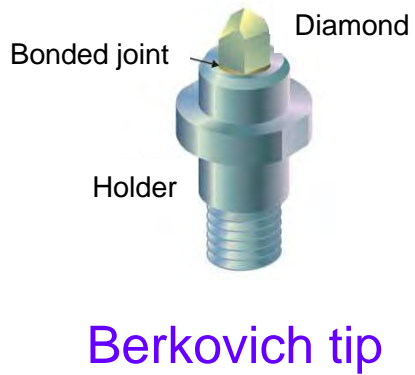


## ➤ Meso-micro scale (on microstructure level)

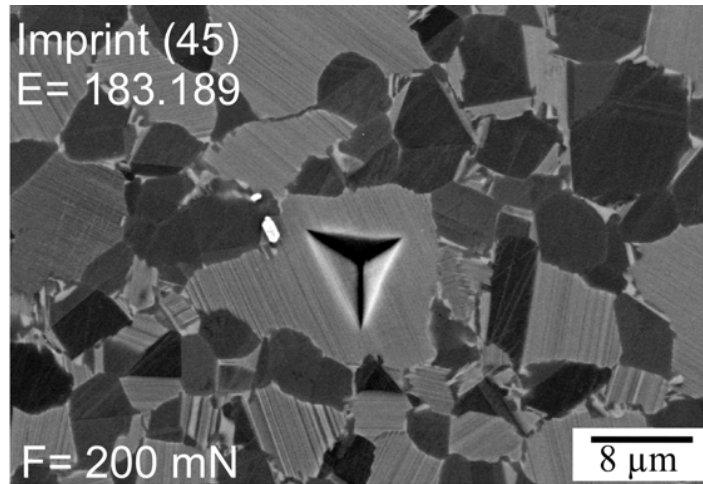
- Scatter in E-modulus
- Inhomogeneous local stresses and strains
- Heterogeneous microcracking



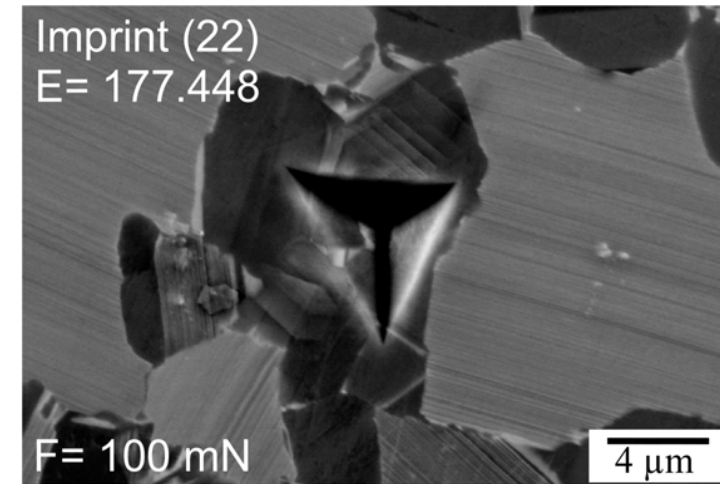
# Material behavior on meso level: Nanoindentation



Poly grains



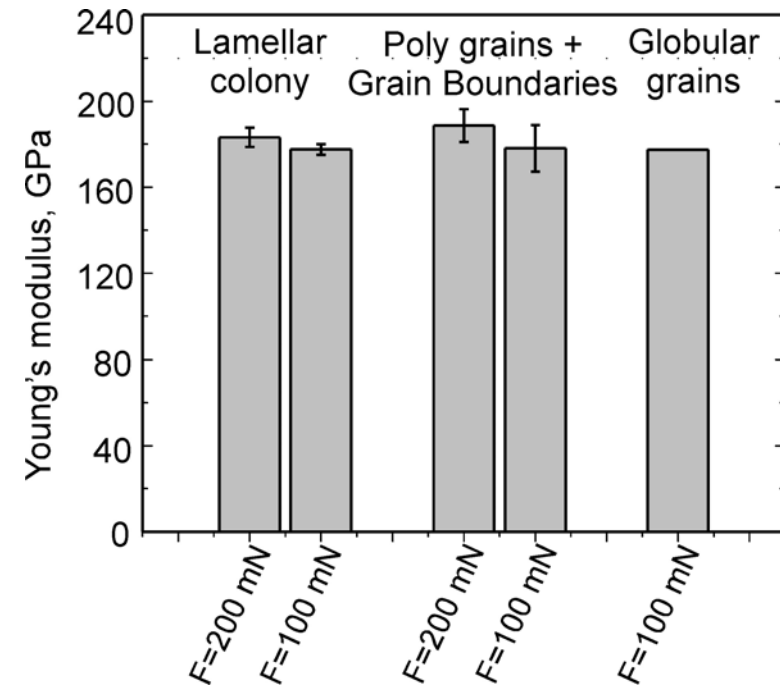
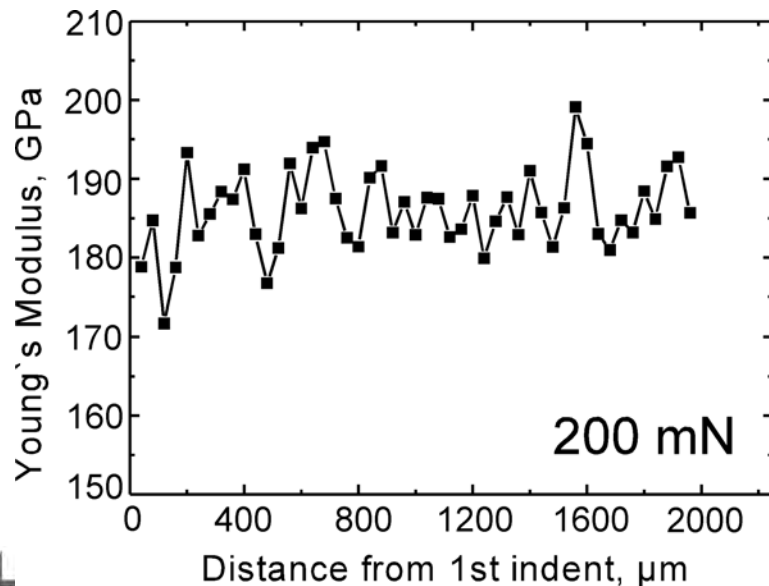
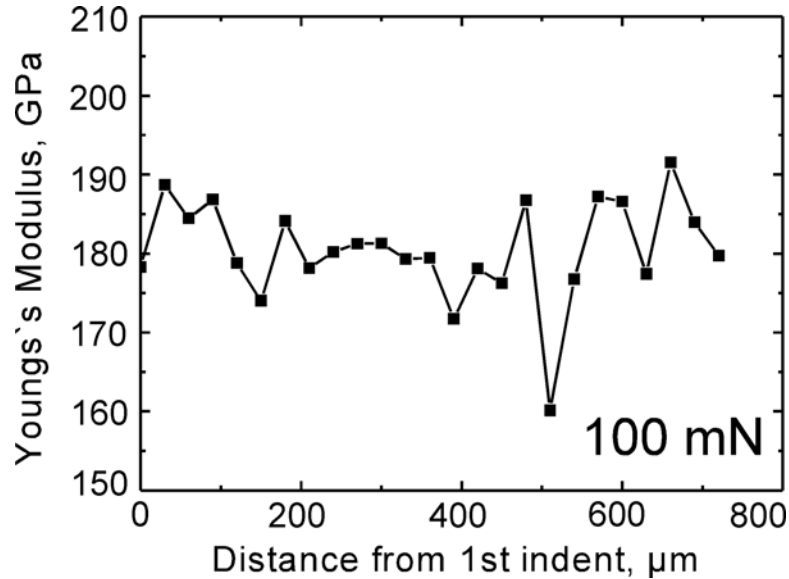
Lamellar colony



Globular grain

# Experimental results: Nanoindentation

E-mod of grains and colonies (Max load: 100 & 200mN)

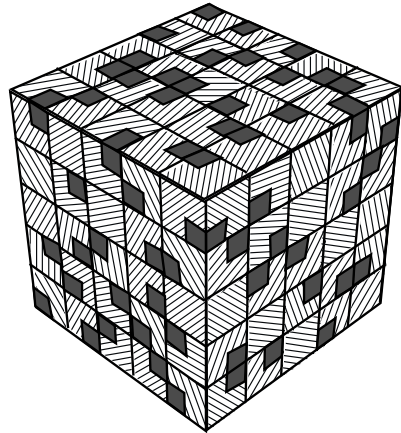


Indentation location	Elastic modulus [GPa] (average value)
Globular grains	169
Lamellar colonies	182
At interfaces between grains/colonies	192

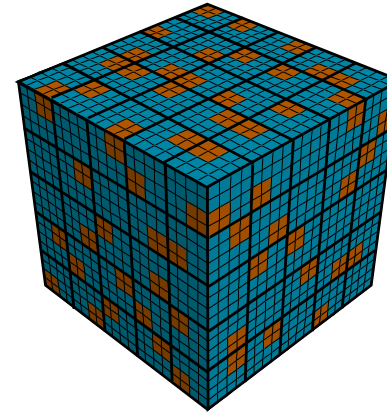


# Representative microstructure for modeling

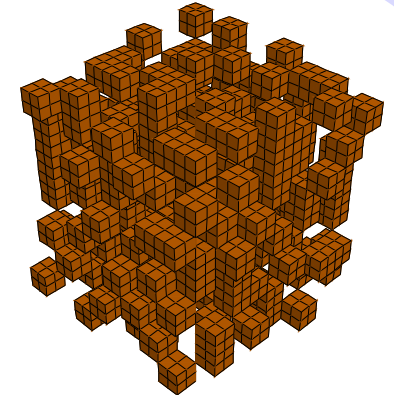
## Meso scale description



Idealization of the microstructure

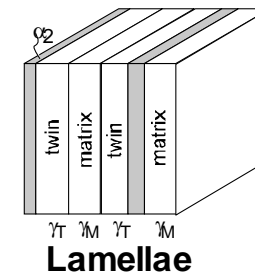
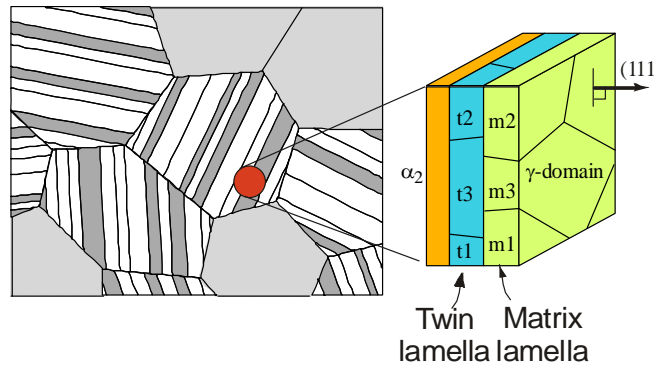


FE Model

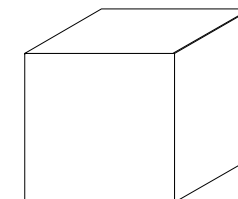


Globular grains

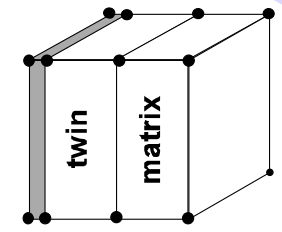
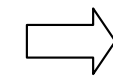
## Micro scale description



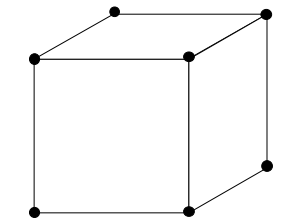
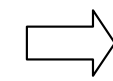
Lamellae



$\gamma$ -grain



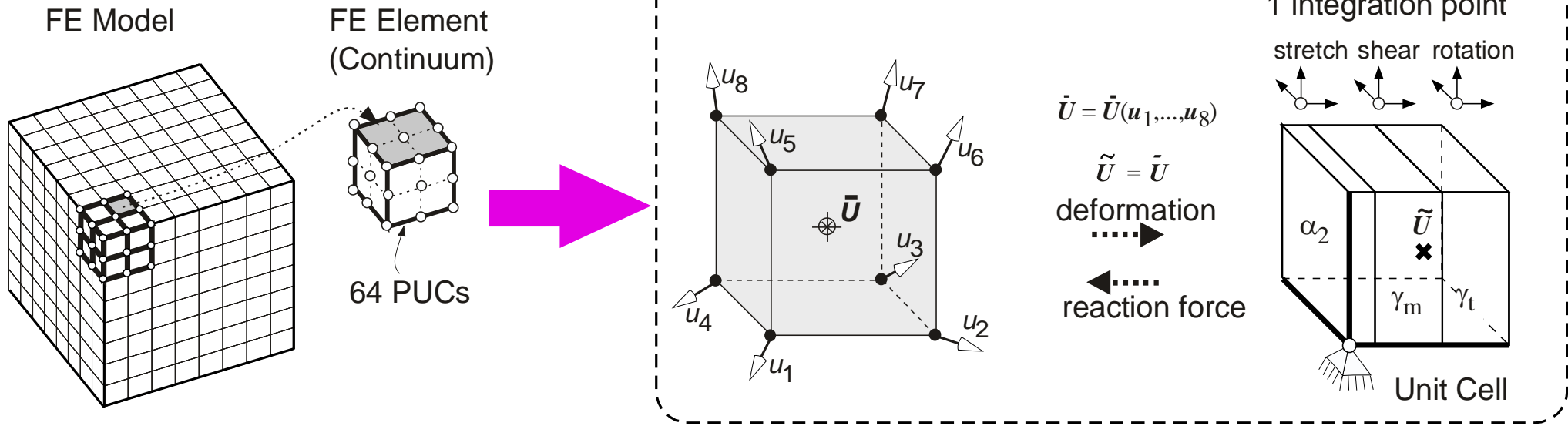
PUC



PUC

# Two scale linking – FE2-method

FE2 model



Periodic Unit Cell - PUC

Crystal plasticity

Crystalline slip is assumed to obey Schmid's law with resolved shear stress:

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

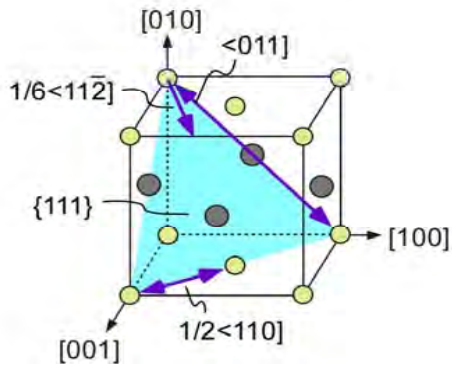
Viscoplastic power law

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



# Applied values for elastic constants of single phases

Experimental values of the phases, after **Yoo and Fu** [\*], determined for binary Ti-49Al alloy

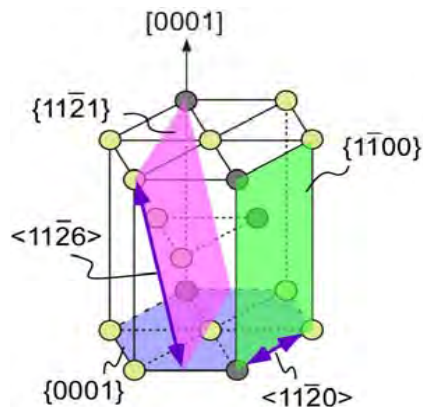


$\gamma$ TiAl

	$E_{1111}$	$E_{1122}$	$E_{2222}$	$E_{1133}$	$E_{3333}$	$E_{1212}$	$E_{1313}$	$E_{2323}$
$\gamma$ -TiAl	190	105	190	90	185	50	120	120
$\alpha_2$ -Ti <sub>3</sub> Al	221	71	221	85	238	75	69	69

Obtained values for TNB (Ti-45Al-5Nb-0.2B) from Simulation

- Simulation of tensile tests
- Adjust crystallographic parameters to satisfy the experimental response

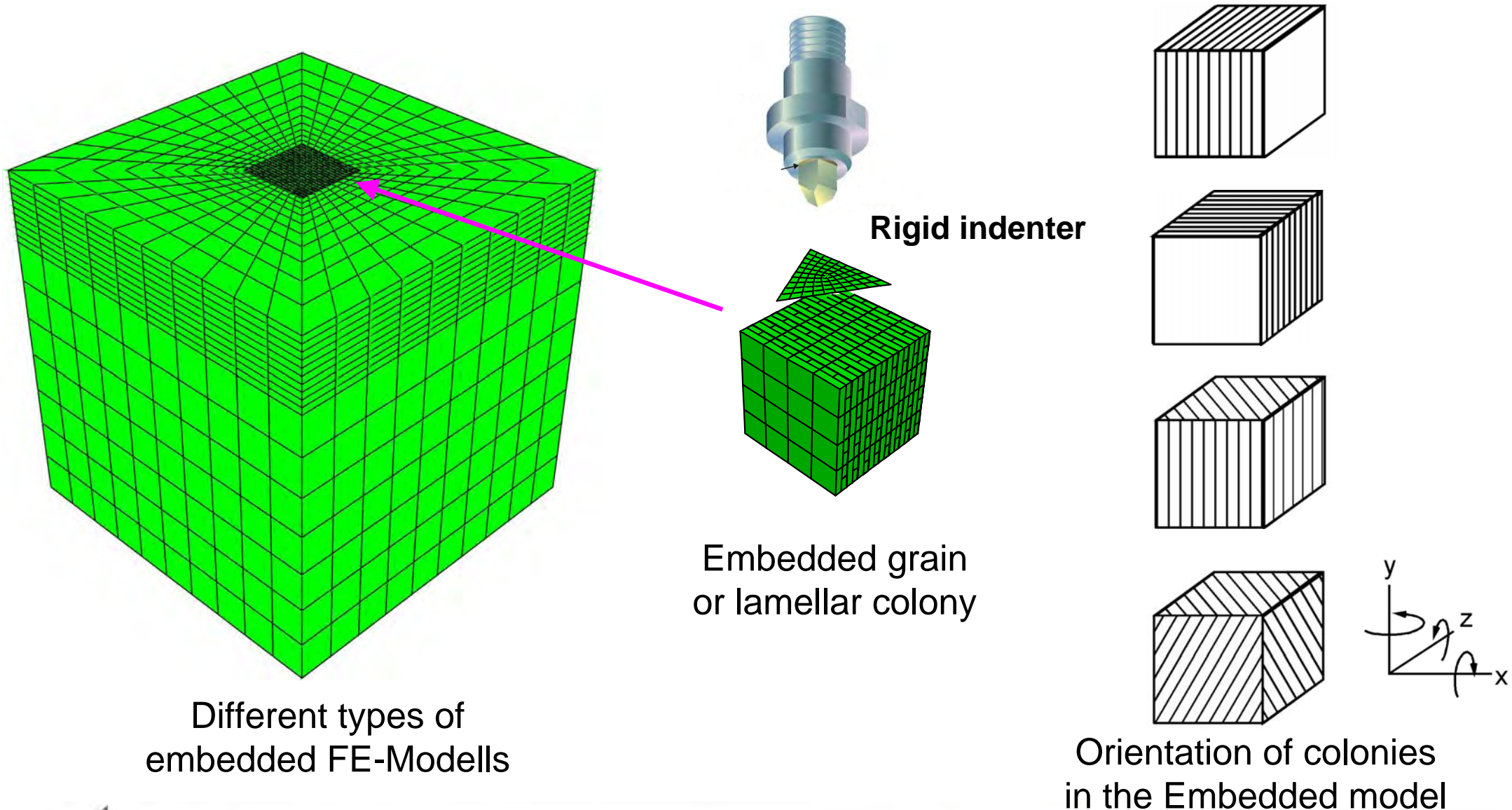


$\alpha_2$  Ti<sub>3</sub>Al

	$E_{1111}$	$E_{1122}$	$E_{2222}$	$E_{1133}$	$E_{3333}$	$E_{1212}$	$E_{1313}$	$E_{2323}$
$\gamma$ -TiAl	161,5	89,25	161,5	76,50	157,25	42,5	102	102
$\alpha_2$ -Ti <sub>3</sub> Al	187.85	60.35	187.85	72,25	202.3	63,75	58,65	58,65

[\*] ISIJ International, Vol. 31 (1991), No. 10, pp. 1049-1062

# Model approximation for nanoindentation simulation

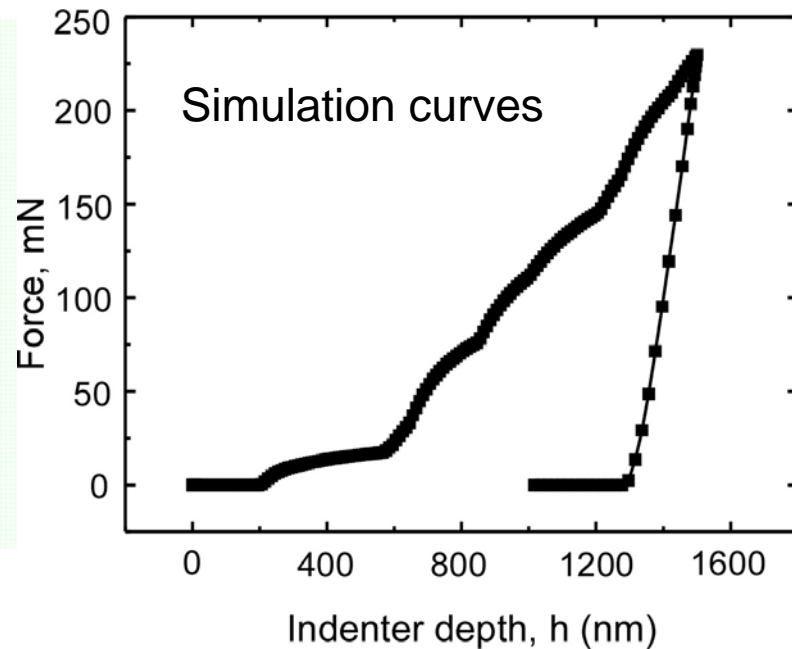


Different types of embedded FE-Modells

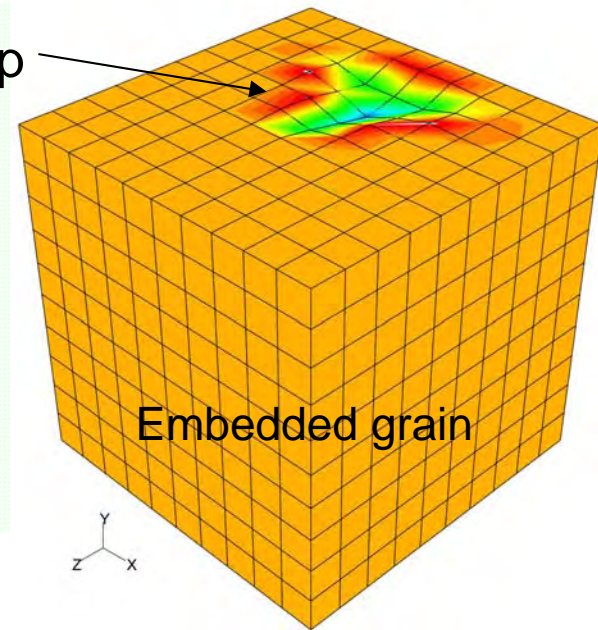
Orientation of colonies in the Embedded model



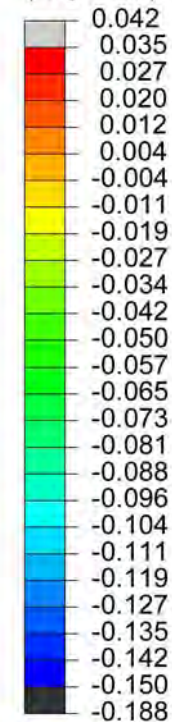
# Calculation of elastic modulus



Pile-up



LE, LE22  
(Avg: 75%)



## Calculation of E-mod:

$$E = (1 - \nu^2) / \left[ 1/E_r - (1 - \nu_d^2)/E_d \right]$$

E = Young's modulus

$\nu$  = poisson's ratio

for diamond:

$$\nu_d = 0.07, E_d = 1140 \text{ GPa}$$

## Oliver-Pharr method:

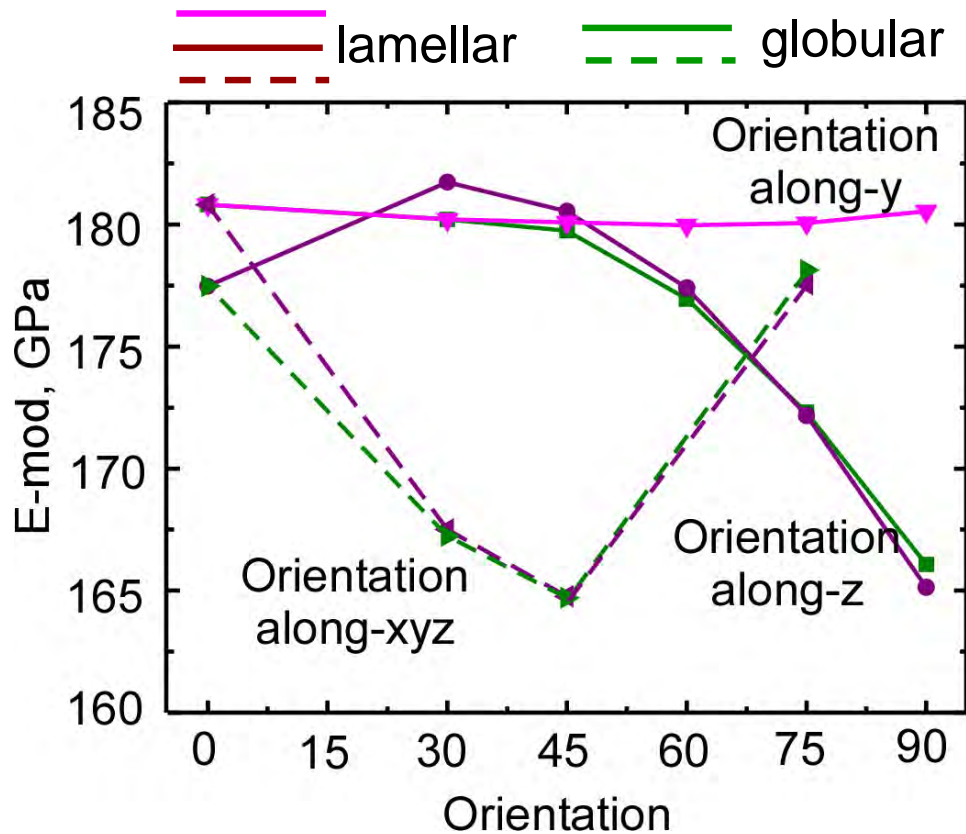
$$E_r = 1/2(\pi/A_c)^{1/2}(1/\beta)S_u$$

$A_c$  = contact area, from ABAQUS

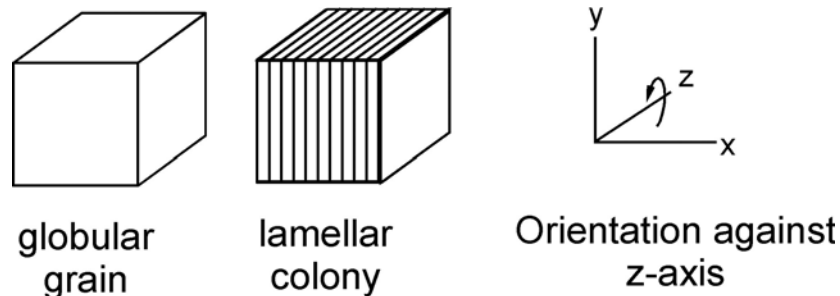
$\beta$  = shape function Berkovich tip = 1.034

$S_u$  = slope, from F-h plot

# Simulation results: Influence of grain/colony orientation

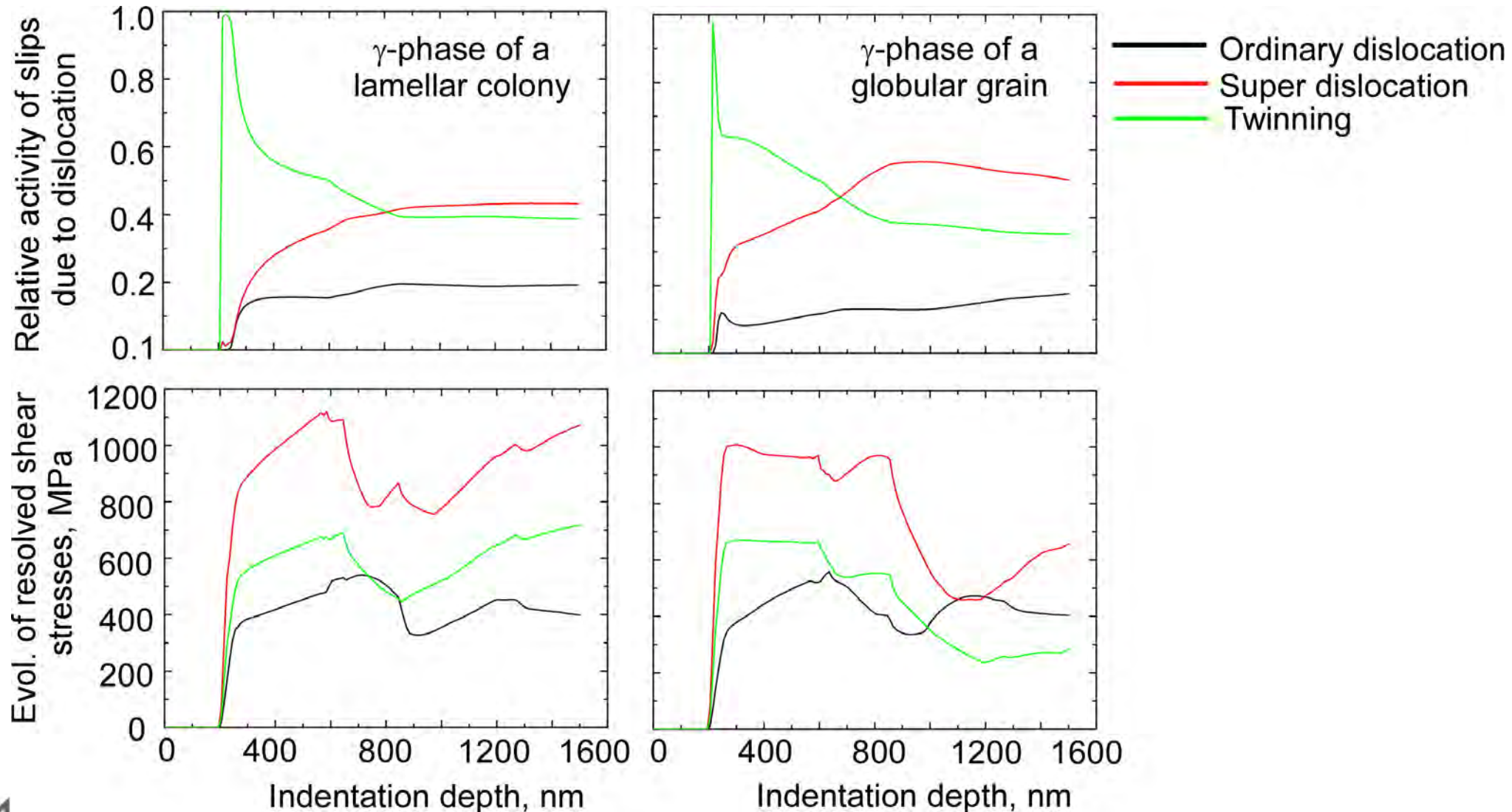


Average - Emod	Exp	Sim.
Macro (Tensile test)	146	142
Meso grain: Lamellar (nanoindentation)	182	177
Meso grain: Globular (nanoindentation)	169	175



Inconsistency:  
Due to model simplicity  
a) Thick lamellae  
b) 4%  $\alpha_2$ -phases

# Simulation results at indenter tip: Slip system activation and shear stress evolution



# Summary and Conclusion

- The nanoindentation experiments showed that the meso scale elastic modulus varies due to microstructural heterogeneity.
- Simulation of nanoindentation showed that
  - Elastic modulus of the colonies and grains vary due to grain orientation
  - The scatter band of elastic modulus due to the influence of colony/grain orientation is  $\pm 25$  GPa
  - Activation of slip systems and the evolution of shear stresses in the crystallographic plane are influenced by deformation constraint of the present phases



# Thank you for your attention

