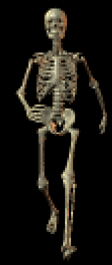

1) Design of new Ti-based biomaterials by using ab-initio simulations, FEM, and experiments

2) Detailed analysis of an indent

B. Sander, D. Ma, M. Friak, F. Roters,
N. Zaafarani, S. Zaefferer,
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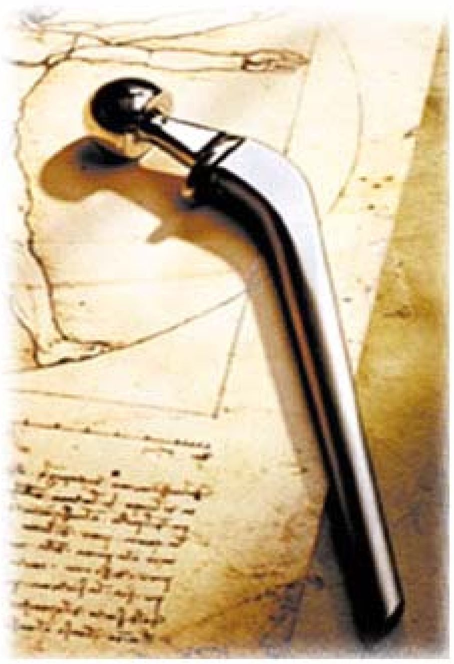
(d.raabe@mpie.de)

lecture, AICES – MIT conference at RWTH Aachen, 08. Oct. 2007

Overview

- **Motivation**
- **Theoretical methods**
- **Experimental methods**
- **Results**
- **Conclusions**



Overview

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Motivation

- **Implant requirements:**

corrosion stability, fatigue resistance, strength-to-weight ratio, ductility, wear resistance ↑

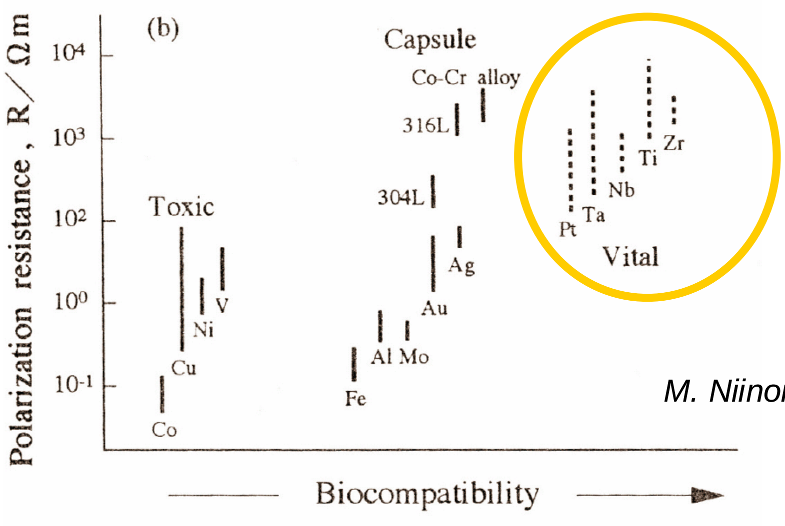
elastic modulus, cytotoxicity, allergic reactions ↓

Aims

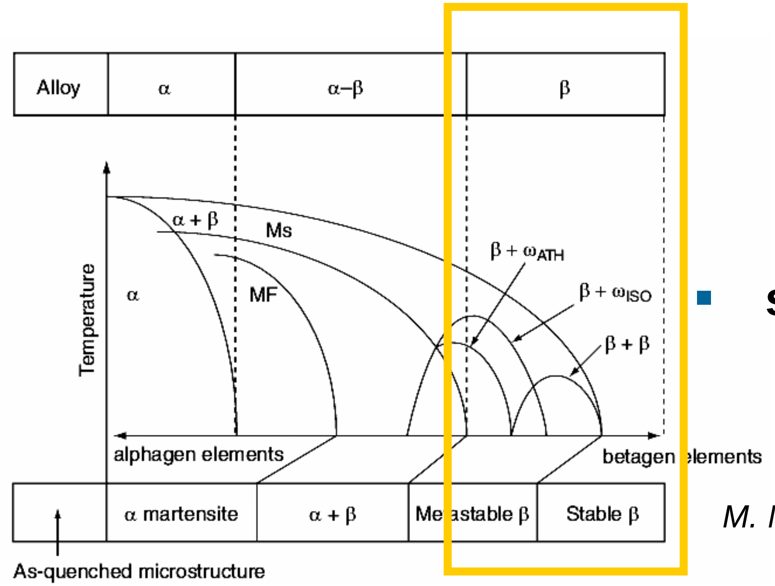
- **Stiffness closer to elastic modulus of human bone**
- **Stabilization of β-Ti**
- **Use only bio-compatible elements**

Boundary Conditions Considered – Some Numbers

- **non-toxic elements**



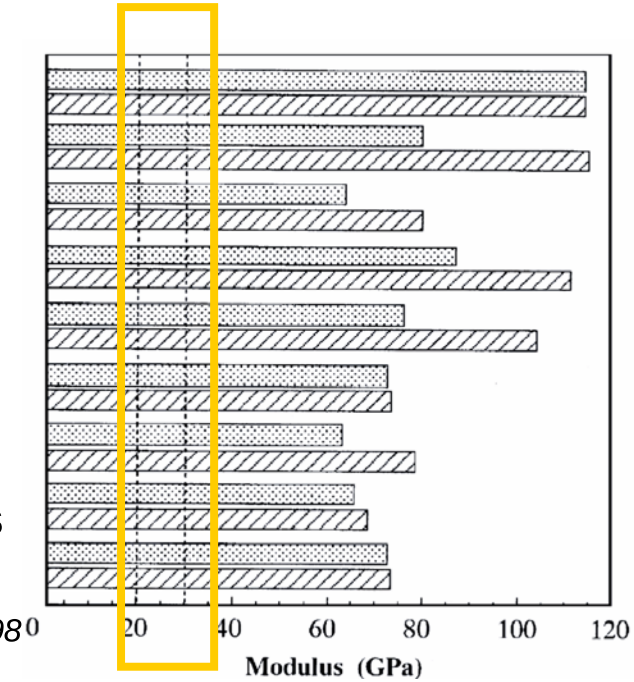
M. Niinomi, JOM,1998



- **stable ß-phase**

M. Niinomi, JOM,1998

- **reduced elastic stiffness**



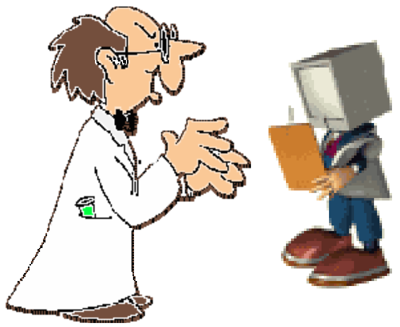
M. Niinomi, JOM,1998

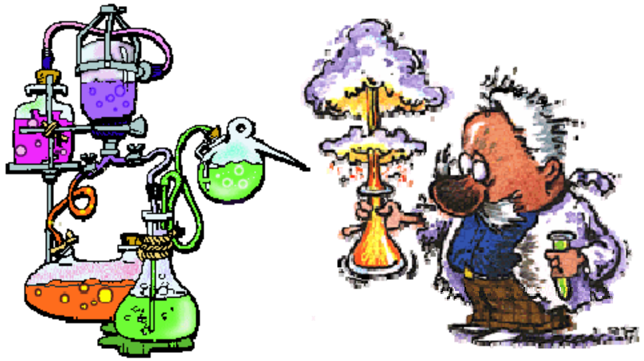
Challenge and Scientific Approach

- <u>Theory – driven</u> guidance in constrained alloy design (non-toxic; ß-phase; reduced stiffness); replace phenomenological rules
- 2 <u>binary</u> alloy systems (Ti-Nb, Ti-Mo) and 2 <u>engineering</u> alloys (Ti-35wt.%Nb-7wt.%Zr-5wt.%Ta and a Ti-20wt.%Mo-7wt.%Zr-5wt.%Ta)
- Combination of ab-initio <u>simulations</u> and <u>experiments</u>

Density functional theory (DFT), generalized gradient approximation (GGA), configurational and vibration entropy

Casting, homogenization, rolling, heat treatment, recrystallization, grain growth, microstructure, mechanics





Overview

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Theoretical methods

- **Free energy $F(x,c,T) = U - T \cdot S$**
- **U: density functional theory (DFT), generalized gradient approximation (GGA)**
- **S: Configurational (mixing) entropy**
- **Ti-Mo and Ti-Nb binary systems**
- **Elastic modulus calculation**
- **Polycrystal homogenization theory**
- **Crystal plasticity finite element method**

Details: Plane wave pseudopotential approach (VASP), plane wave cutoff energy: 170 eV, 8×8×8 Monkhorst mesh to sample Brillouin zone, relaxation until cell stress free, supercells of 2×2×2 elementary cubic unit cells with a total of 16 atoms, variety of alloys by replacing Ti by either Nb or Mo (from 6.25 %, 1 Nb/Mo atom in a 16 atom supercell), variation of local arrangements: 48 bcc and 28 hcp configurations, further details on poster

Overview

- Motivation
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Experimental

- **Use ab-initio results as guideline for alloy composition**
- **2 binary systems (Ti-Nb, Ti-Mo) and 2 engineering alloys (Ti-35wt.%Nb-7wt.%Zr-5wt.%Ta and a Ti-20wt.%Mo-7wt.%Zr-5wt.%Ta)**
- **Thermomechanical processing: electric arc furnace (Ar), 4 × repeated remelting and solidification, cast into copper mold (60mm×32,6mm×10mm), homogenization (1200°C), hot rolling (750°C), recrystallization treatment**
- **Characterization: OM, SEM, EBSD, EDX, XRD, ultrasonic resonance frequency, mechanical testing**

Details: furnace evacuated and flooded with Ar at 300 mbar; water cooled copper crucible; arc temperature 3000°C; melt at peak temperature 1830-1850°C; intense stirring; 30-60s melting time; solidifcation+tilting+remeltinged 4 times; all heat treatments under Ar or vacuum; SEM, EBDS, EDX: JEOL / ZEISS HR-SEM; XRD: Co-radiation

Overview

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- **Results**
- Conclusions

Overview

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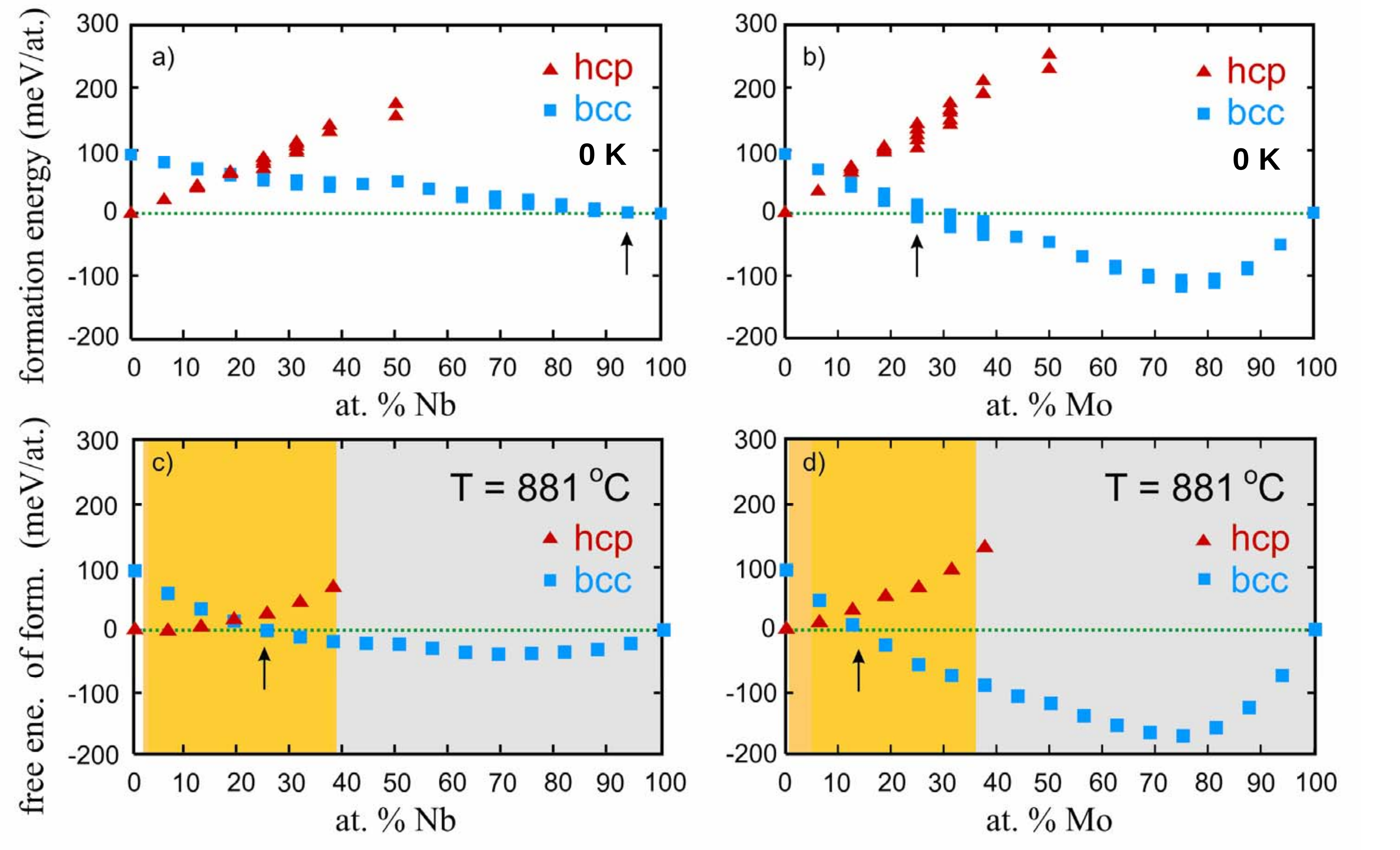
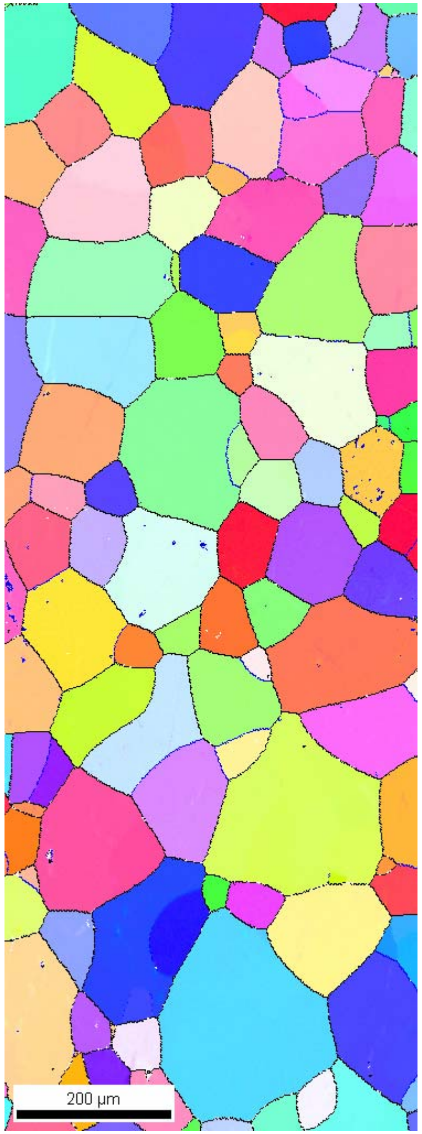
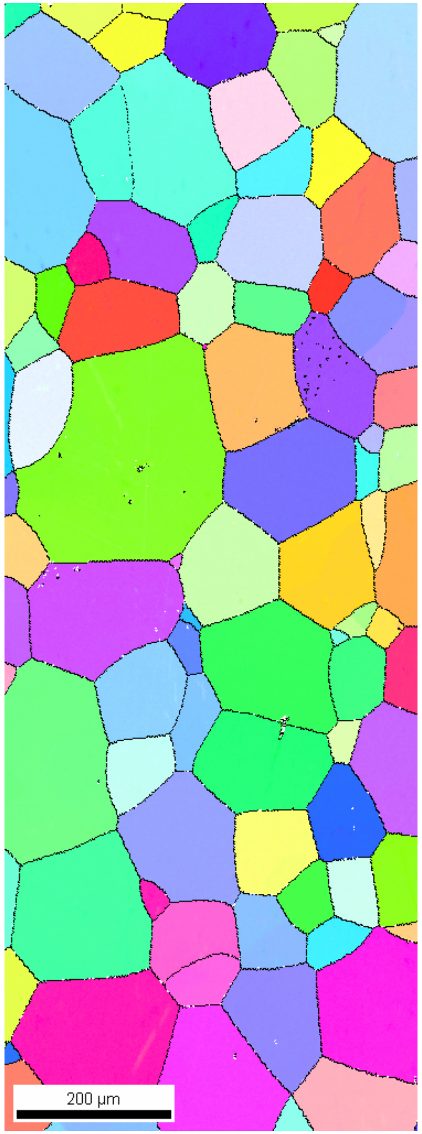
- **Results** → 2 binary systems; 2 engin. alloys
- Conclusions

Results from theory – binary alloys

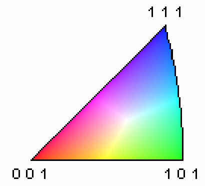


Experimental – results – microstructure, EBSD

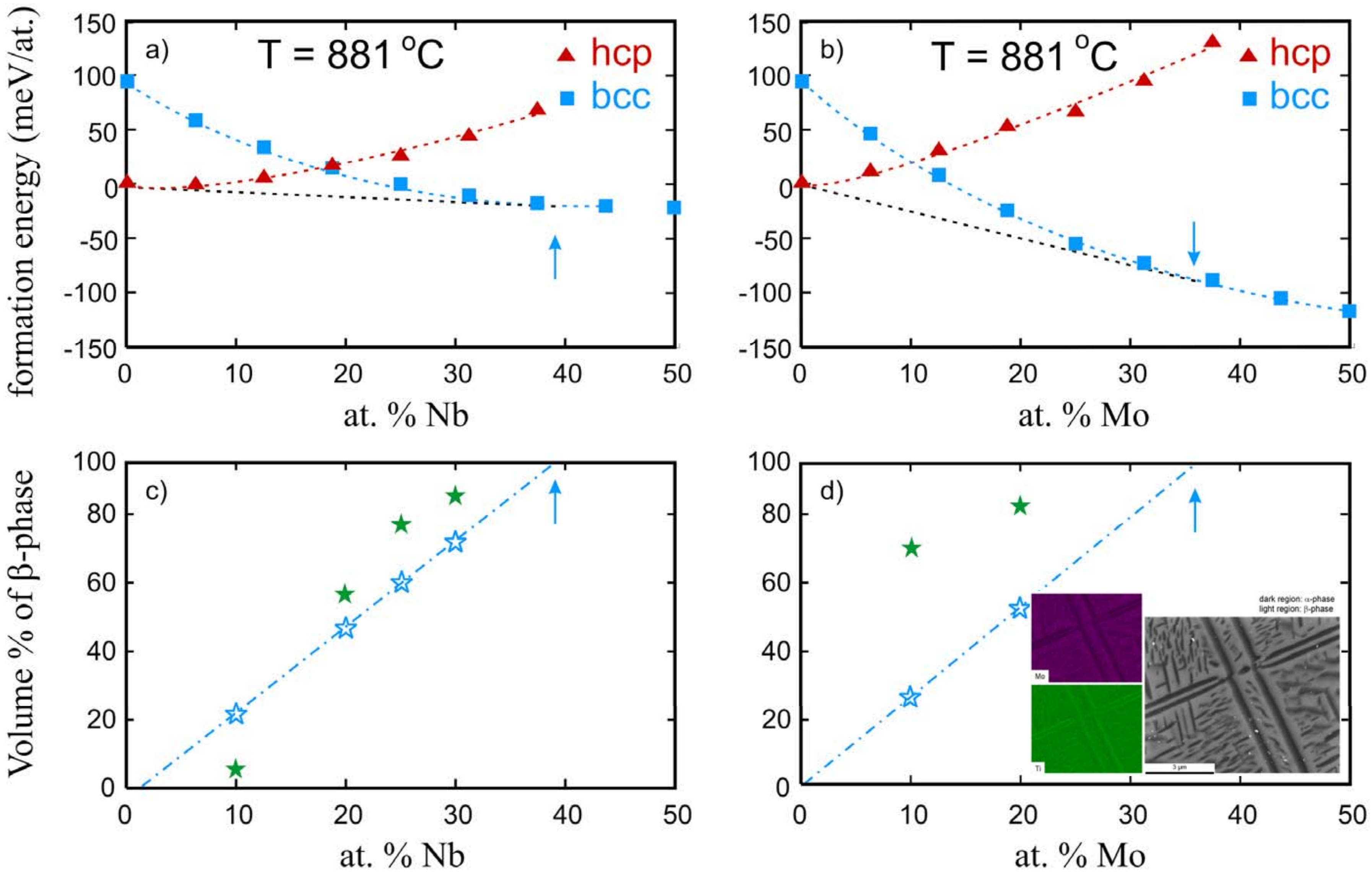




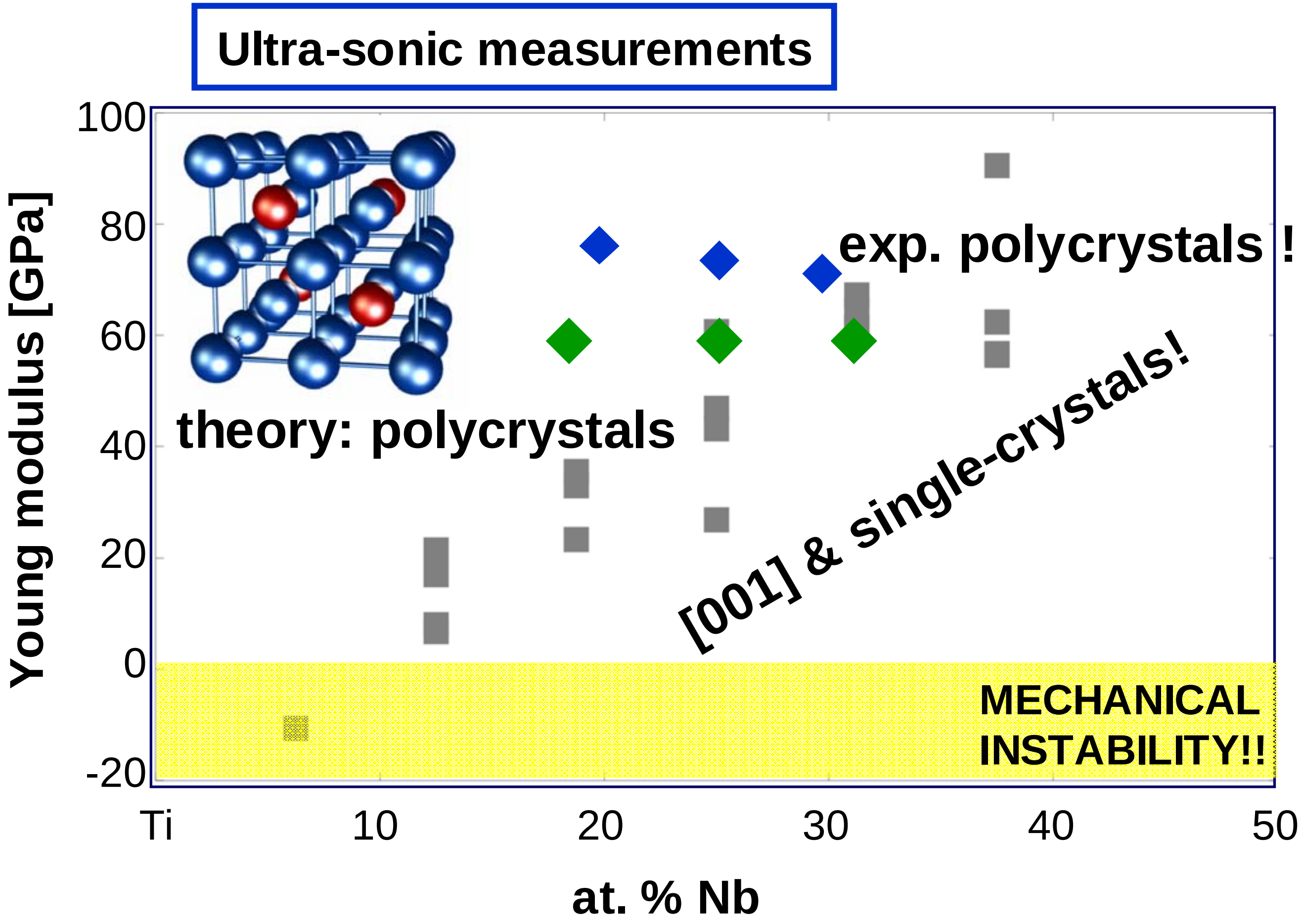
- **Ti-30at%Nb (as cast)**



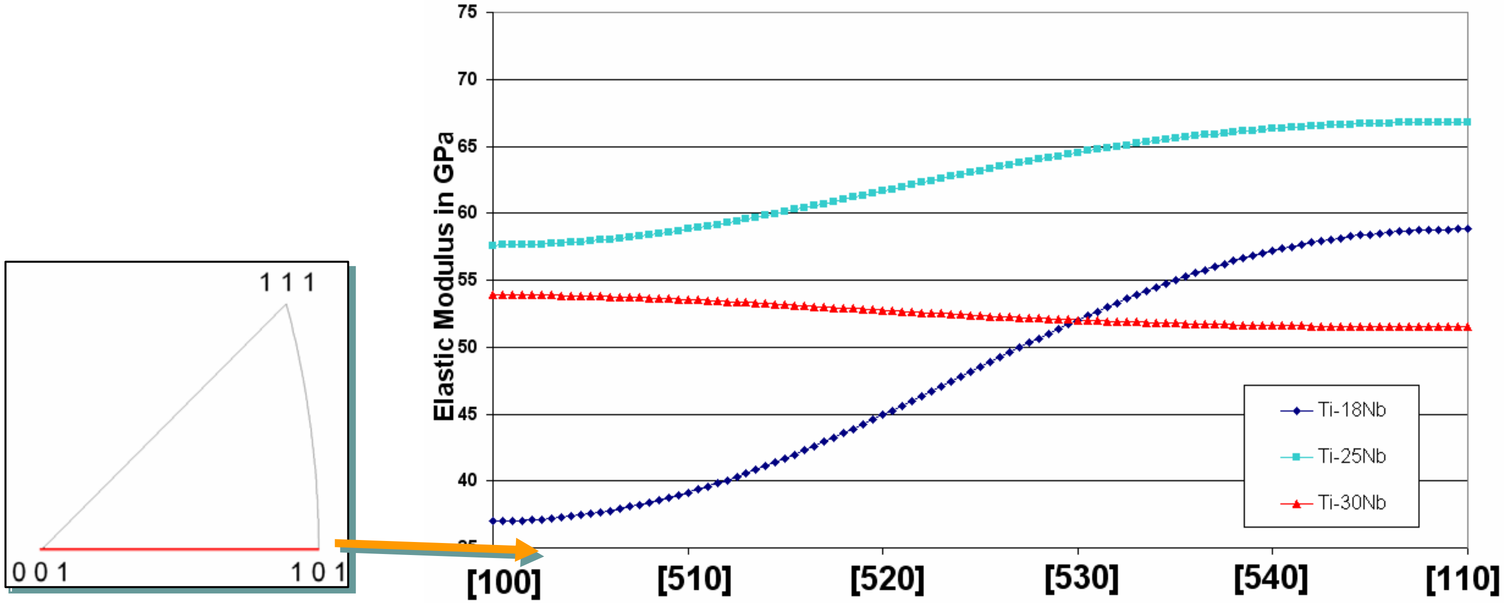
Ab initio inspired alloy design

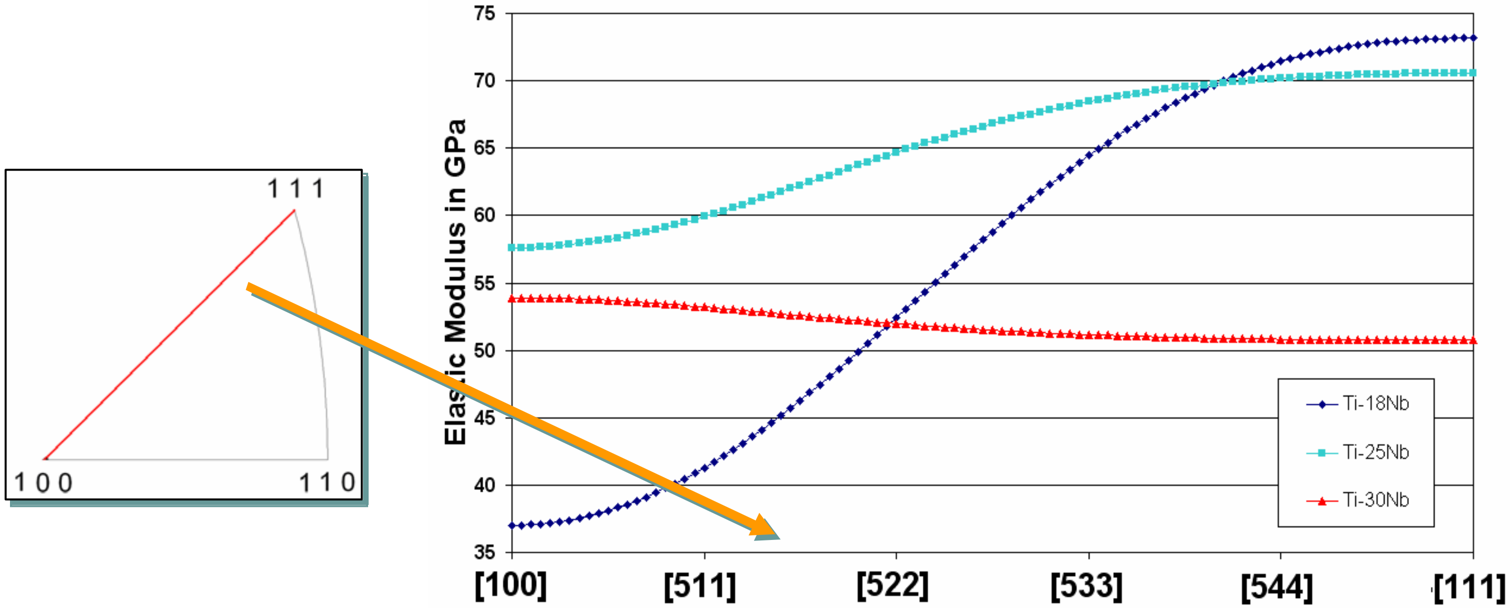


Results, theory and experiment – elastic modulus



Ab initio inspired alloy design: tensor (an)isotropy





Overview

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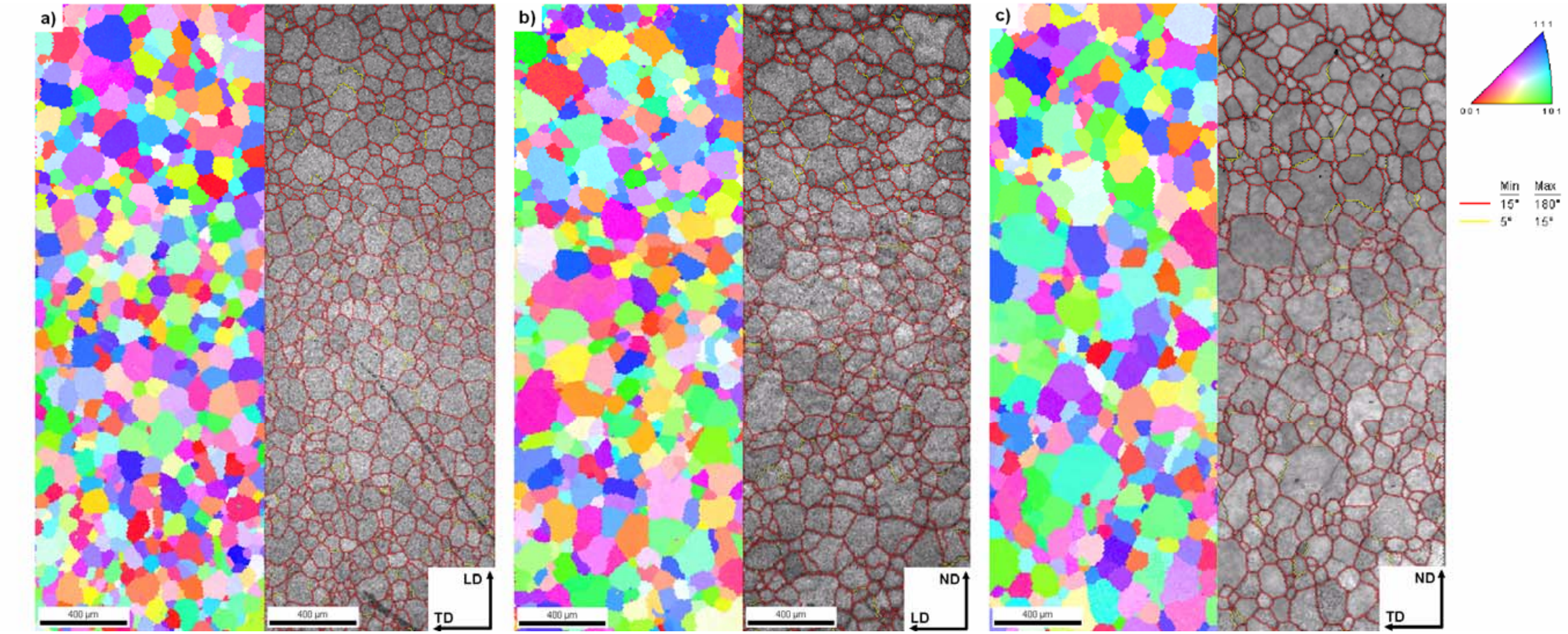
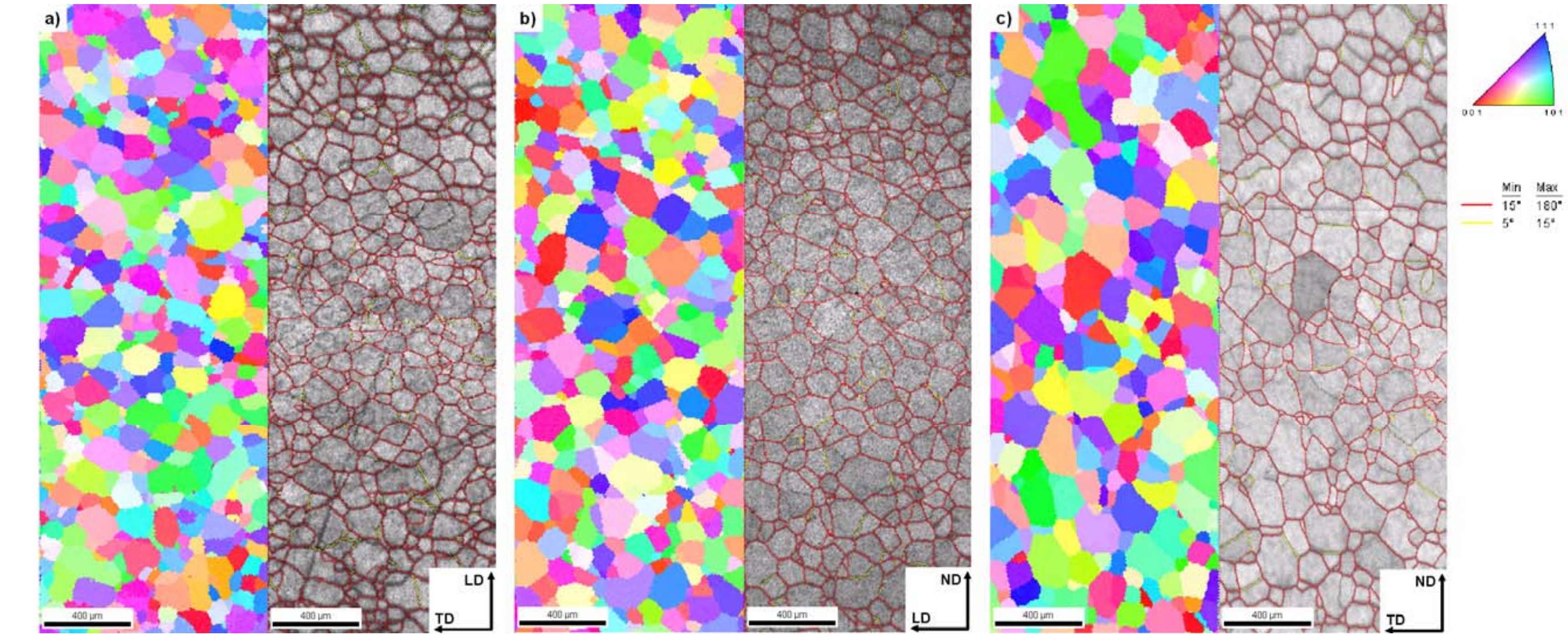
Experimental – results – microstructure Mo

- **Ti-20wt.%Mo-7wt.%Zr-5wt.%Ta – as cast**

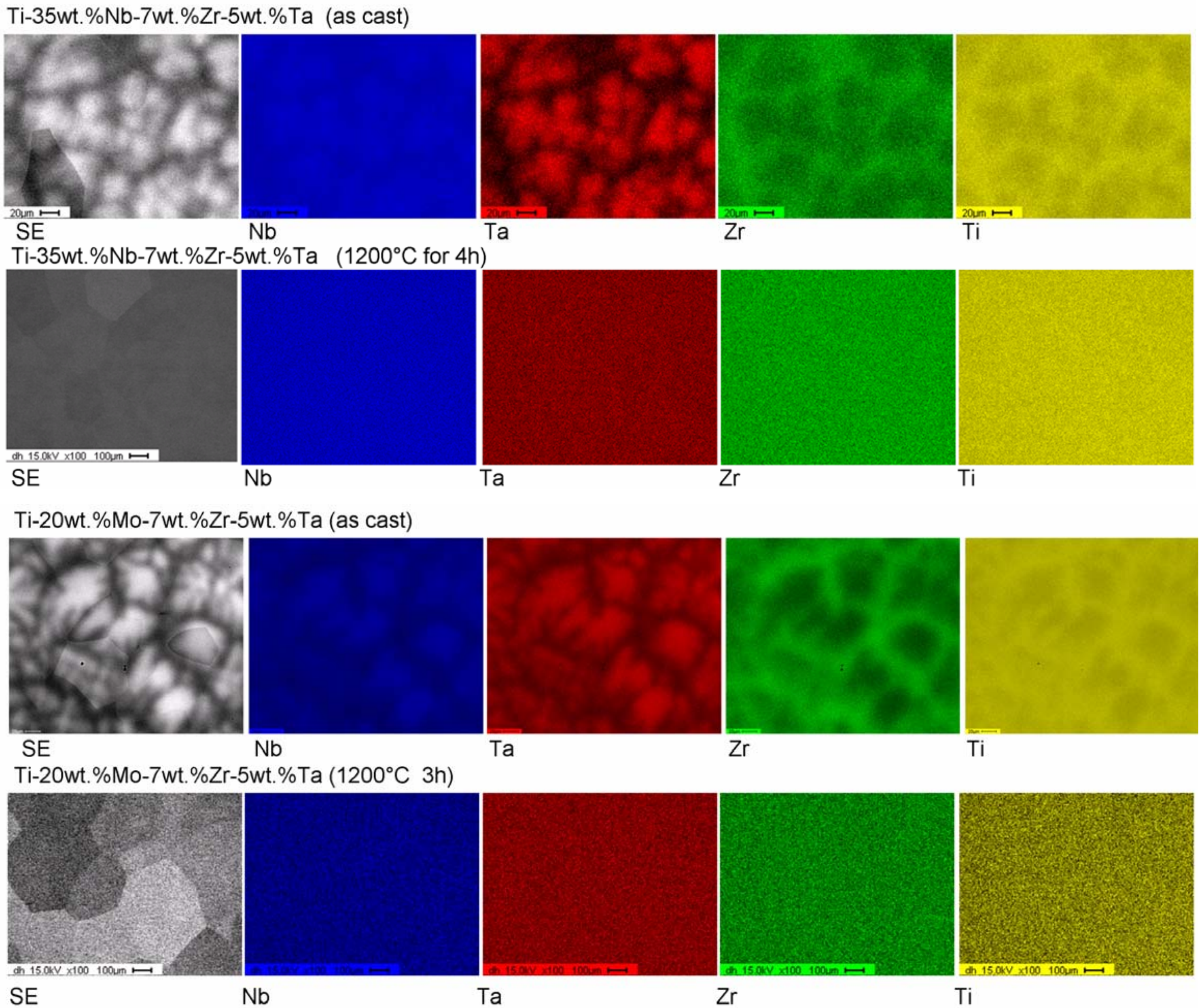


Experimental – results – microstructure Nb

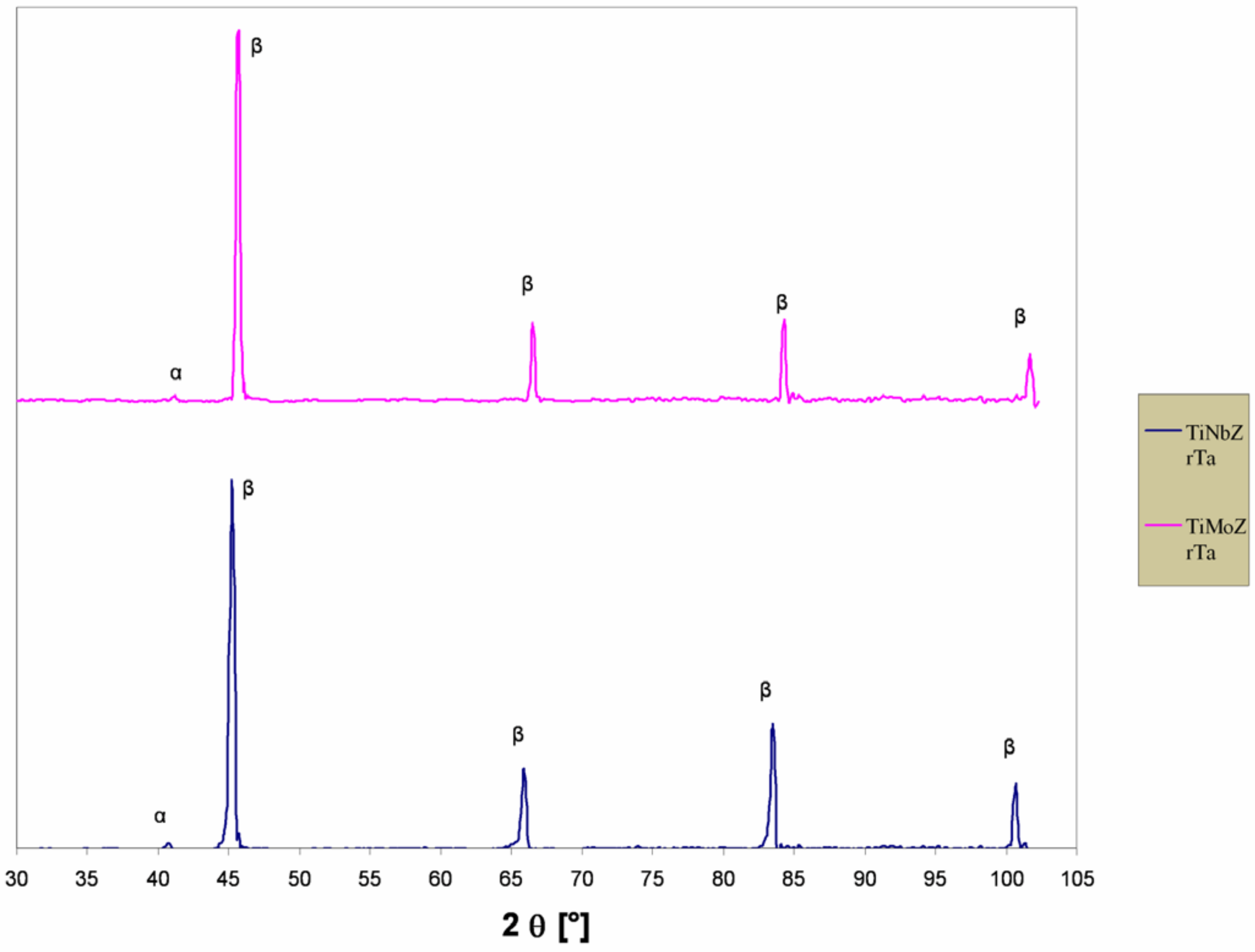
- **Ti-35wt.%Nb-7wt.%Zr-5wt.%Ta - as cast**



Experimental – Results – Microstructure, Segregation



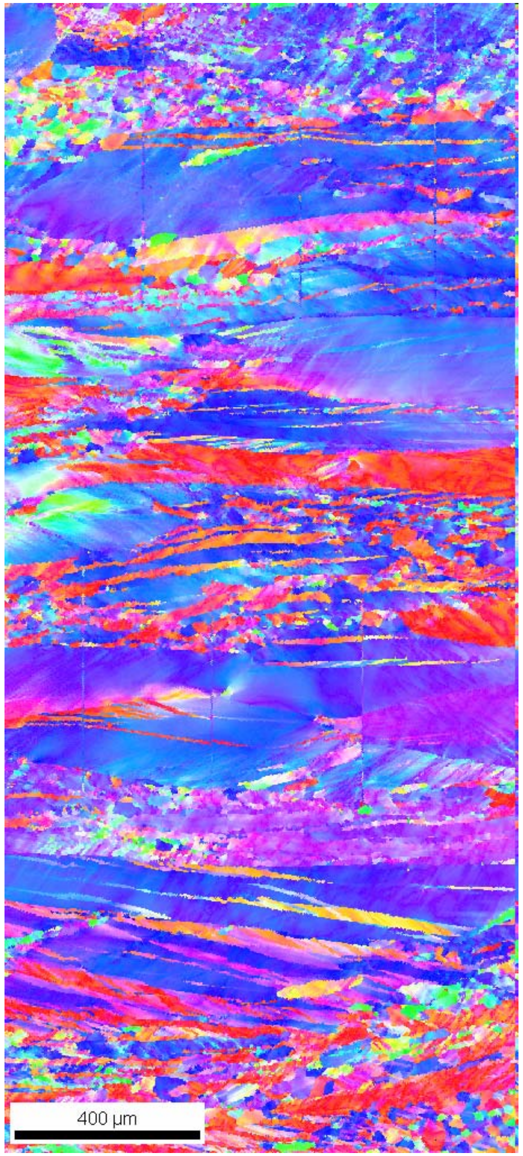
Experimental – Results – Phases



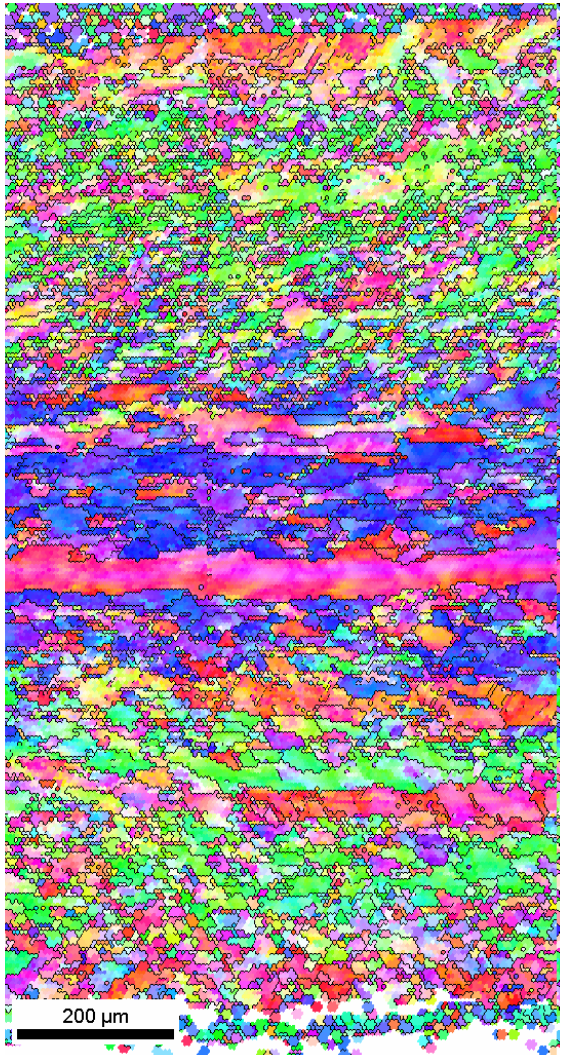
Experimental – results – microstructure

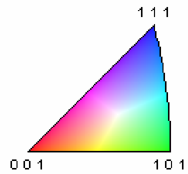
- **Ti-35wt.%Nb-7wt.%-Zr-5wt.%-Ta (rolled at 750°C)**

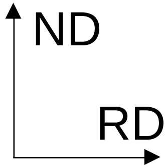
70%



90%





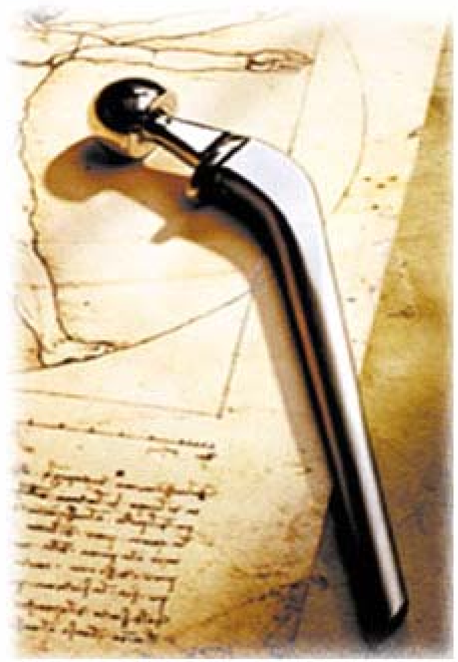


Results, elastic modulus

- **Ti: 114.7 GPa**
- **Ti-20wt.%Mo-7wt.%Zr-5wt.%Ta: 81.5 GPa**
- **Ti-35wt.%Nb-7wt.%Zr-5wt.%Ta: 59.9 GPa**

Conclusions

- **ab – initio prediction works (TD, modulus)**
- **Good fit between experiments and theory**
- **Next generation alloy design**
- **Ti, Steels, Mg, Chitin**



1) Design of new Ti-based biomaterials by using ab-initio simulations, FEM, and experiments
2) Detailed analysis of an indent

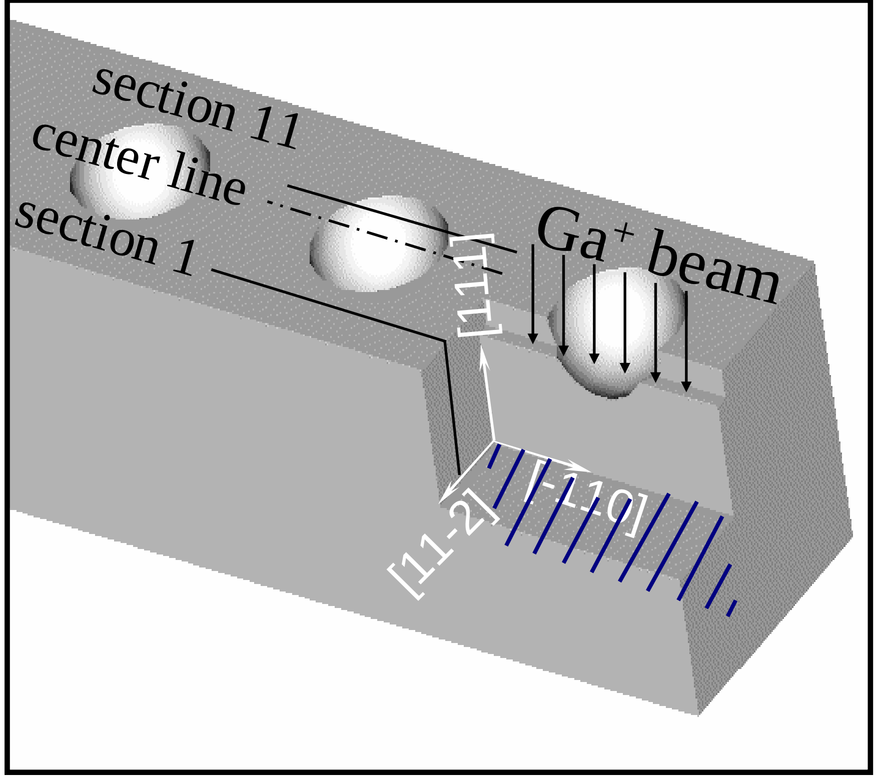
Experimental Procedure

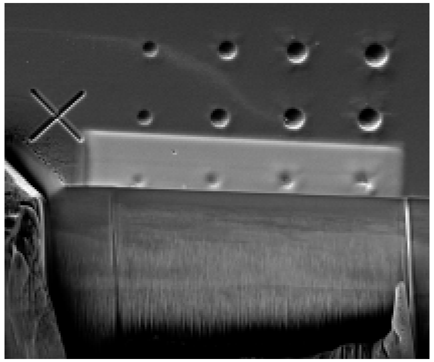
1 micron diamond polishing along {11-2} plane followed by 5 min ultrasonically in acetone cleaning

Milling by FIB

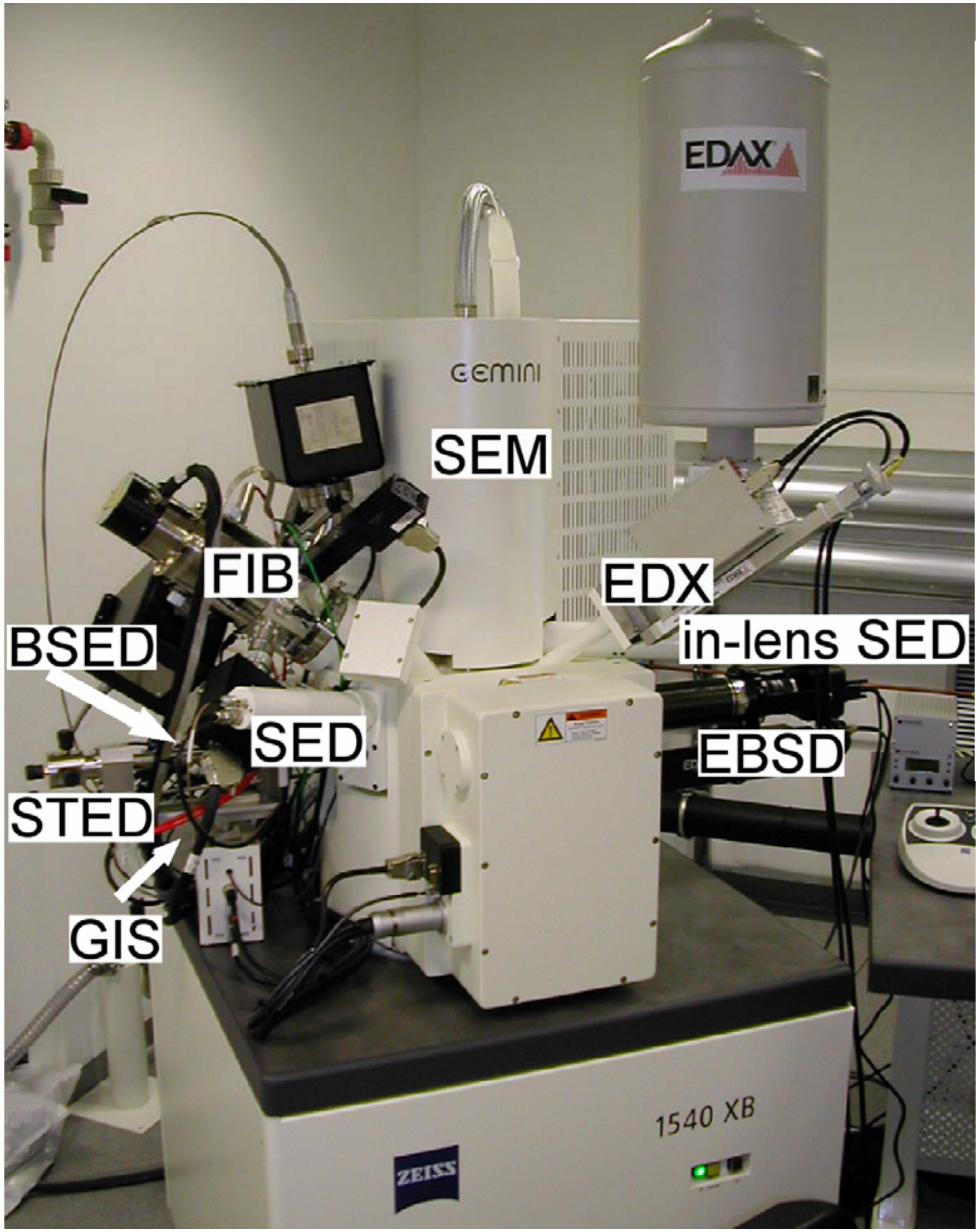
EBSD in each slice

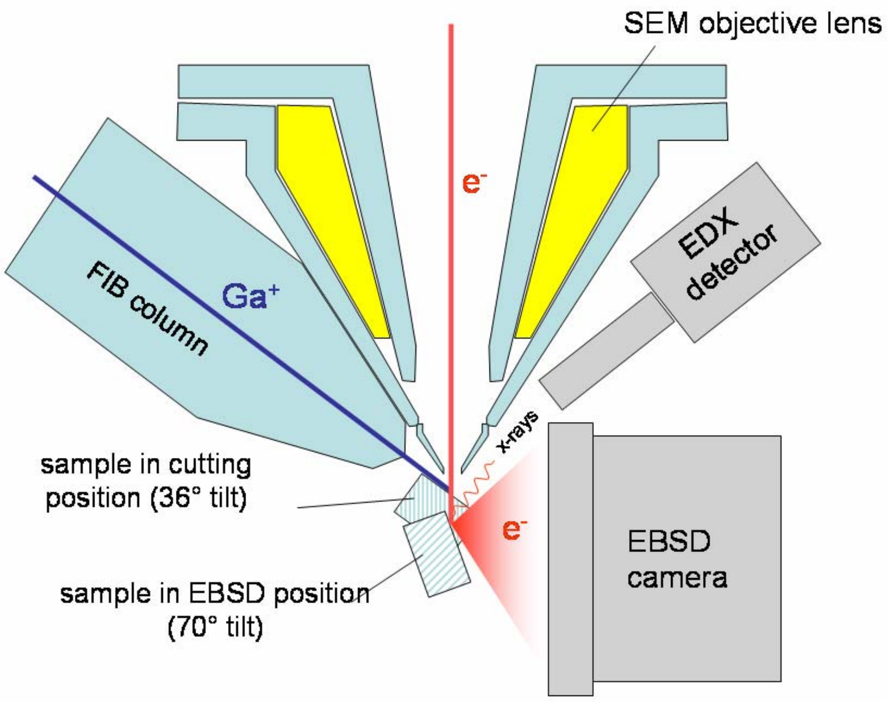
Layout of the FIB milling through indents

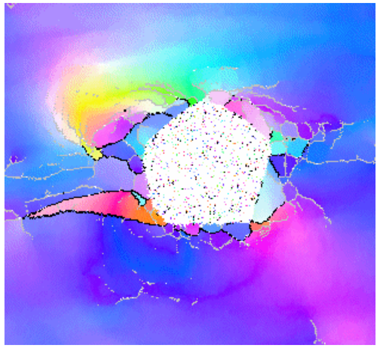




3D EBSD - electron orientation microscopy

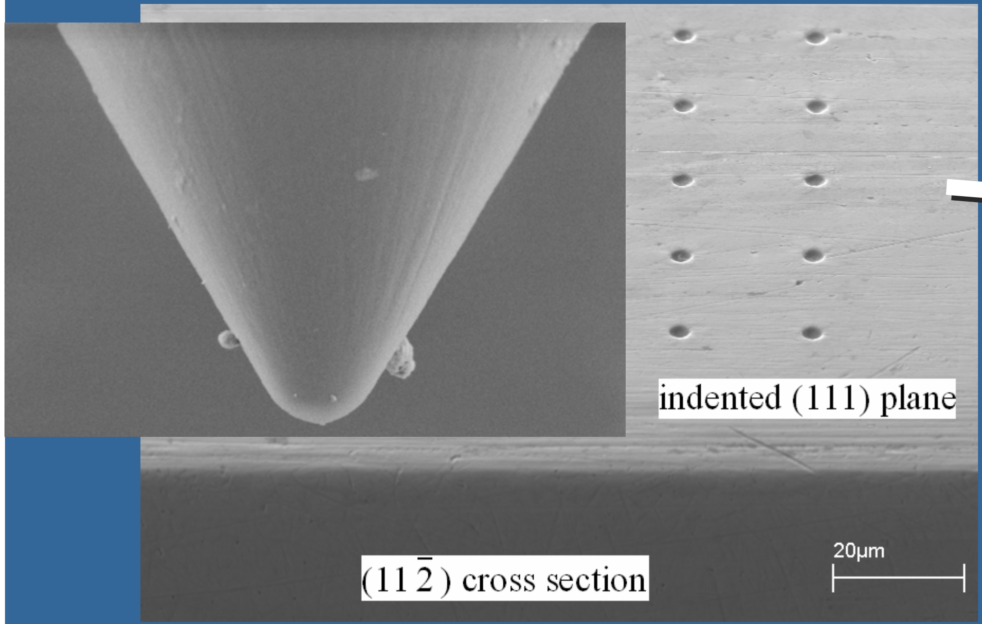


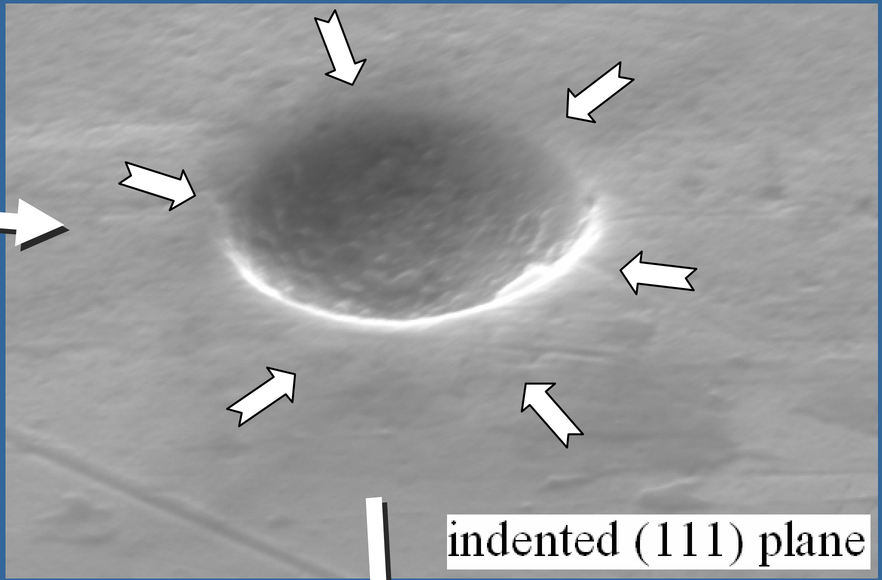


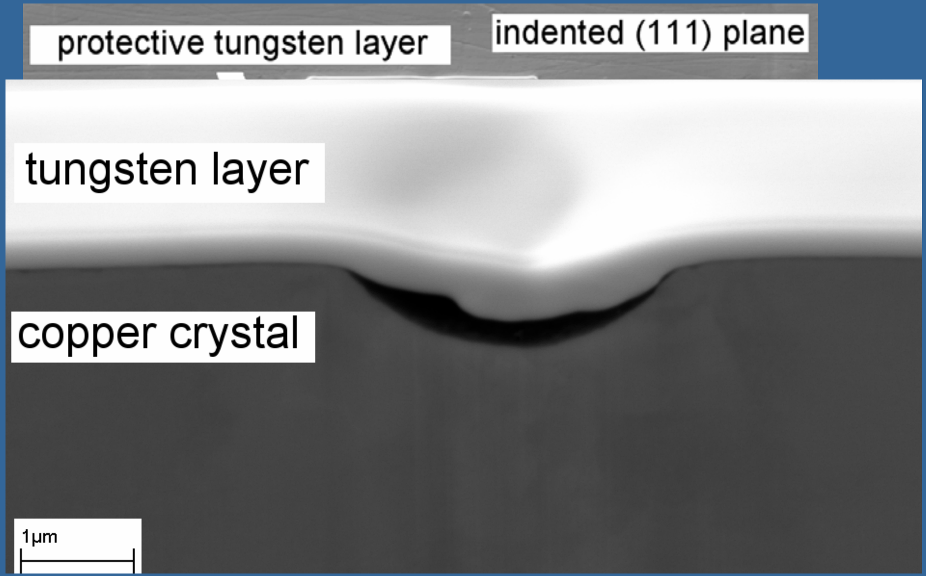


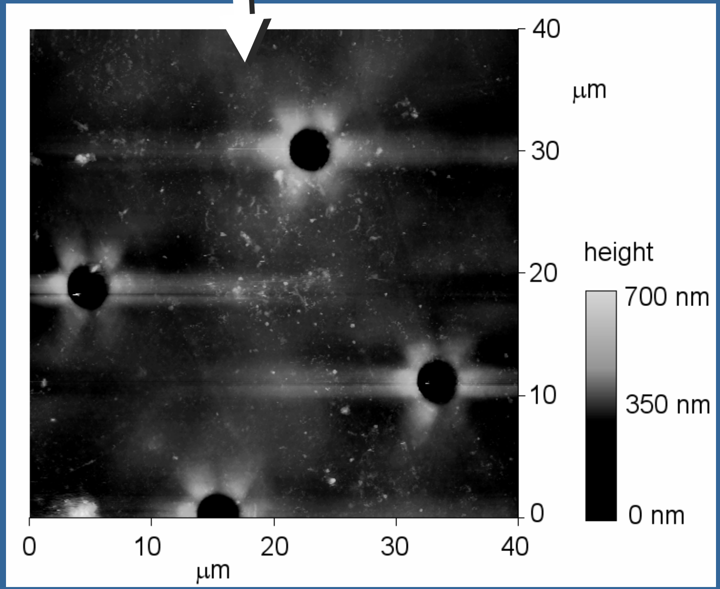
Nanoindentation - 3D

10 mN, no holding time , rate: 1.82 mN/s



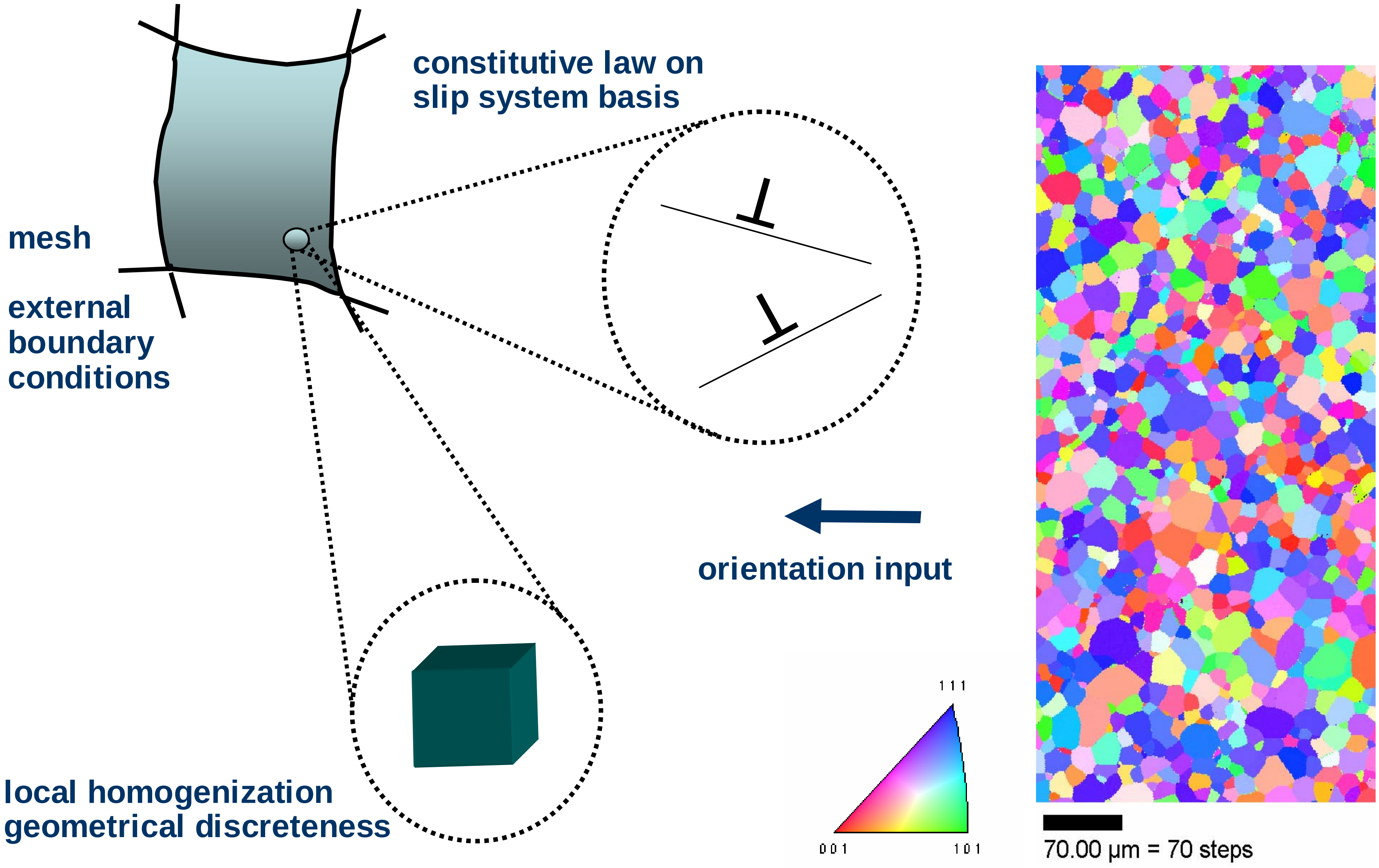




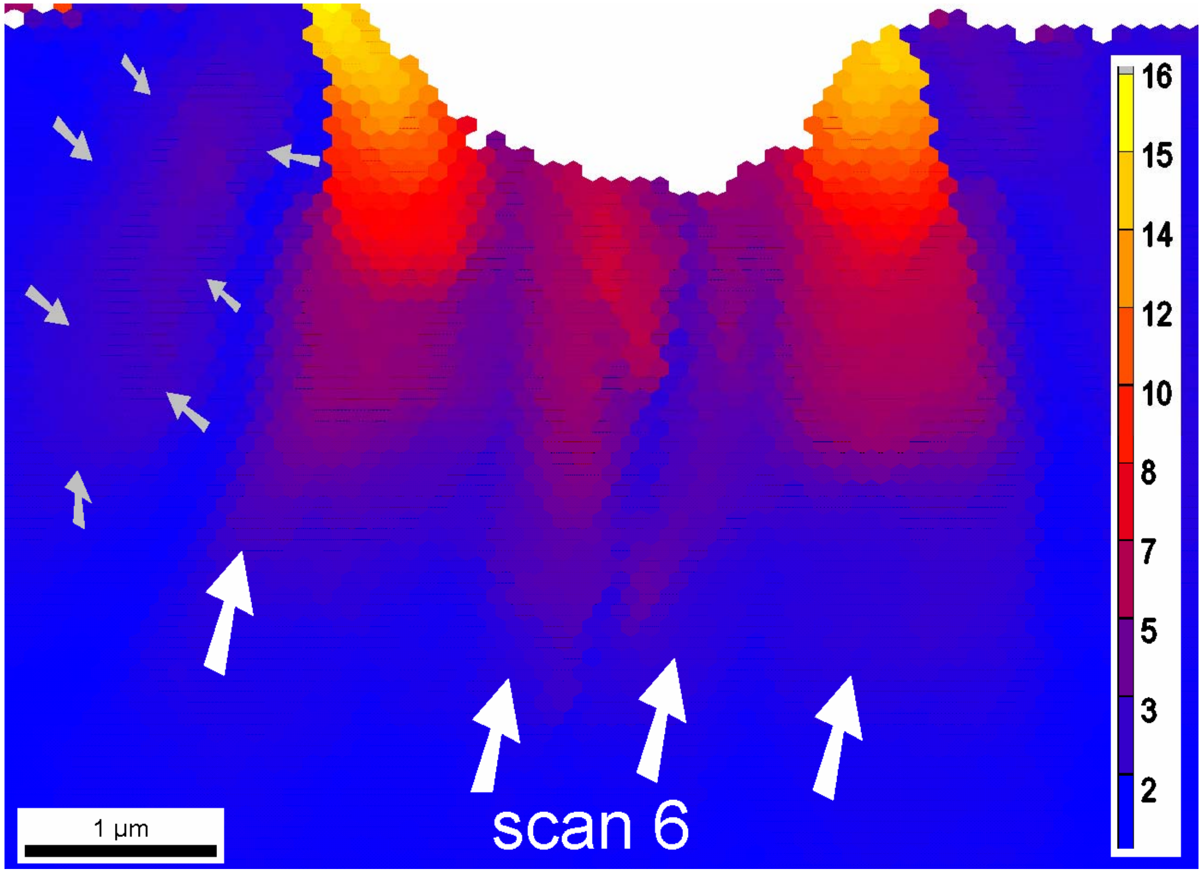


crystal mechanics FEM (general)

crystal plasticity FEM (CPFEM) - family

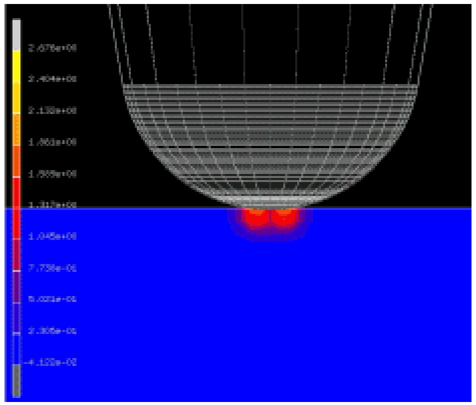


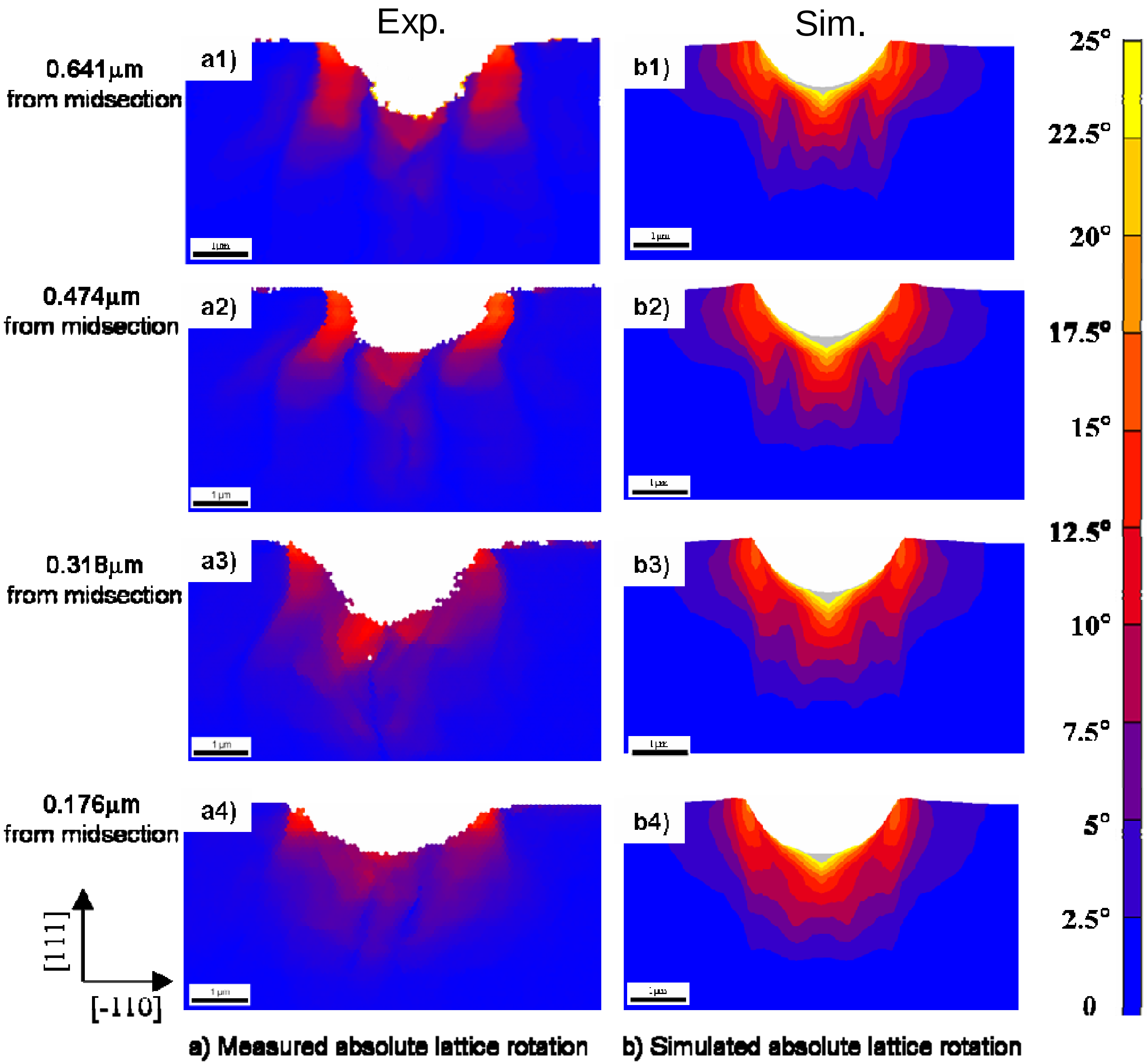
Misorientation map



Closer view of the experimentally observed pattern of the absolute values of the deformation-induced crystalline lattice rotations in ° in the vicinity of the indent

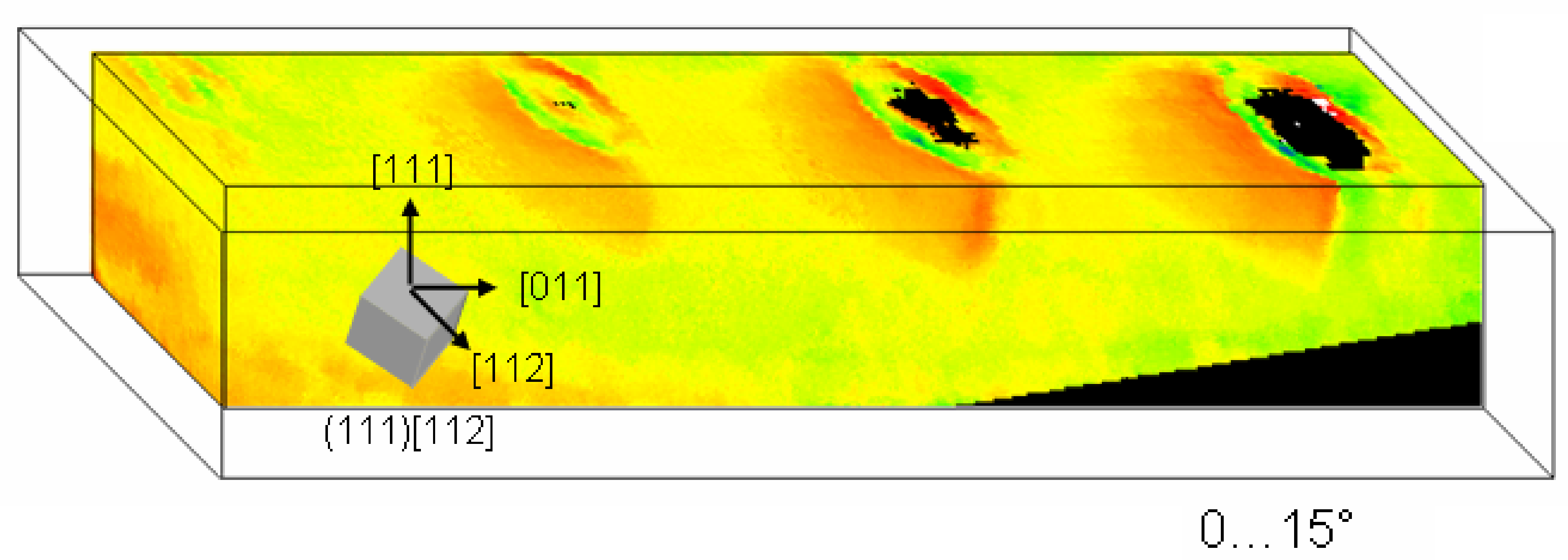
Comparison: magnitude of orientation changes





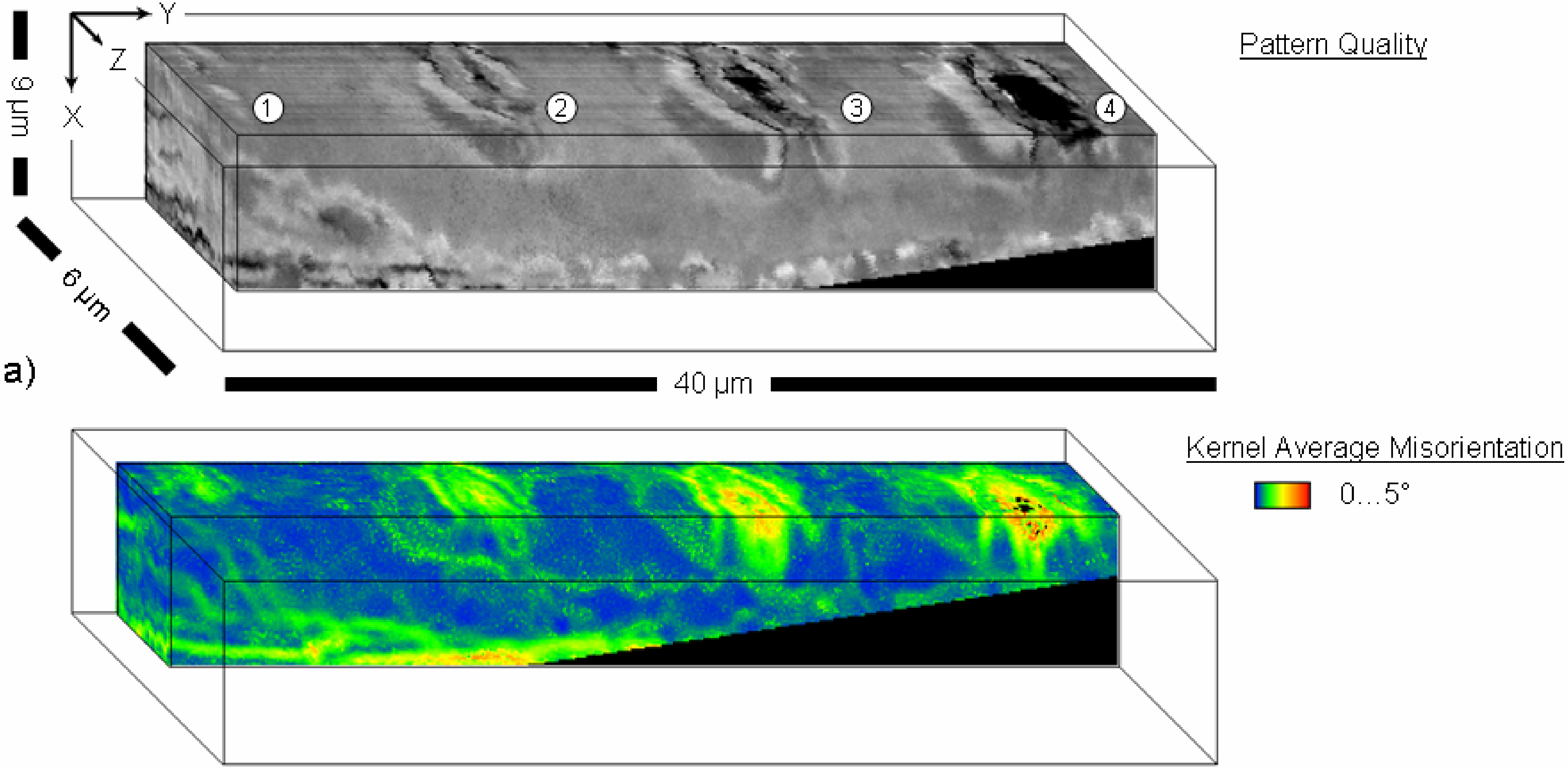
Experimental : Forces: 4, 6, 8, and 10 mN

Gradual evolution during indentation ?
Experiment



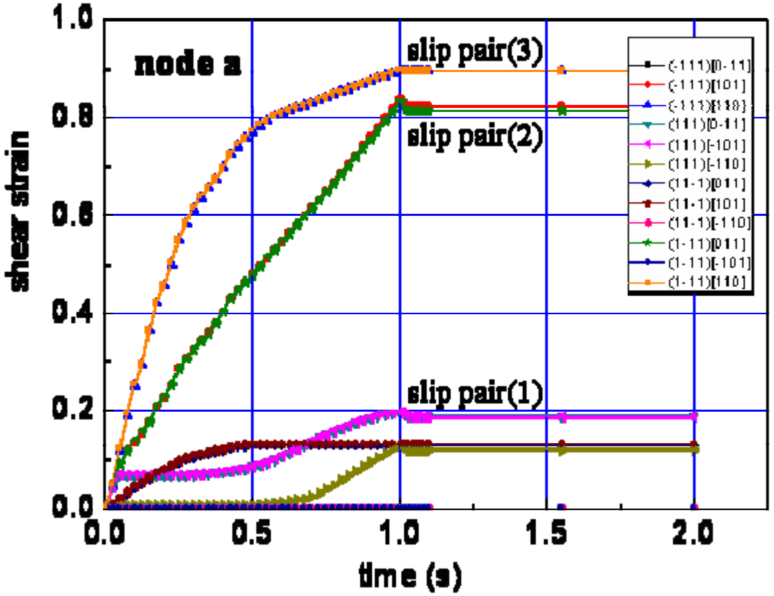
self-similarity, same type of pattern from early beginning

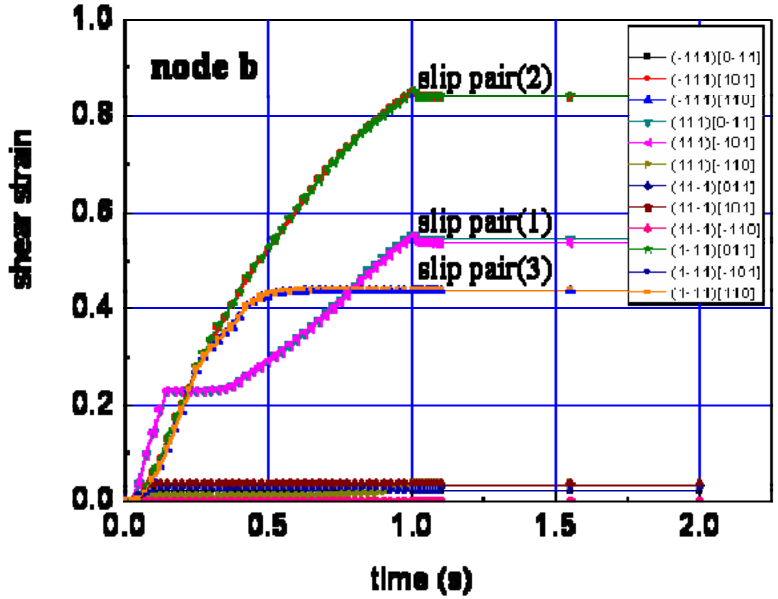
Experimental : Forces: 4, 6, 8, and 10 mN

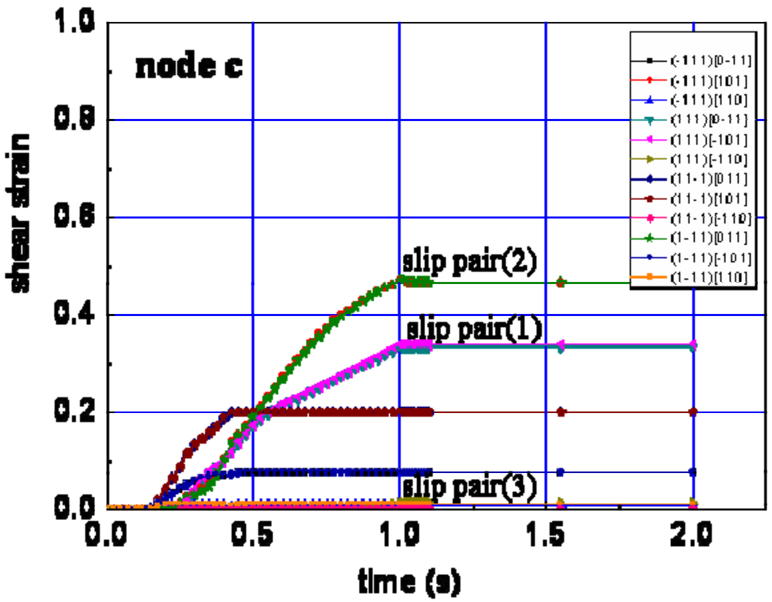


local !! curvature seems NOT to be larger for very small indents

Local active slip systems (simulation)

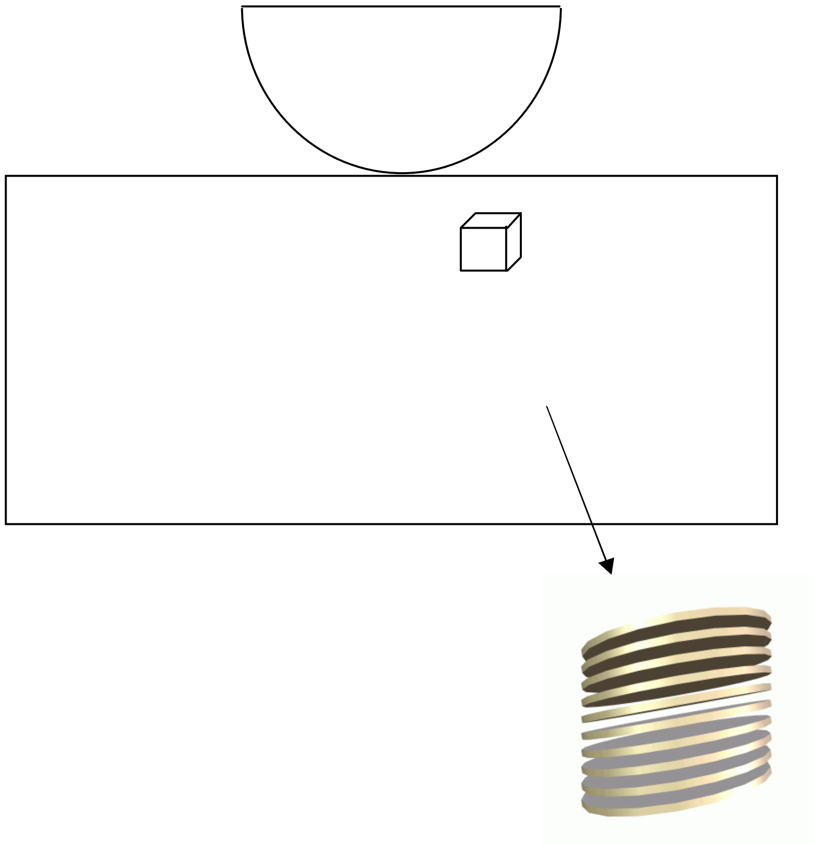


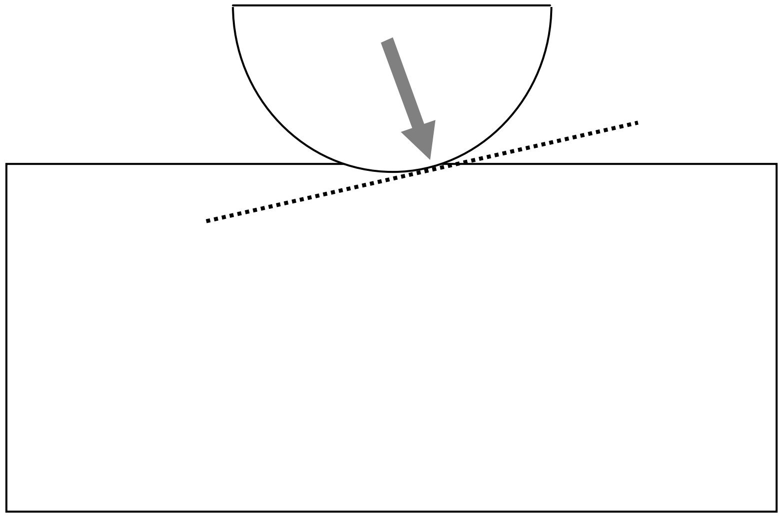


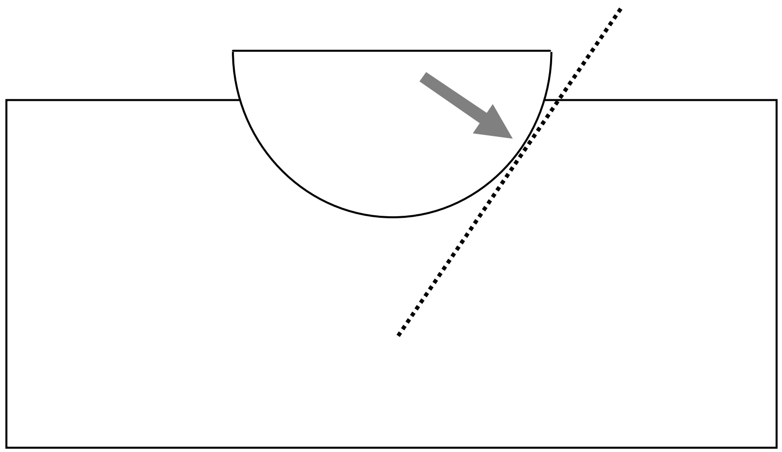


The active slip systems during indentation at these nodes

Sachs case under compression tangential to contact







Simplify: single crystal kinematics for a Sachs case under compression tangential to local contact interface