



Texture Evolution during Casting and Hot Rolling of a β -Ti-Nb alloy

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International Conference on the Texture of Materials

ICOTOM 15

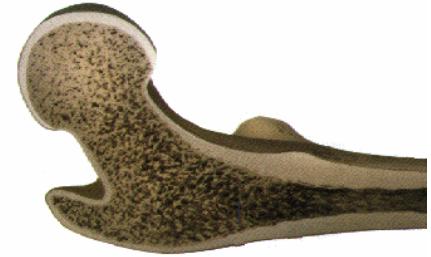
Pittsburgh, June 2008



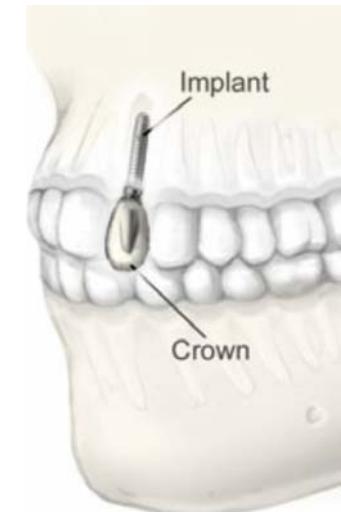
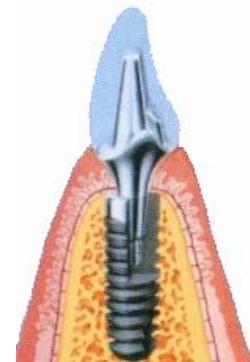
- Motivation 
- Experimental
- Simulations
- Conclusions

Motivation – BCC Ti alloys as biomaterials (implants)

- Bone: 20-25 GPa
- Current implant alloys: 115 GPa
- Stress shielding, bone degeneration
- Lower elastic stiffness
- β -Ti (BCC: Ti-Nb, Ti-Mo, Ti-V,...)
- Bio-compatible alloy elements



- here: Anisotropy and texture
- Ti-35Nb-7Zr-5Ta (wt.%)



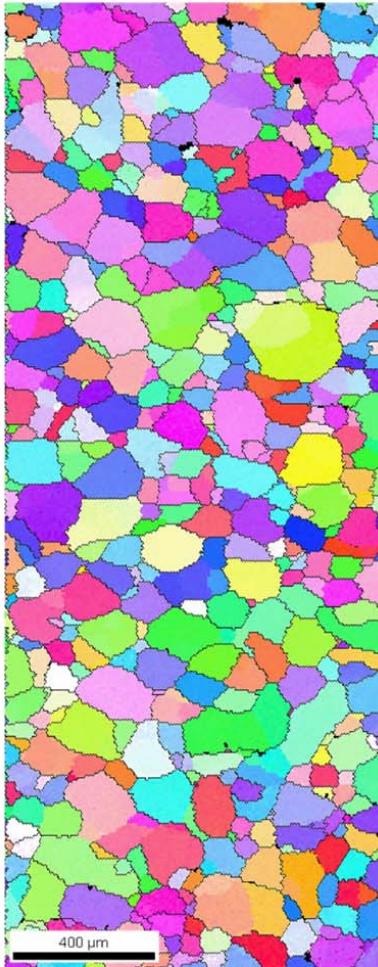


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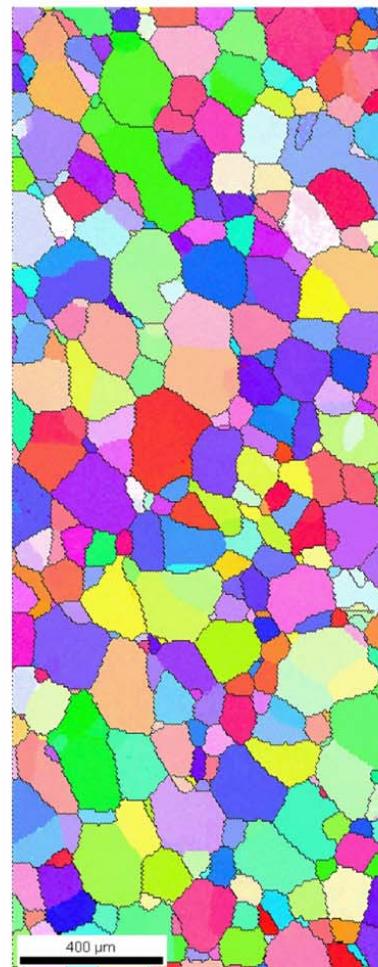


Ti-35wt.%Nb-7wt.%Zr-5wt.%Ta

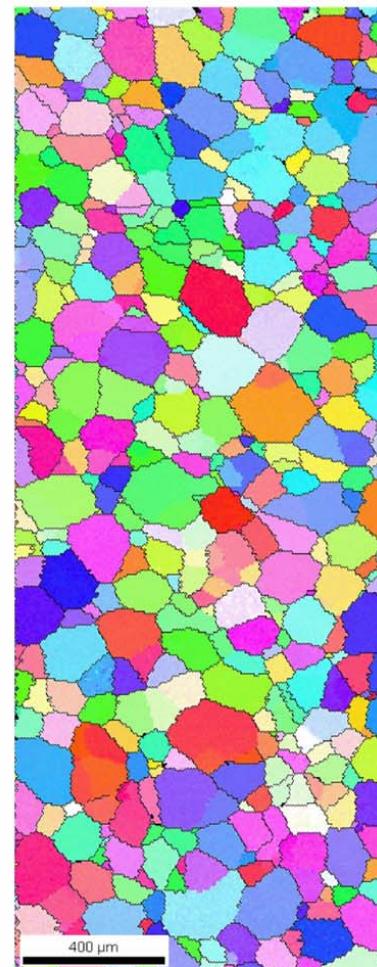
as cast alloy



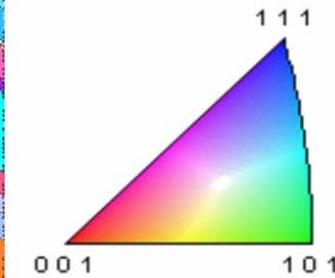
TD
↑
RD



ND
↑
TD



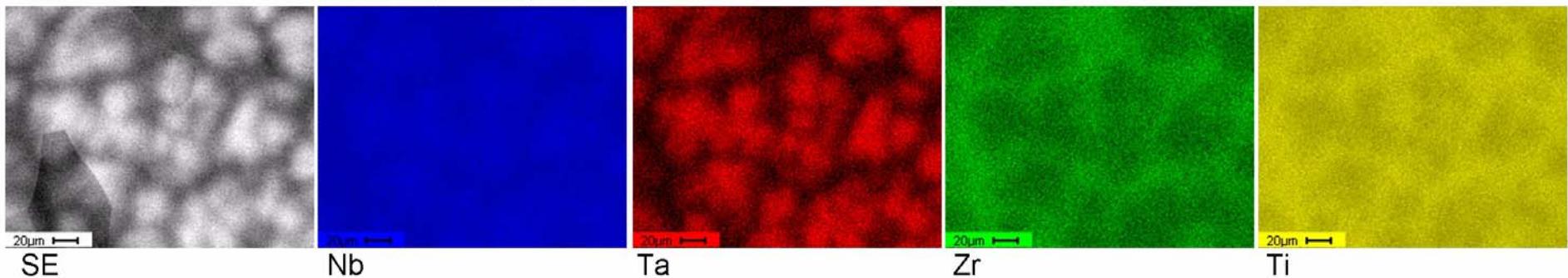
ND
↑
RD



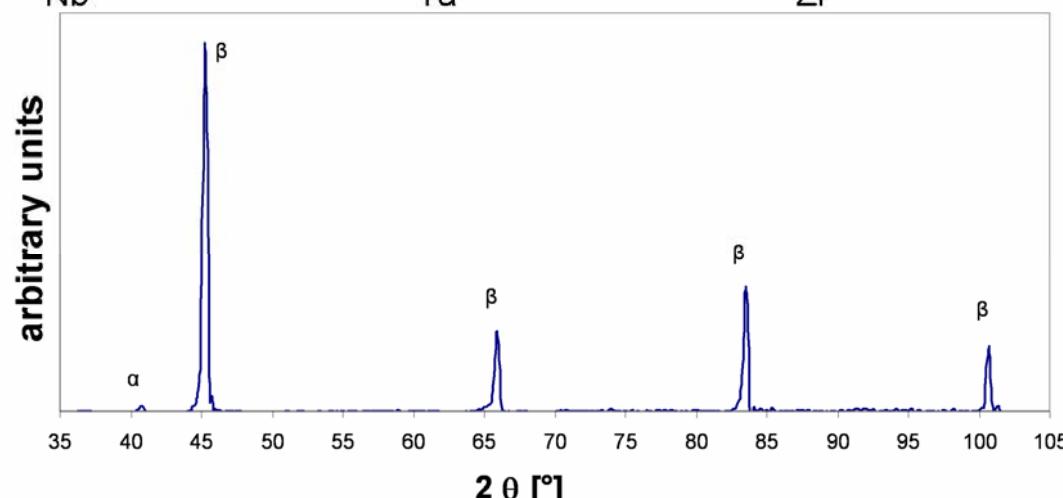
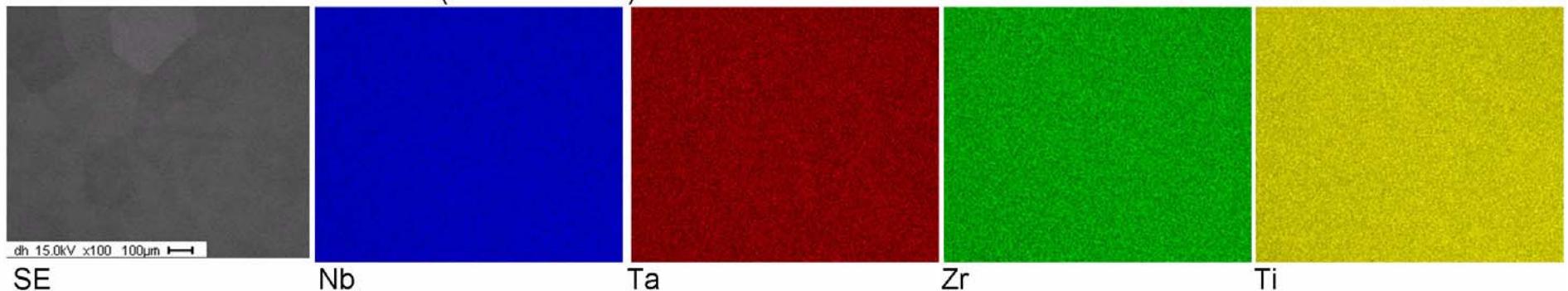


Ti-35wt.%Nb-7wt.%Zr-5wt.%Ta

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

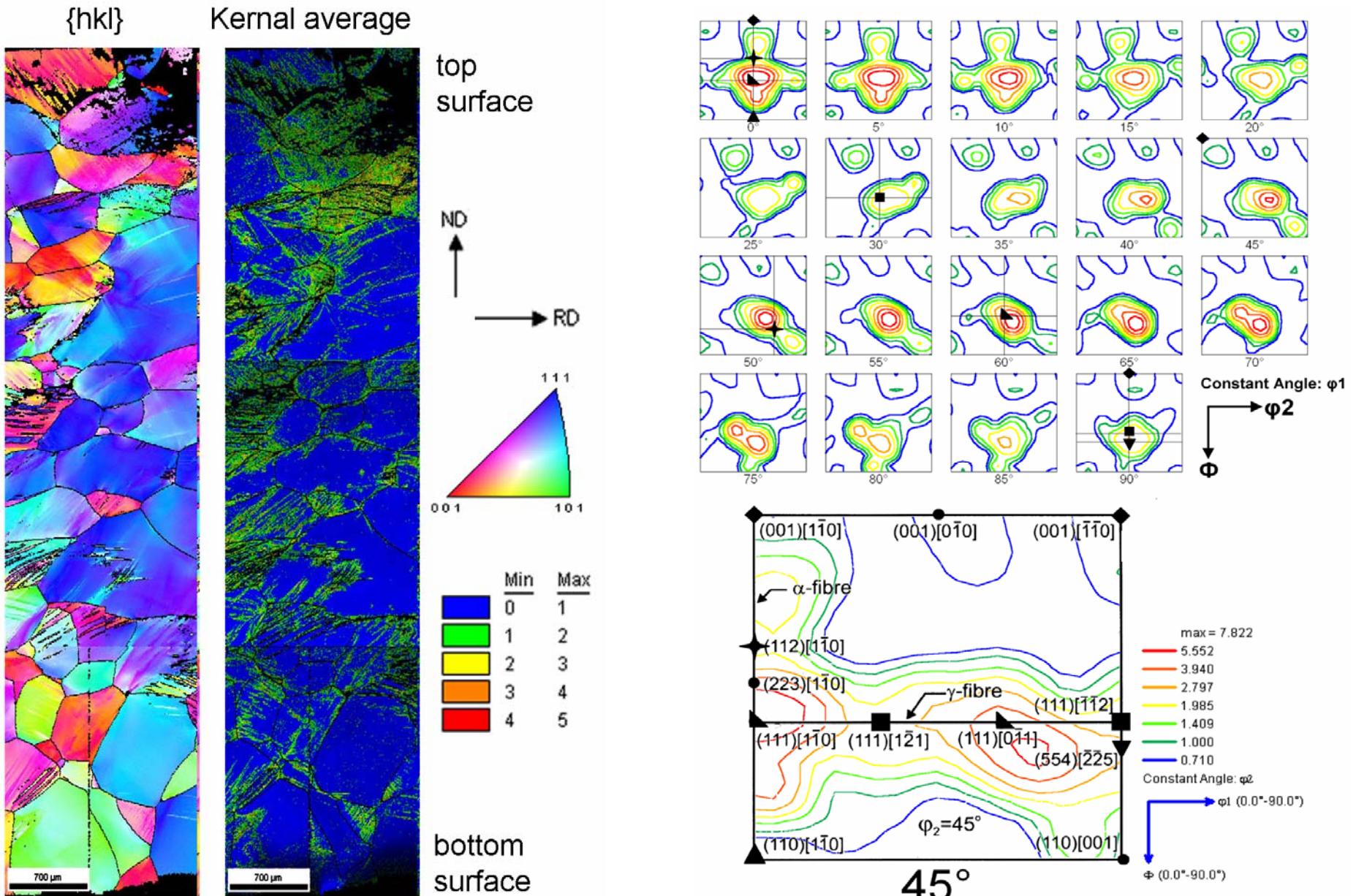


Ti-35wt.%Nb-7wt.%Zr-5wt.%Ta (1200°C for 4h)

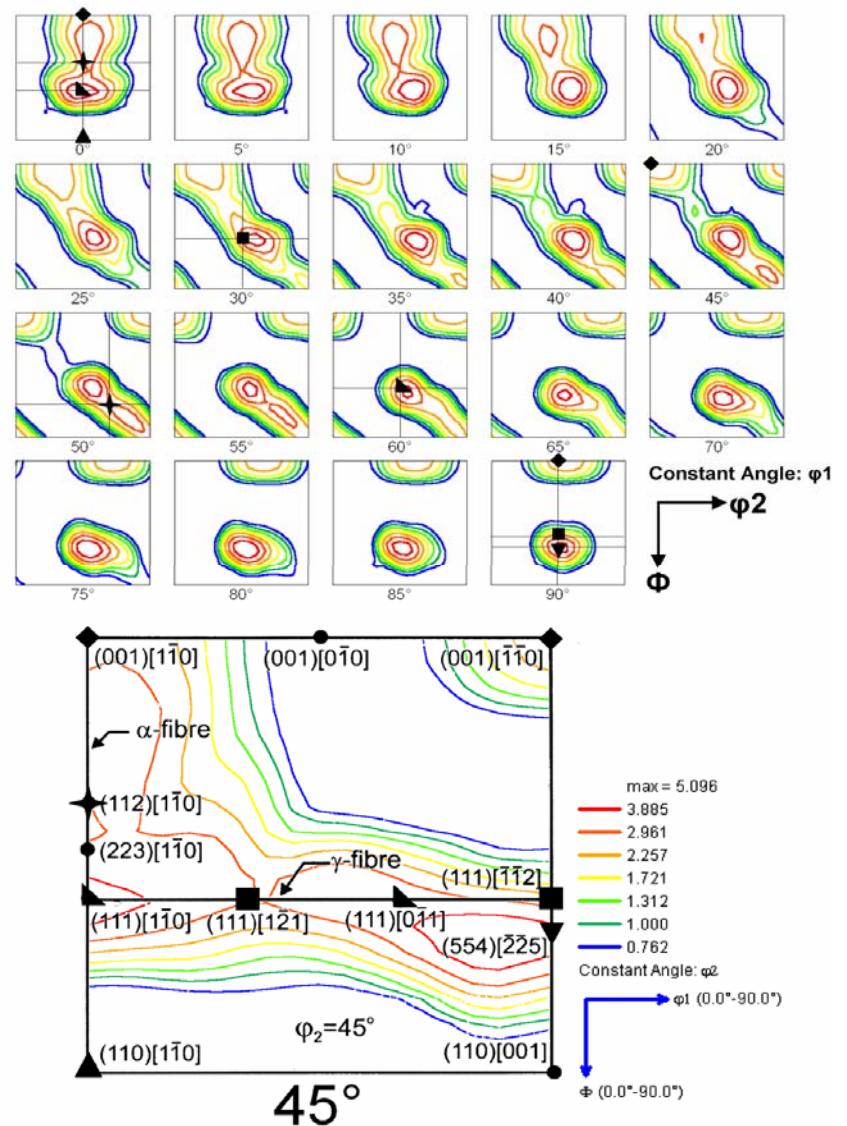
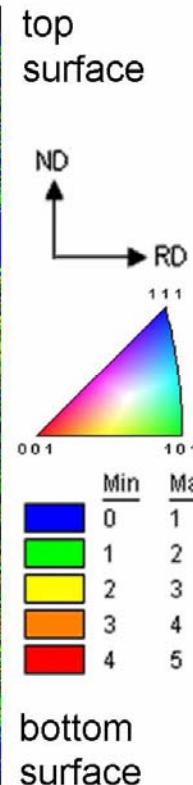
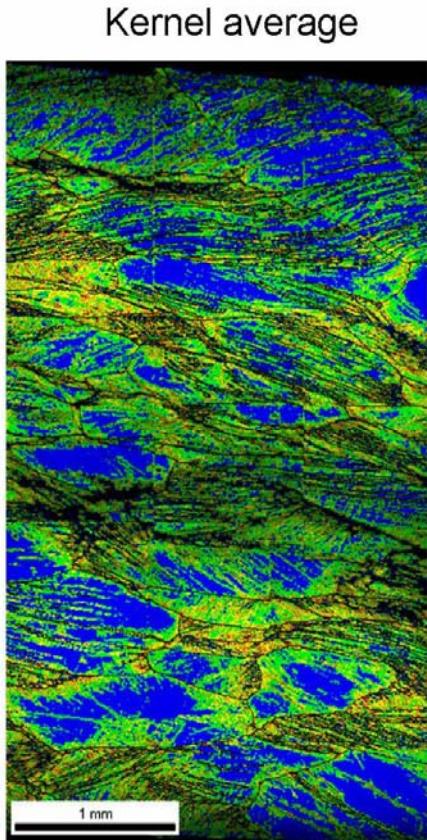
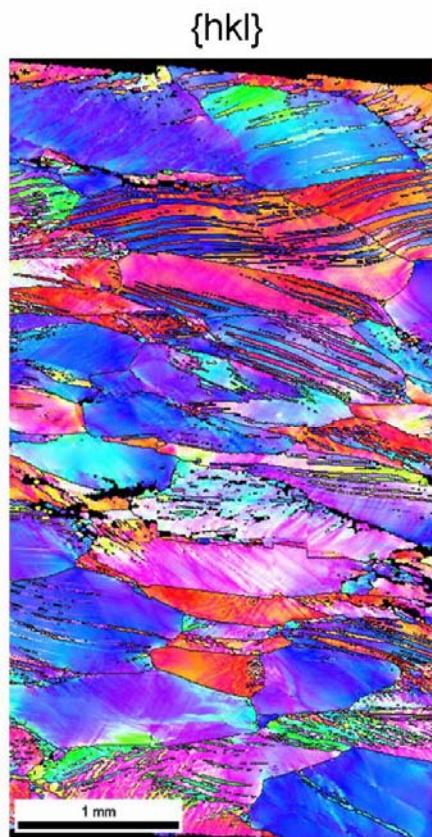


D. Raabe, lecture, ICOTOM 15, June 2008

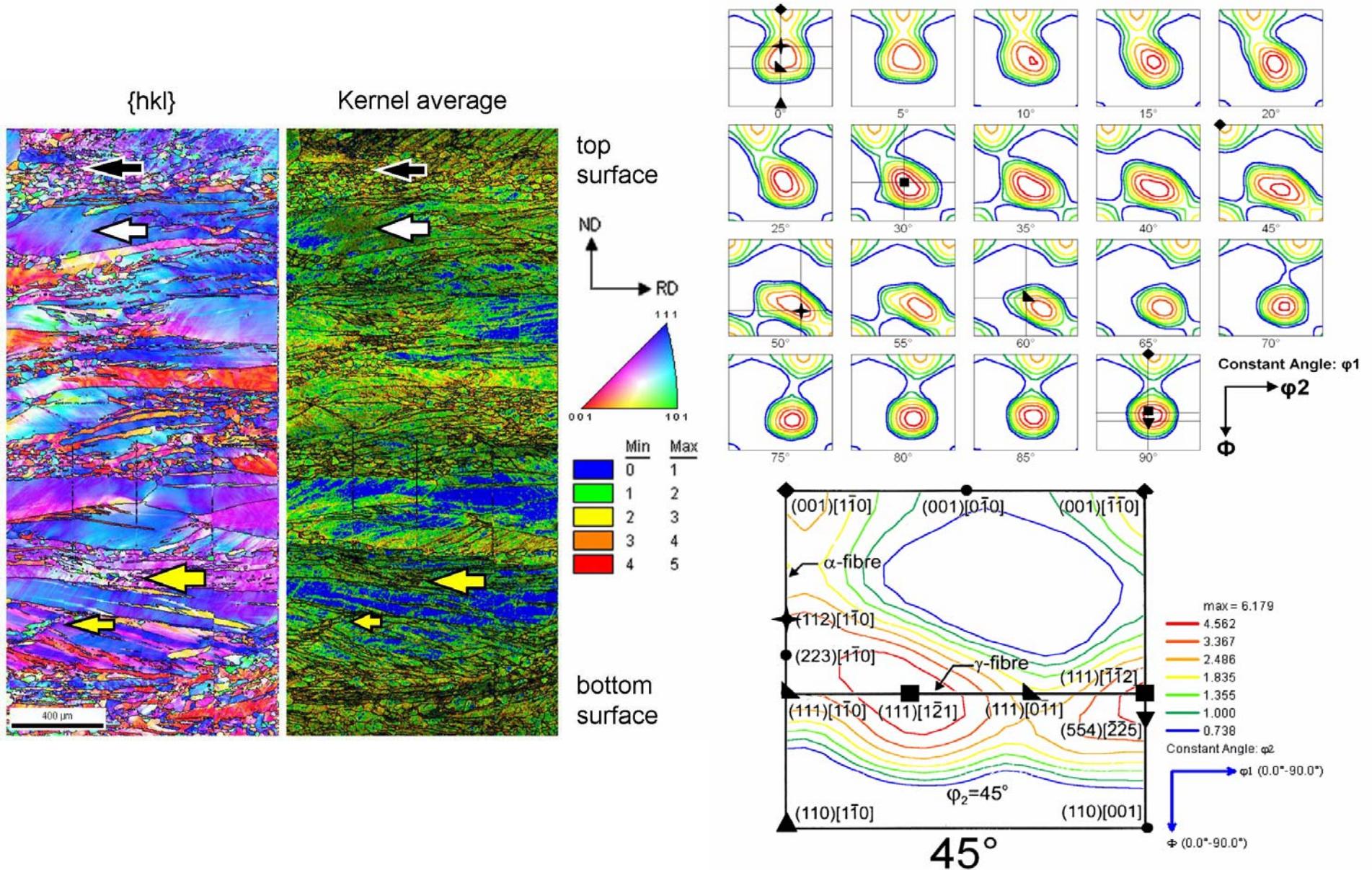
Ti-35wt.%Nb-7wt.%Zr-5wt.%Ta - 20% warm rolled (850°C)



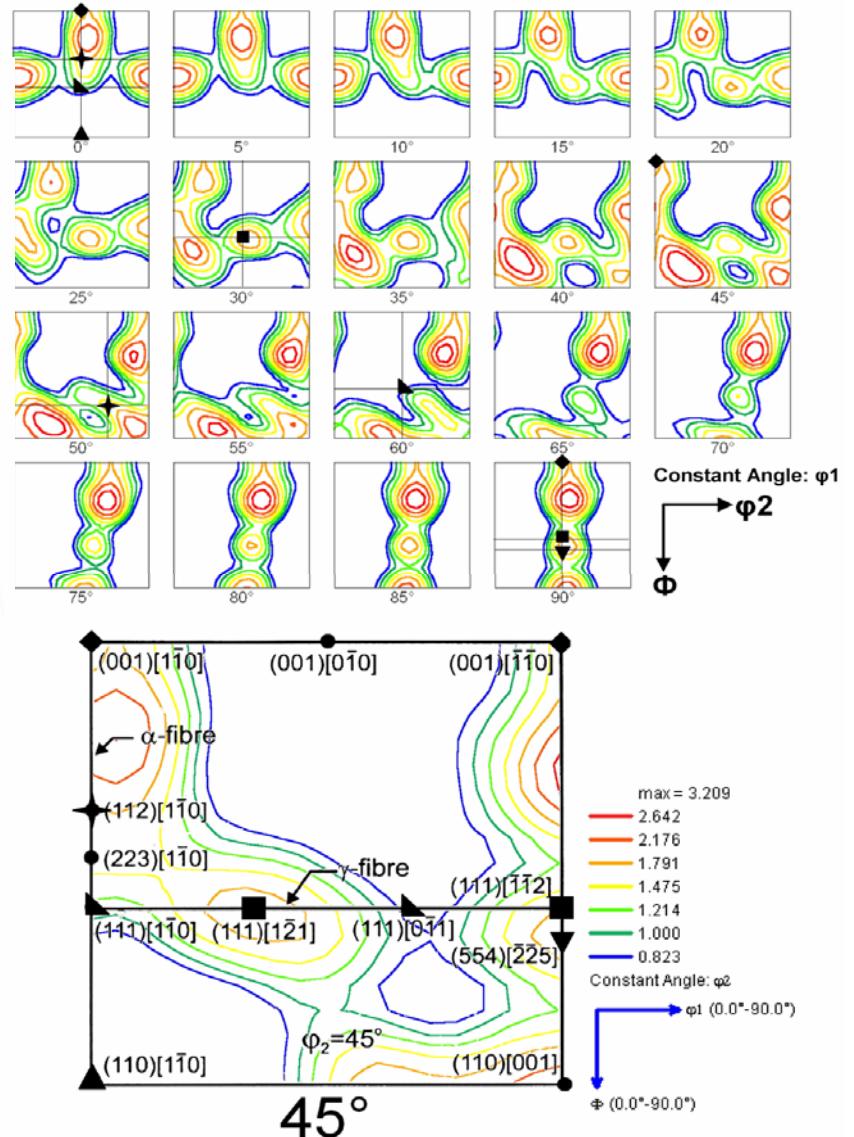
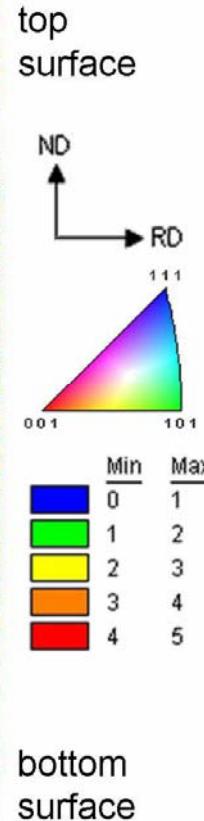
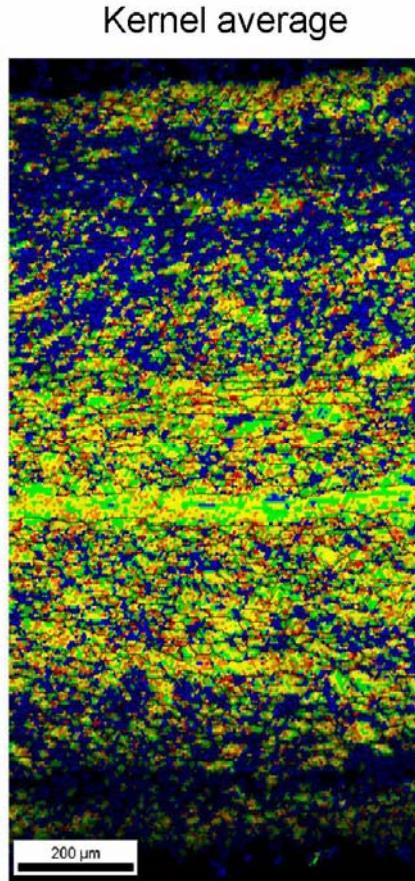
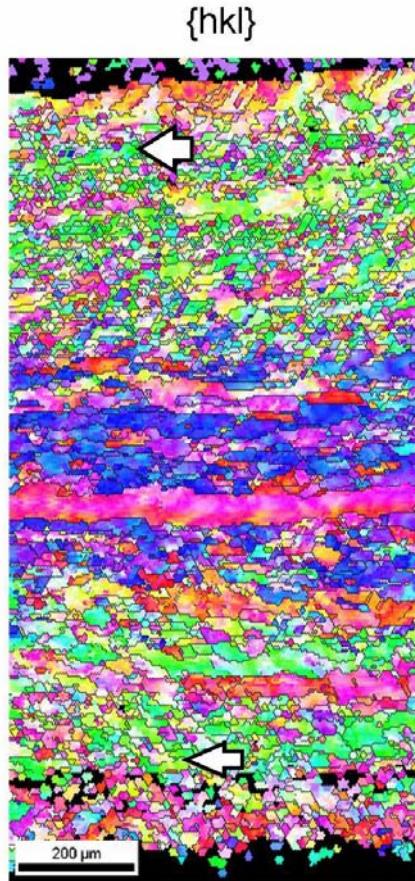
Ti-35wt.%Nb-7wt.%Zr-5wt.%Ta - 50% warm rolled (850°C)



Ti-35wt.%Nb-7wt.%Zr-5wt.%Ta - 70% warm rolled (850°C)



Ti-35wt.%Nb-7wt.%Zr-5wt.%Ta - 90% warm rolled (850°C)





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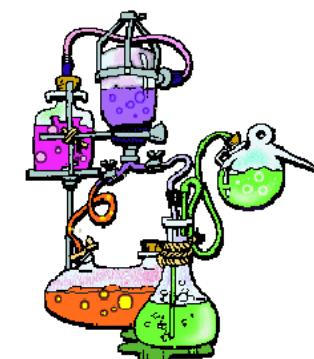
Scientific approach

- **Theory – driven guidance (non-toxic; BCC; low stiffness); replace phenomenological rules**
- **2 binary (Ti-Nb, Ti-Mo); 2 engineering (Ti-35wt.%Nb-7wt.%Zr-5wt.%Ta and a Ti-20wt.%Mo-7wt.%Zr-5wt.%Ta)**
- **Combination of ab-initio simulations, homogenization and experiments**
- **Characterization: OM, SEM, EBSD, EDX, XRD, ultrasonic resonance, mechanical testing**

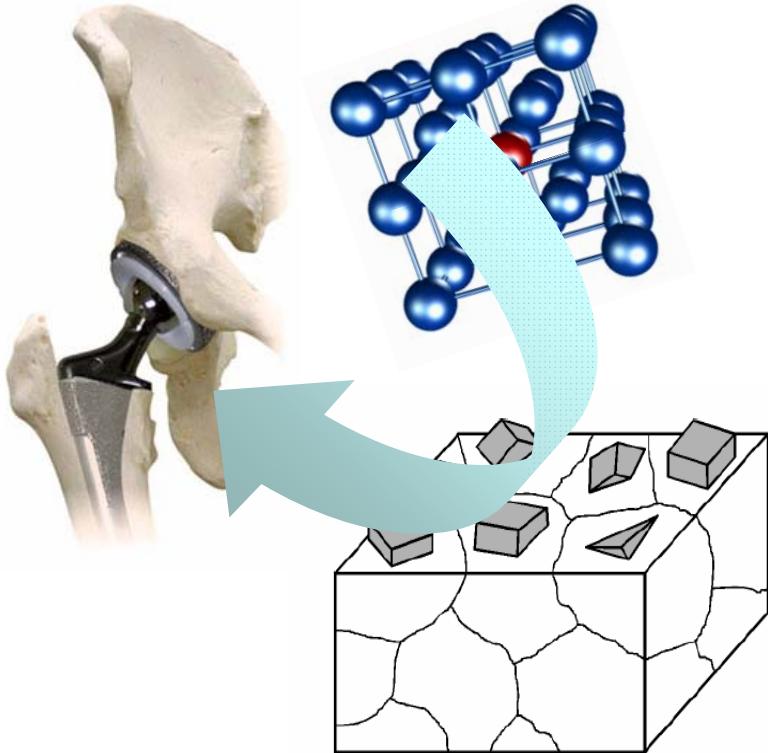
Density functional theory (DFT)
FEM, analytical bounds



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



Theoretical methods



- Free energy $F(x,c,T) = U - T \cdot S$
- U: density functional theory (DFT)
- S: configuration entropy
- BCC: Ti-Mo and Ti-Nb
- Elastic tensor
- Polycrystal homogenization

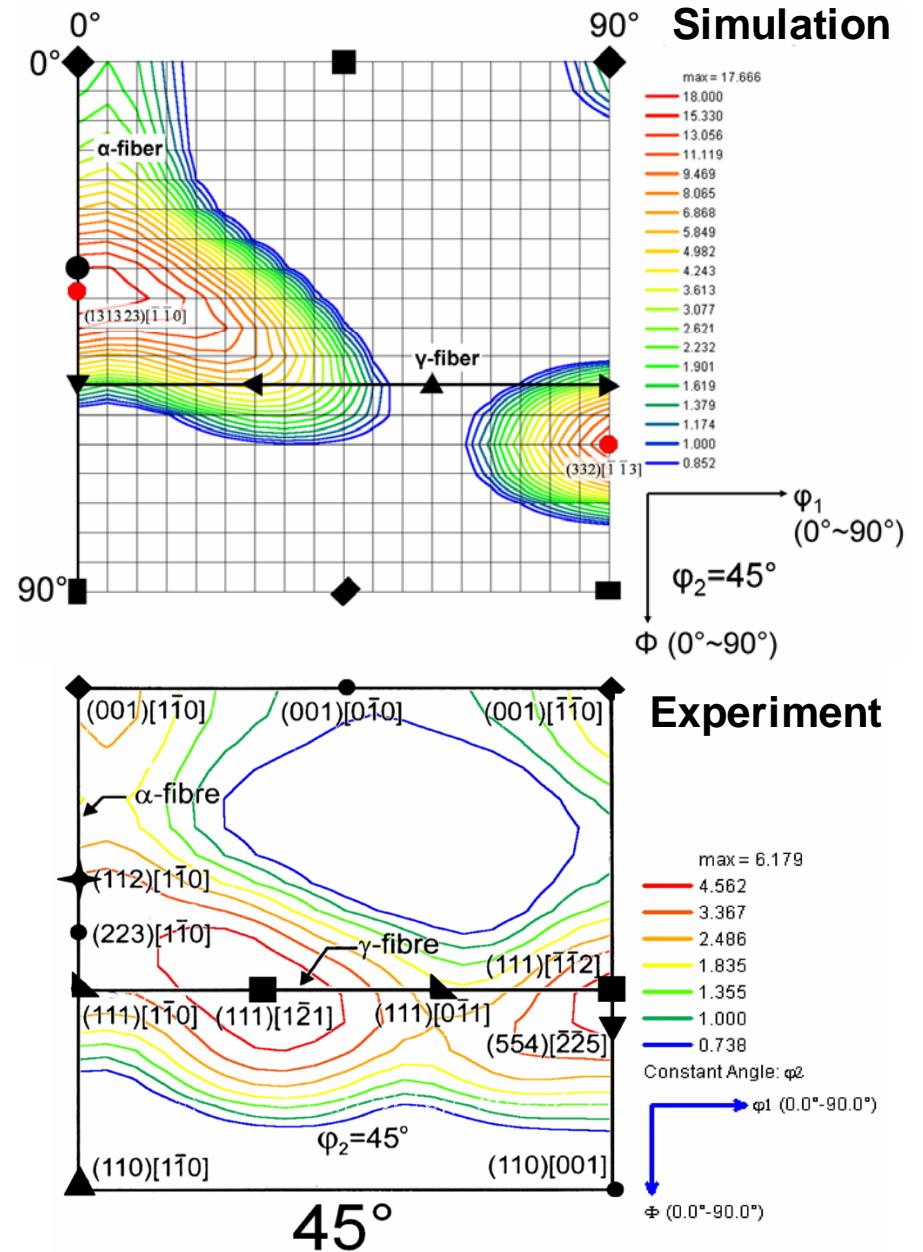
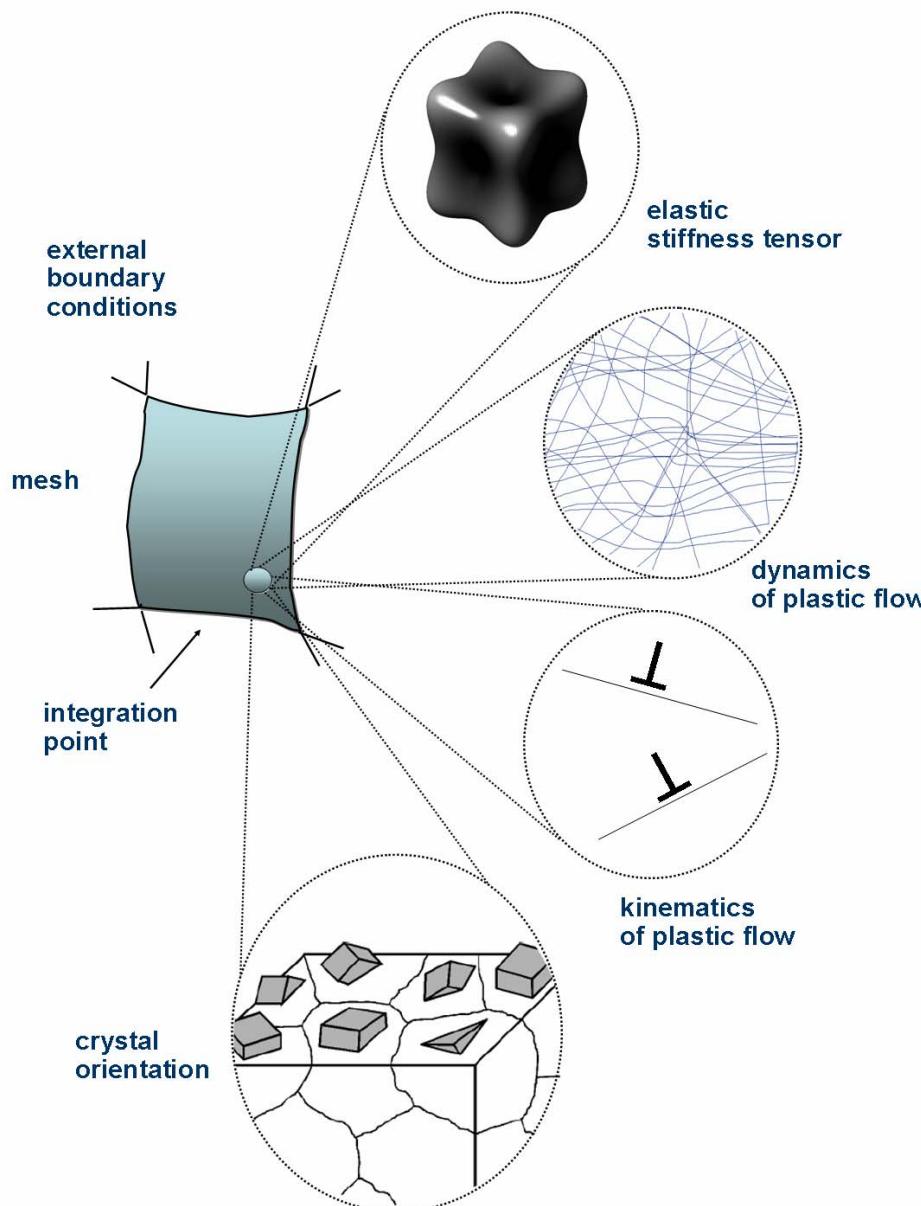
Details:

DFT: GGA, plane wave pseudopotential approach (VASP), plane wave cutoff energy:

170 eV, $8 \times 8 \times 8$ and $9 \times 9 \times 6$ Monkhorst k-point mesh, relaxation until cell stress free, supercells of $2 \times 2 \times 2$ 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

Polycrystal homogenization: Voigt, Reuss, HS, Hershey, CPFEM

Simulation: DFT (ab initio) and CPFEM (continuum)





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Conclusions

- Texture and microstructure of BCC Ti-35Nb-7Zr-5Ta
- Warm rolling (850°C)
- Up to 50% rolling the texture and microstructure did not reveal pronounced gradients through thickness
- Texture similar to other bcc
- Recrystallization negligible below 50% reduction
- After 70% reduction typical bcc warm rolling components, partial recrystallization
- After 90% thickness reduction strong through-thickness texture and microstructure gradients, explained in terms of heavy shear at the surface and plane strain deformation in the center followed by strong recrystallization in the surface layers (top, bottom) and strong recovery in center



Further reading

- D. Raabe, B. Sander, M. Friák, D. Ma, J. Neugebauer, *Acta Materialia* 55 (2007) 4475–4487, “Theory-guided bottom-up design of beta-titanium alloys as biomaterials based on first principles calculations: theory and experiments”
- B. Sander, D. Raabe, *Texture inhomogeneity in a Ti-Nb-based beta-titanium alloy after warm rolling and recrystallization*, *Materials Science & Engineering A* 479 (2008) 236–247