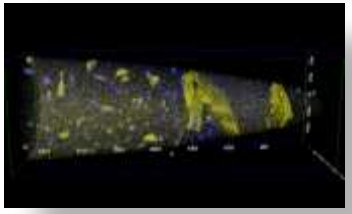
Multiscale Modeling in Materials Science

F. Roters, M. Friak, T. Hickel, J. Neugebauer, D. Raabe

WWW.MPIE.DE
d.raabe@mpie.de
Max-Planck-Institut
für Eisenforschung GmbH
Düsseldorf, Germany

theory

experiment



MPIE research focus: multiscale modeling in the CPTS

M. Jansen (Festkörperforschung), K. Kremer (Polymerforschung), S. Müller (Mathematik i. d. Naturwissenschaften), J. Neugebauer (Eisenforschung) , D. Raabe (Eisenforschung), K. Reuter (Fritz-Haber), M. Scheffler (Fritz-Haber), W. Thiel (Kohlenforschung)

Answering societies' grand challenges with complex alloys

70% of all **industrial innovations** are associated with progress in **materials science**

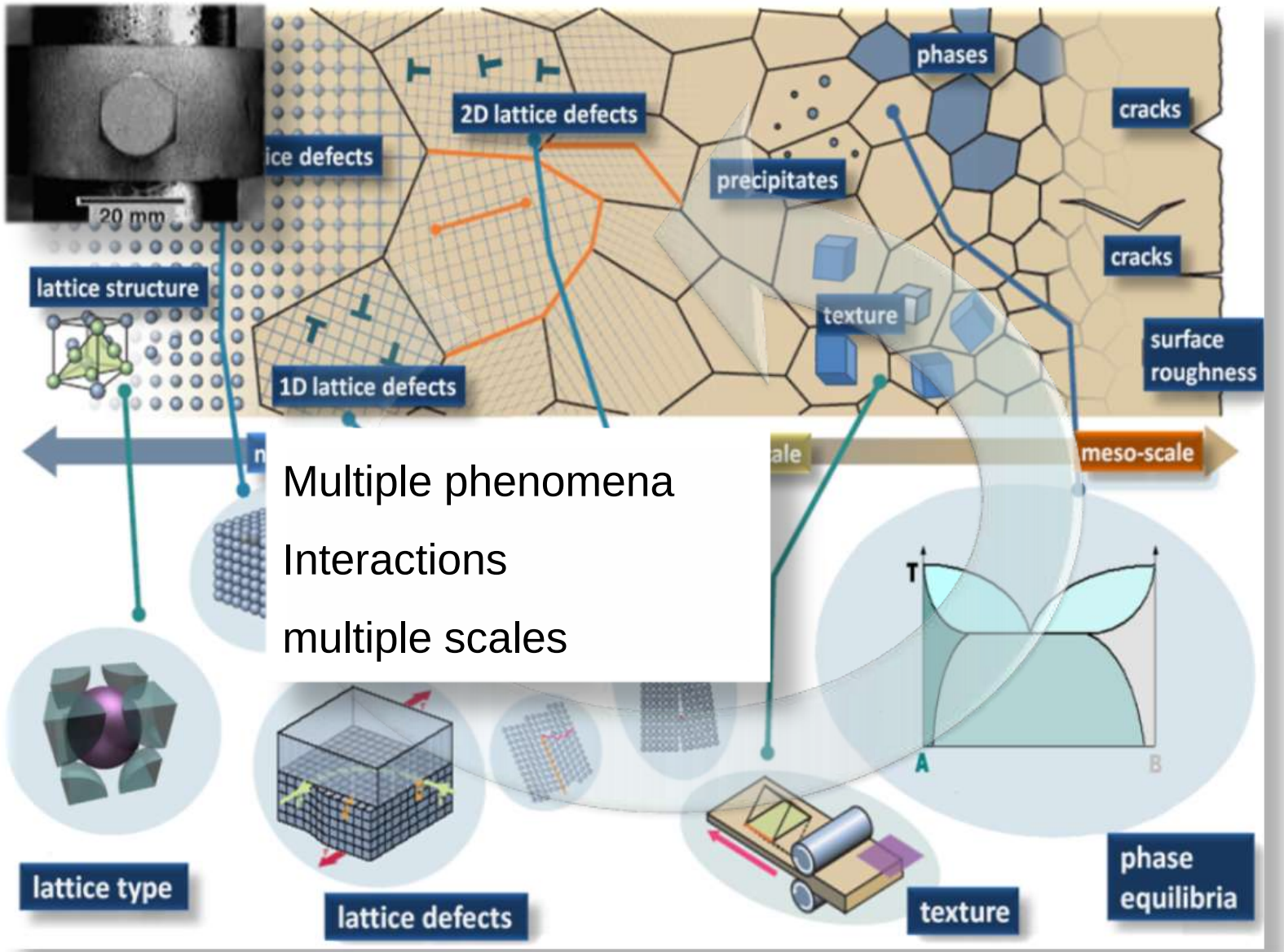
Complex Materials occupy key roles
(energy, transportation, health, safety, infrastructure)

Materials-related industries account for 46% of all EU manufacturing value and 11% of the EU's total domestic product

3.5 billion € per day in the EU
World Trade Organisation

Mission: Understanding and designing complex materials from first principles

Scientific mission: complex materials in real environments

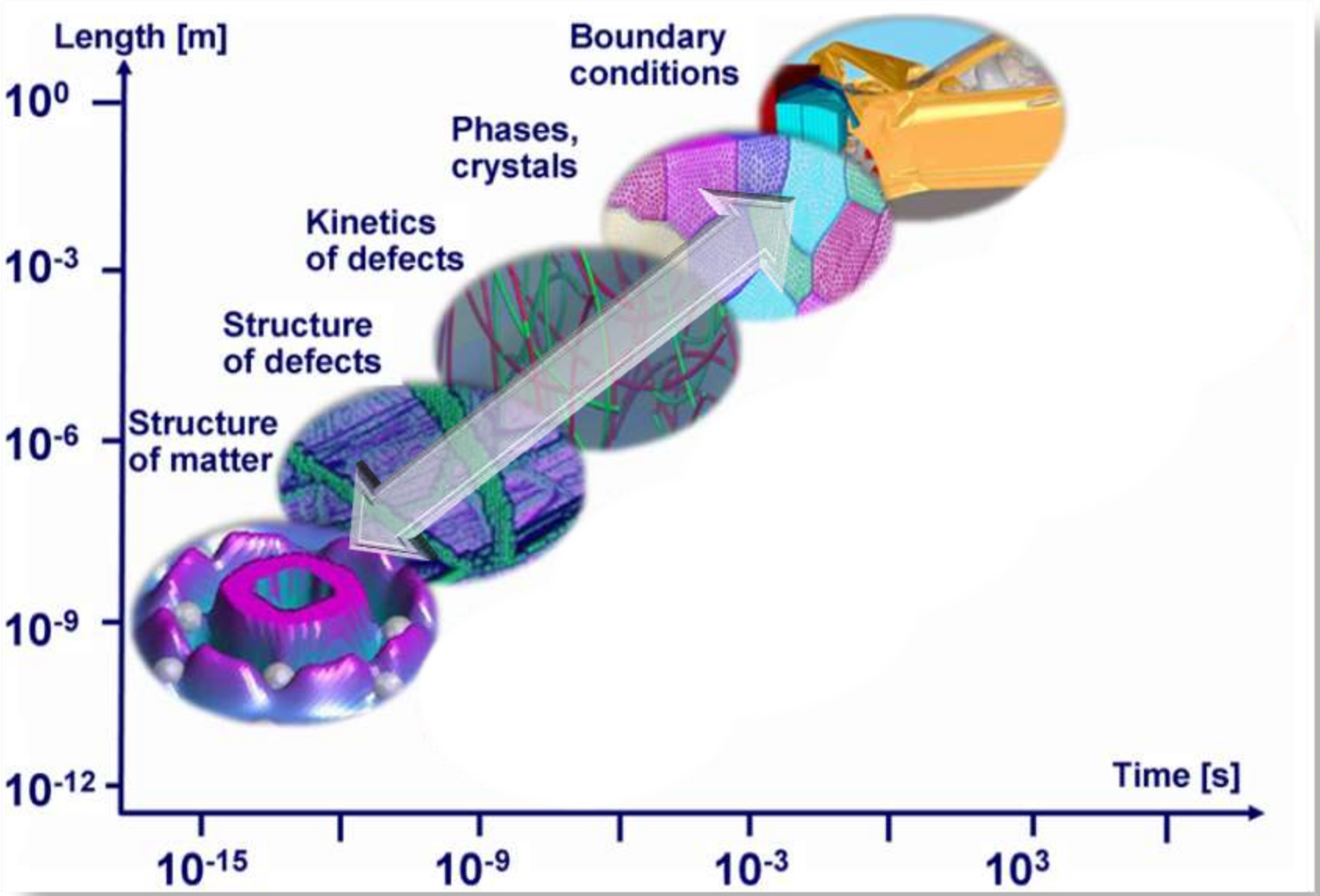


Multiple phenomena

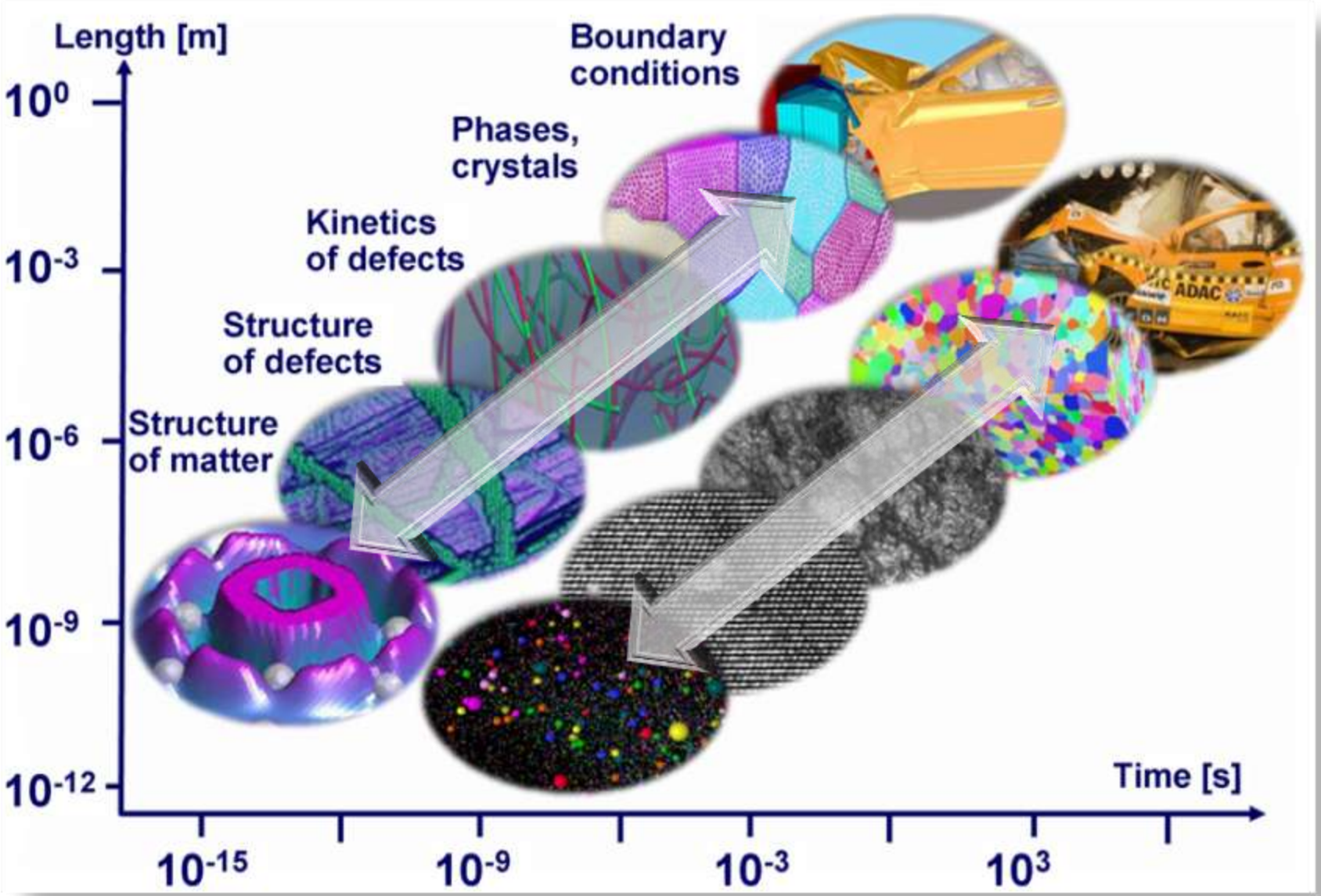
Interactions

multiple scales

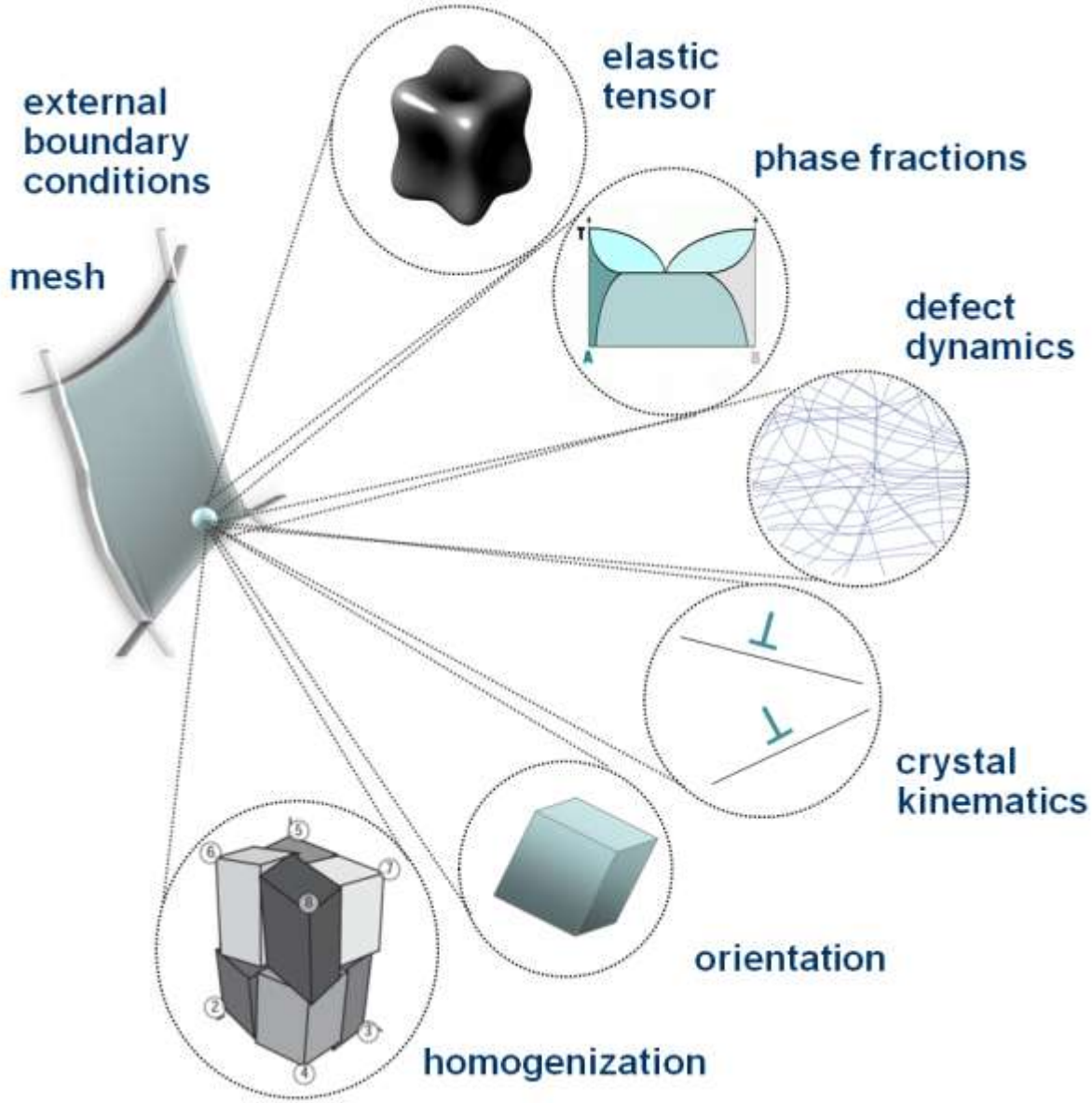
Multiscale Modeling and Experimentation



Multiscale Modeling and Experimentation



Multiscale crystal plasticity FEM



PDE solver:

FEM

MC

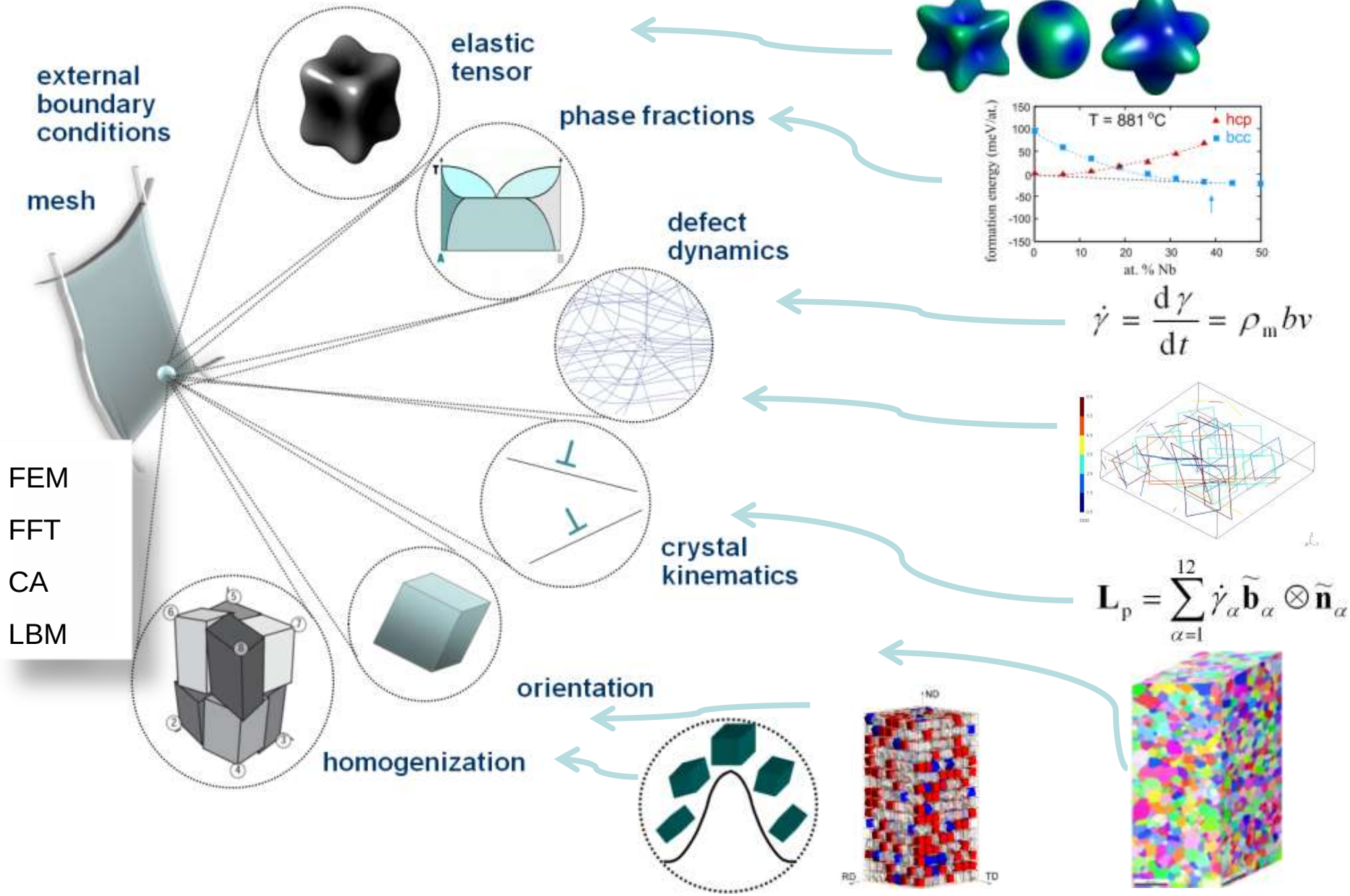
FFT

CA

LBM

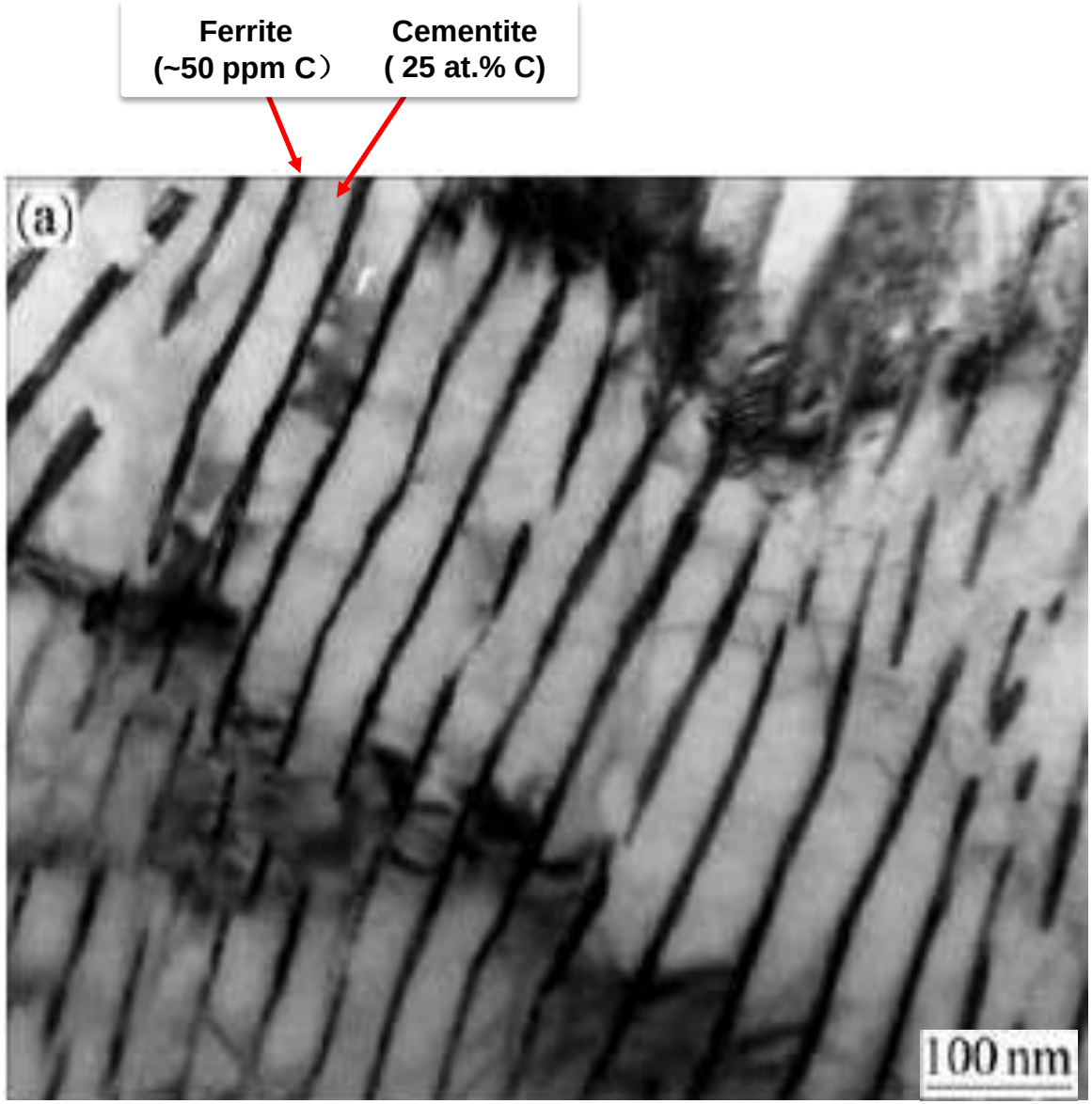
Raabe, Zhao, Park, Roters: Acta Mater. 50 (2002) 421

Multiscale crystal plasticity FEM



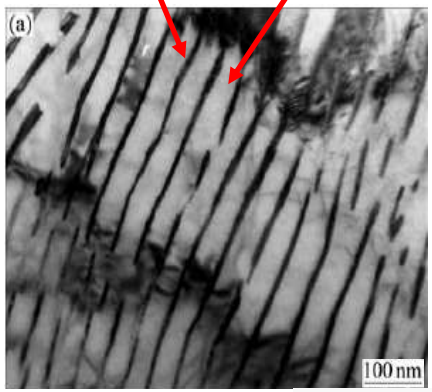
Raabe, Zhao, Park, Roters: Acta Mater. 50 (2002) 421

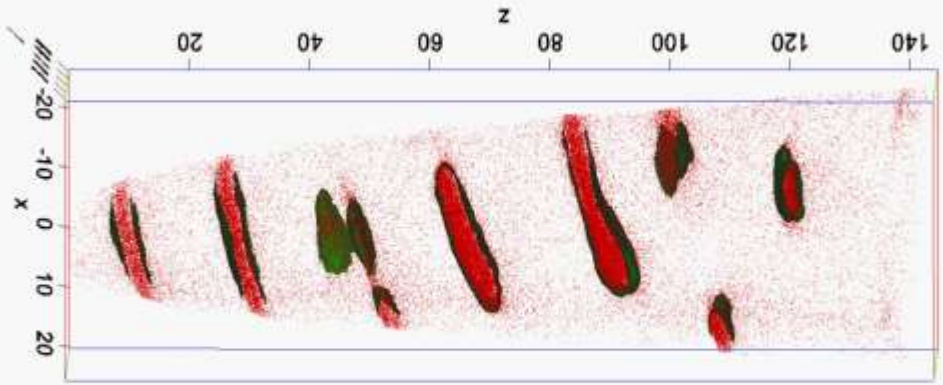
Towards the limits of strength: cold-drawn pearlitic steel



Towards the limits of strength: cold-drawn pearlitic steel

Ferrite (~50 ppm C) **Cementite (25 at.% C)**



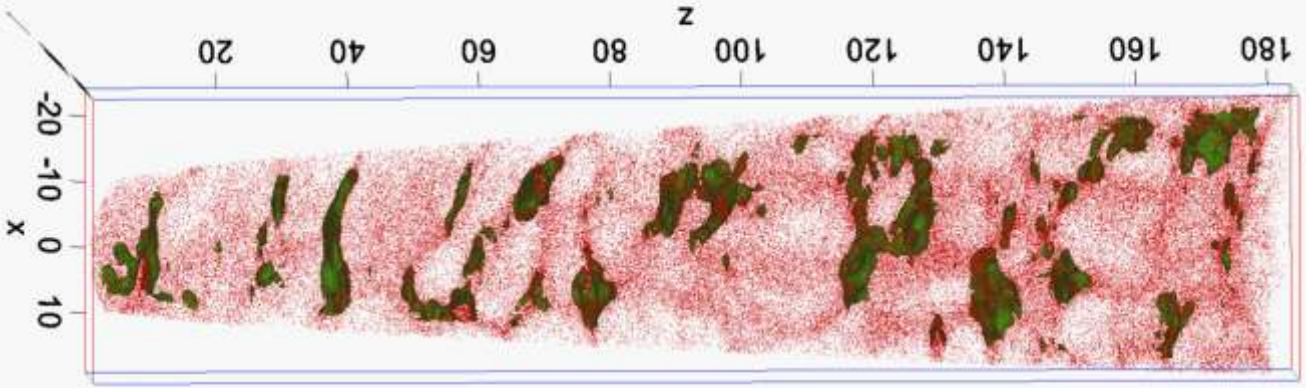


(ε = 2)

Scale: nm

C iso-concentration (7 at.%)

• C

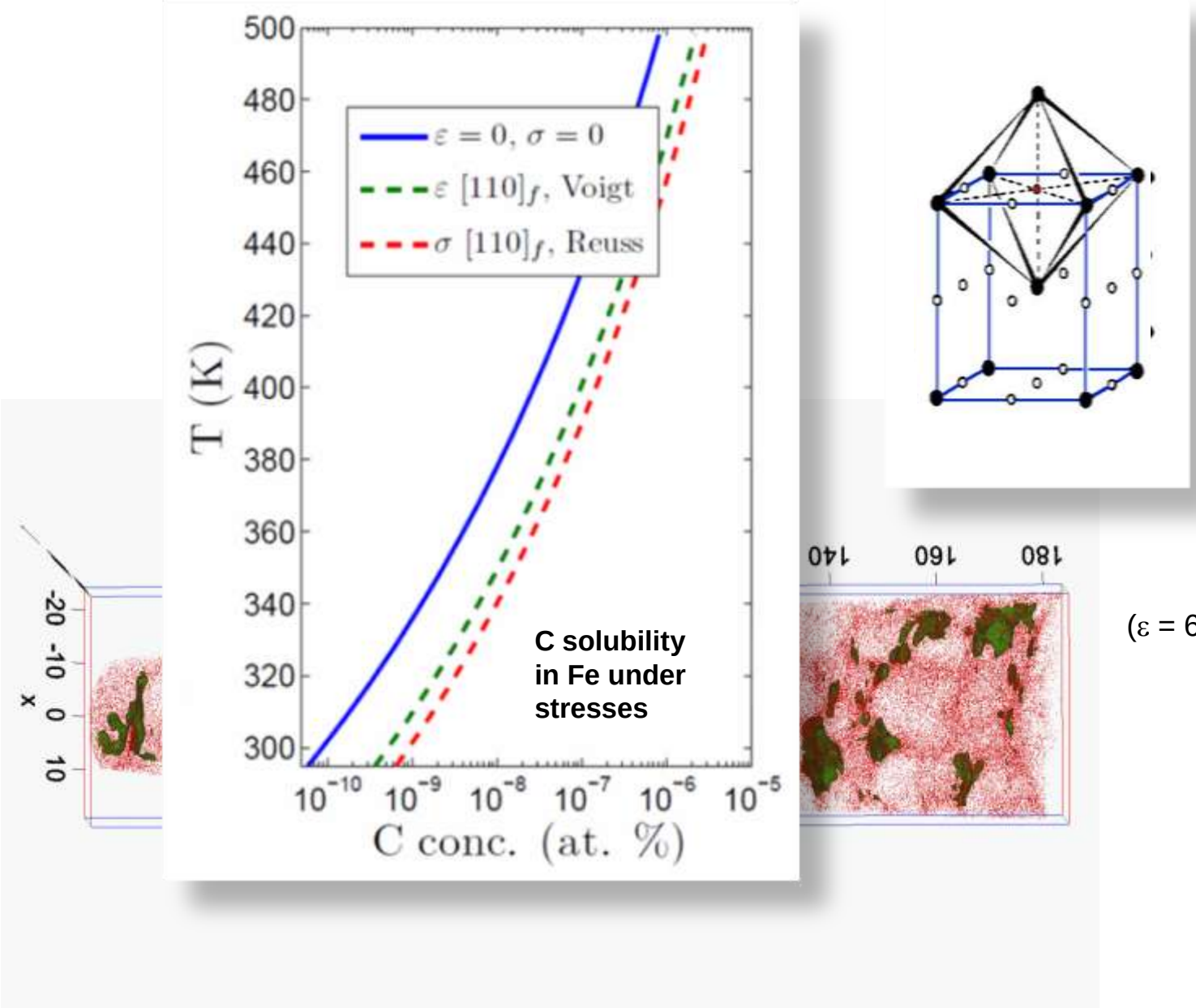


(ε = 6.5)

Towards the limits of strength: cold-drawn pearlitic steel

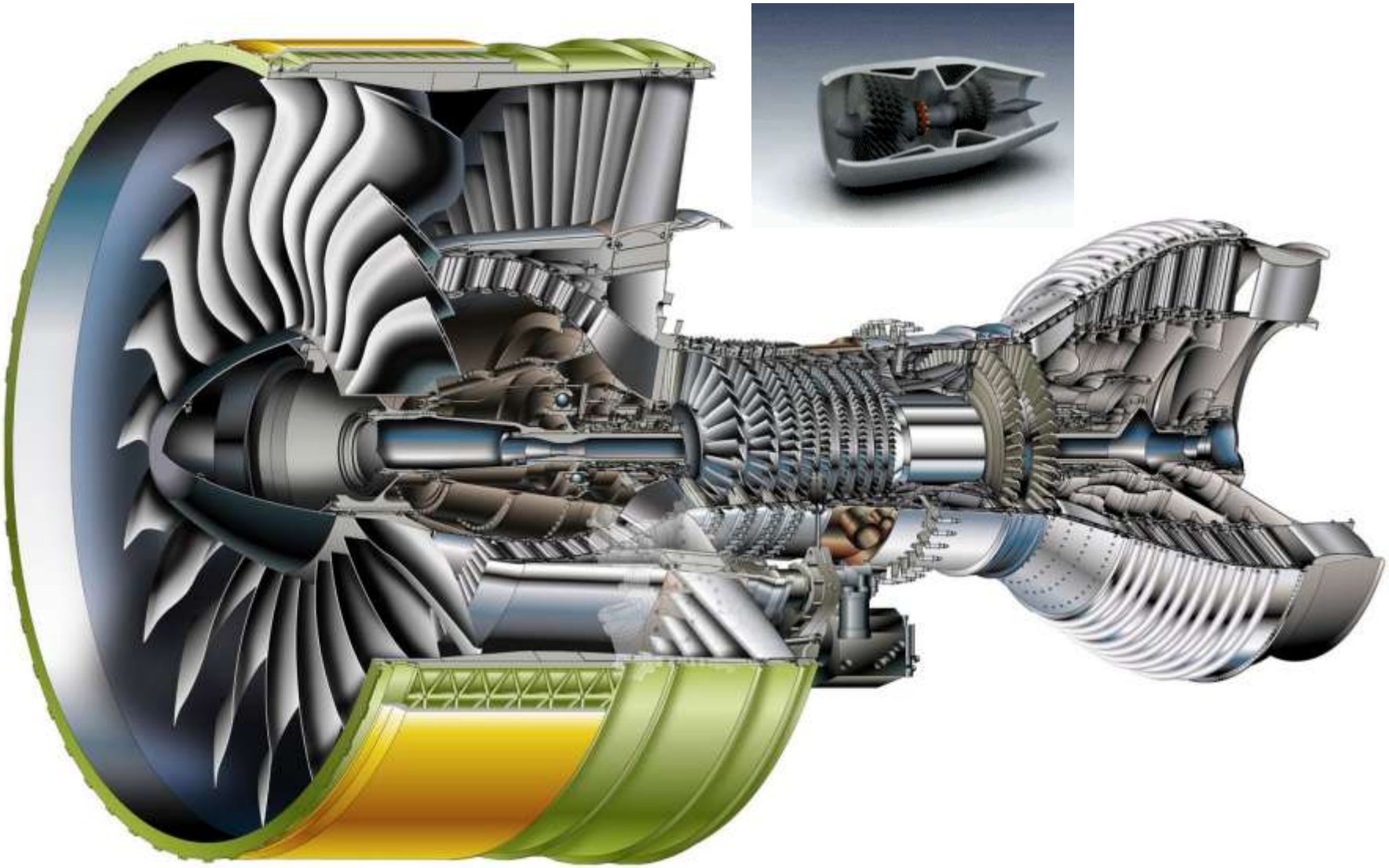
C iso-concentration (7 at.%)

• C



(ε = 6.5)

New materials for key technologies: Aero-space

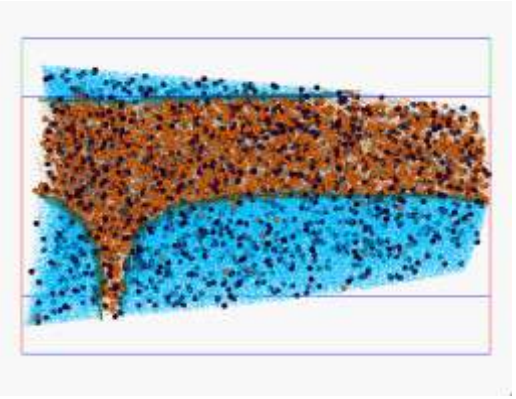


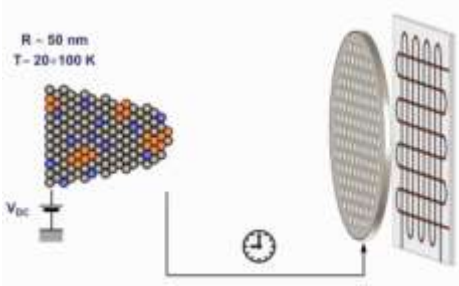
New materials for key technologies: Aero-space

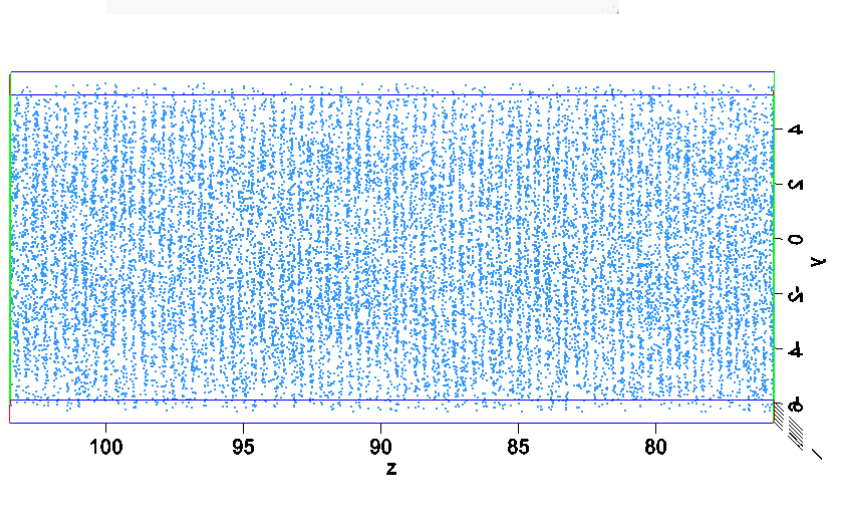
Complex Ni-based superalloy (ERBO, CMSX-4)

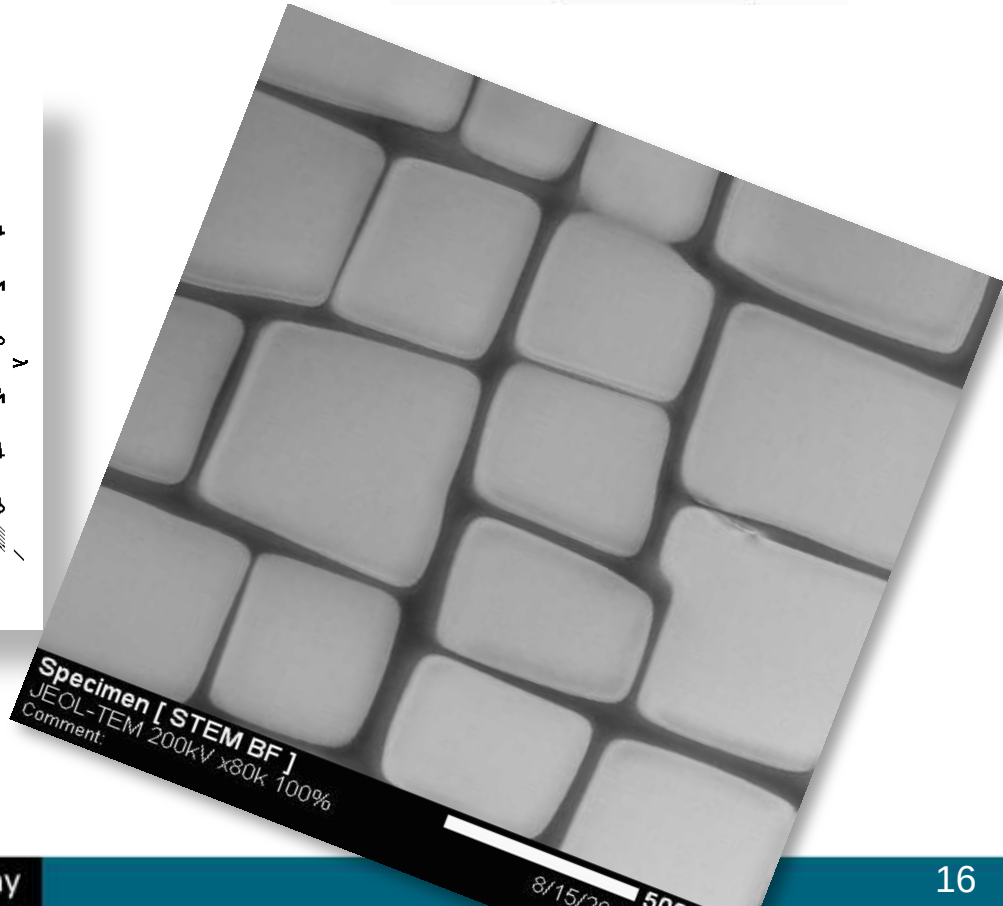
Complex Ni-based superalloy (ERBO, CMSX-4)

Al Re W Ni-iso (56 at.%)

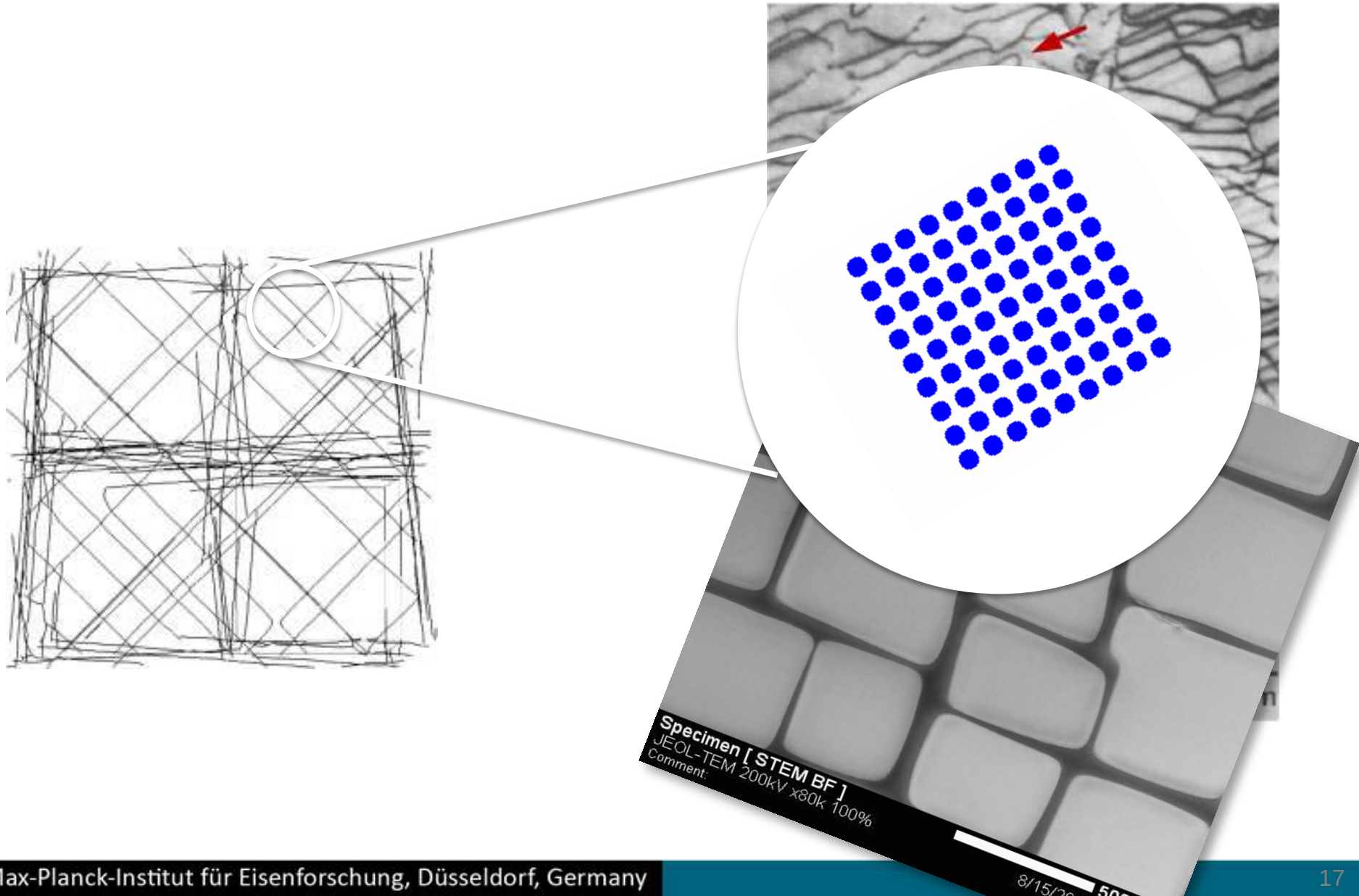






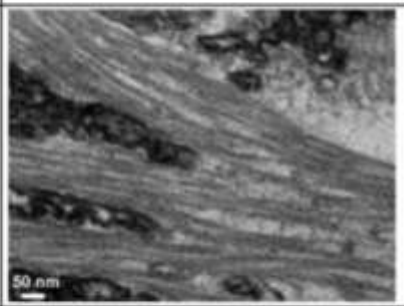
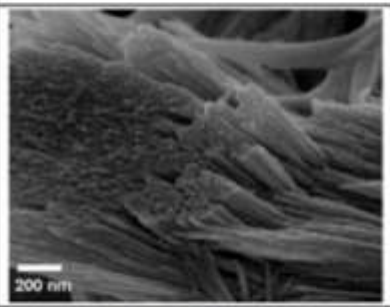
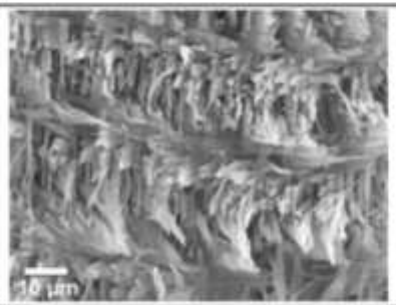
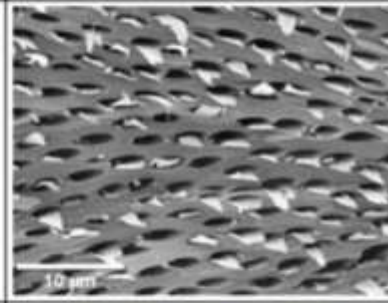
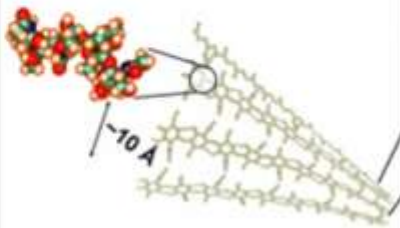
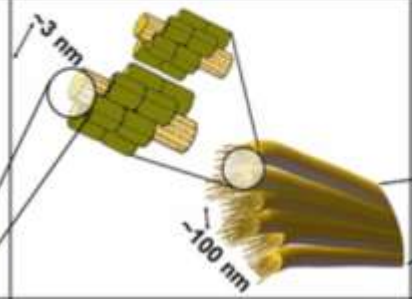
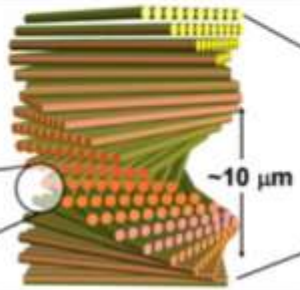
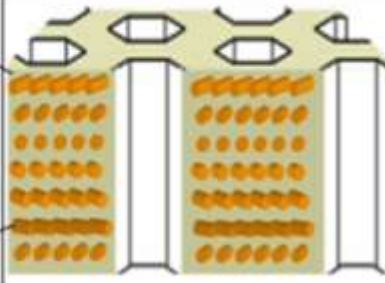
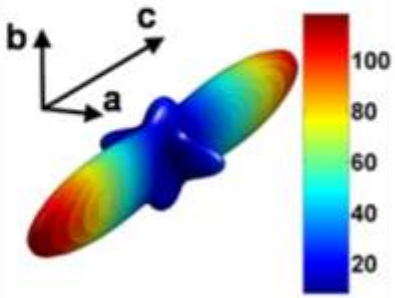
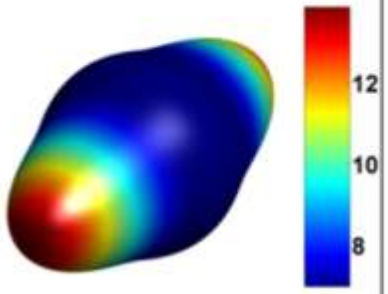
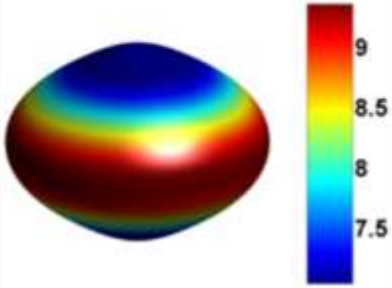
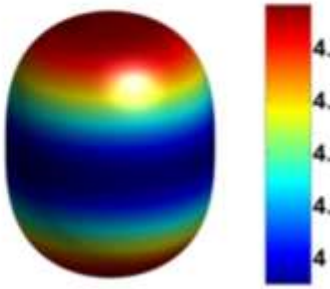


Change of microstructure

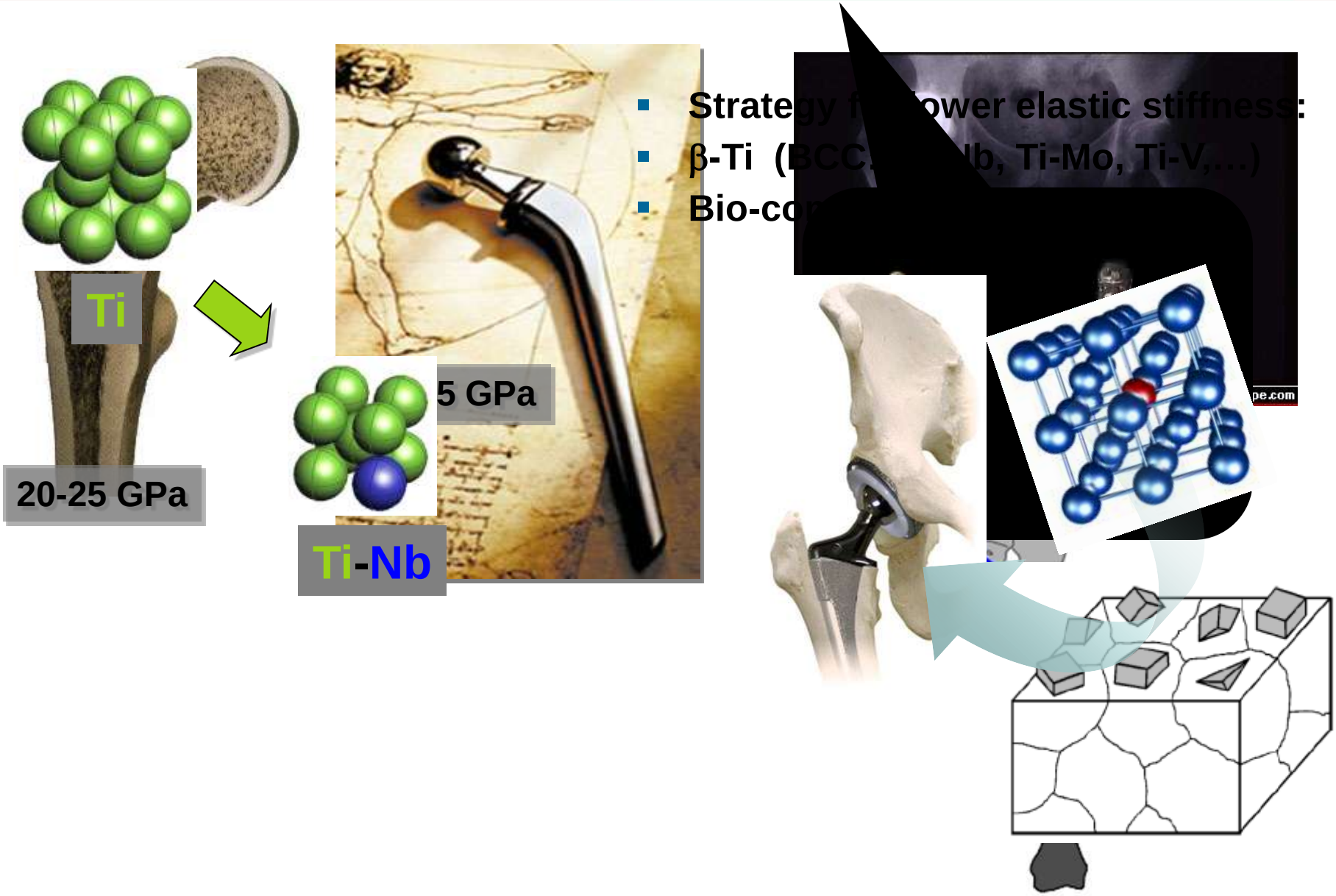


Exoskeleton component of more than 90% of all species …

adaptive material → candidate for bio-inspired material

Scale	0.1 nm – 10 nm	10 nm – 100 nm	100 nm – 10 μm	10 μm – 1 mm
Hierarchical structure unit	α-chitin (H-bonded anti-parallel N-acetyl-glucosamine molecular chains)	Mineralized chitin-protein nanofibrils in a planar array	Twisted plywood stack of mineralized chitin-protein planes without pore canals	Twisted plywood stack of mineralized chitin-protein planes with pore canals
Experimental method	Transmission electron microscope	Field emission scanning electron microscope	Field emission scanning electron microscope	Field emission scanning electron microscope
Microstructure				
Schematic				
Simulation method	Ab initio; density functional theory	Mori-Tanaka scheme (chitin-protein fiber); Torquato 3-point scheme (mineral-protein matrix)	Voigt estimate, tensor rotation	Torquato 3-point homogenization
Elastic behavior, 3D map of Young's modulus [GPa] a,b-axis: basal directions of chitin cell c-axis: longitudinal axis of molecule				

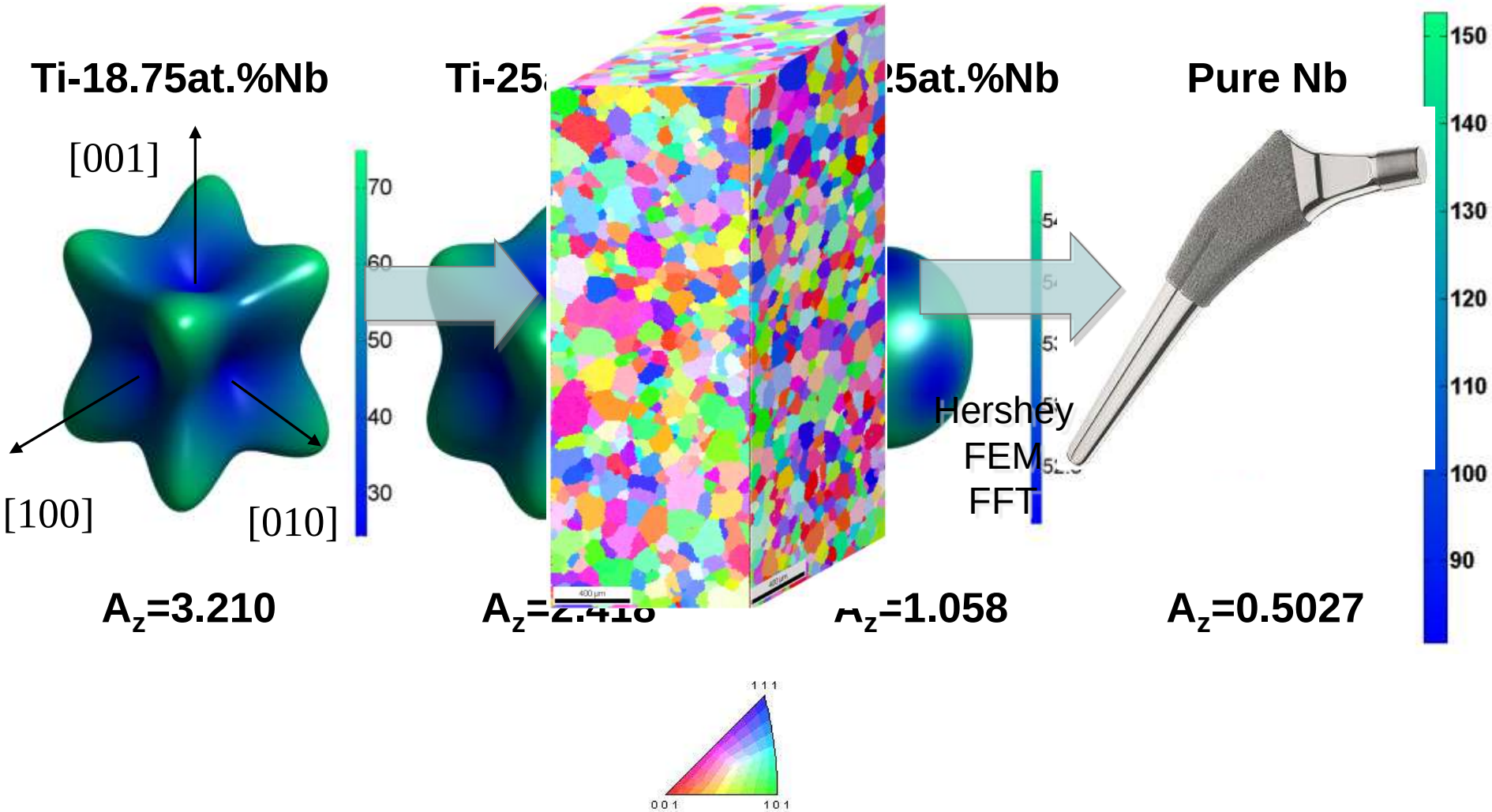
BCC Ti alloys as biomaterials (implants)



- Strategy f ower elastic stiffness:
- β-Ti (BCC, b, Ti-Mo, Ti-V,…)
- Bio-co

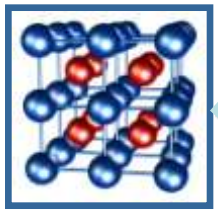
Young's modulus surface plots

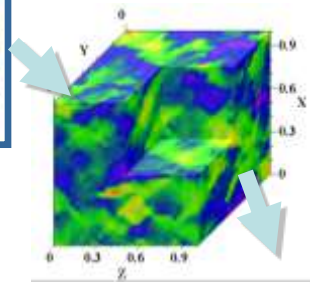
$A_z = 2\,C_{44}/(C_{11} - C_{12})$



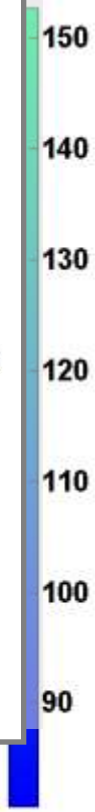
Young's modulus surface plots

$A_z = 2\,C_{44}/(C_{11} - C_{12})$

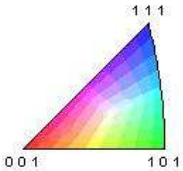




- Ti: <u>115 GPa</u>
- Ti-35wt.%Nb: <u>59.9 GPa</u>



A_z=3.210 A_z=2.418 A_z=1.058 A_z=0.5027



Successfully dealing with:

Complexity, multiple scales, interaction with experiments

Grand challenges / quo vadis:

Massive parallelization of PDE models

Exchange-correlation functions in DFT

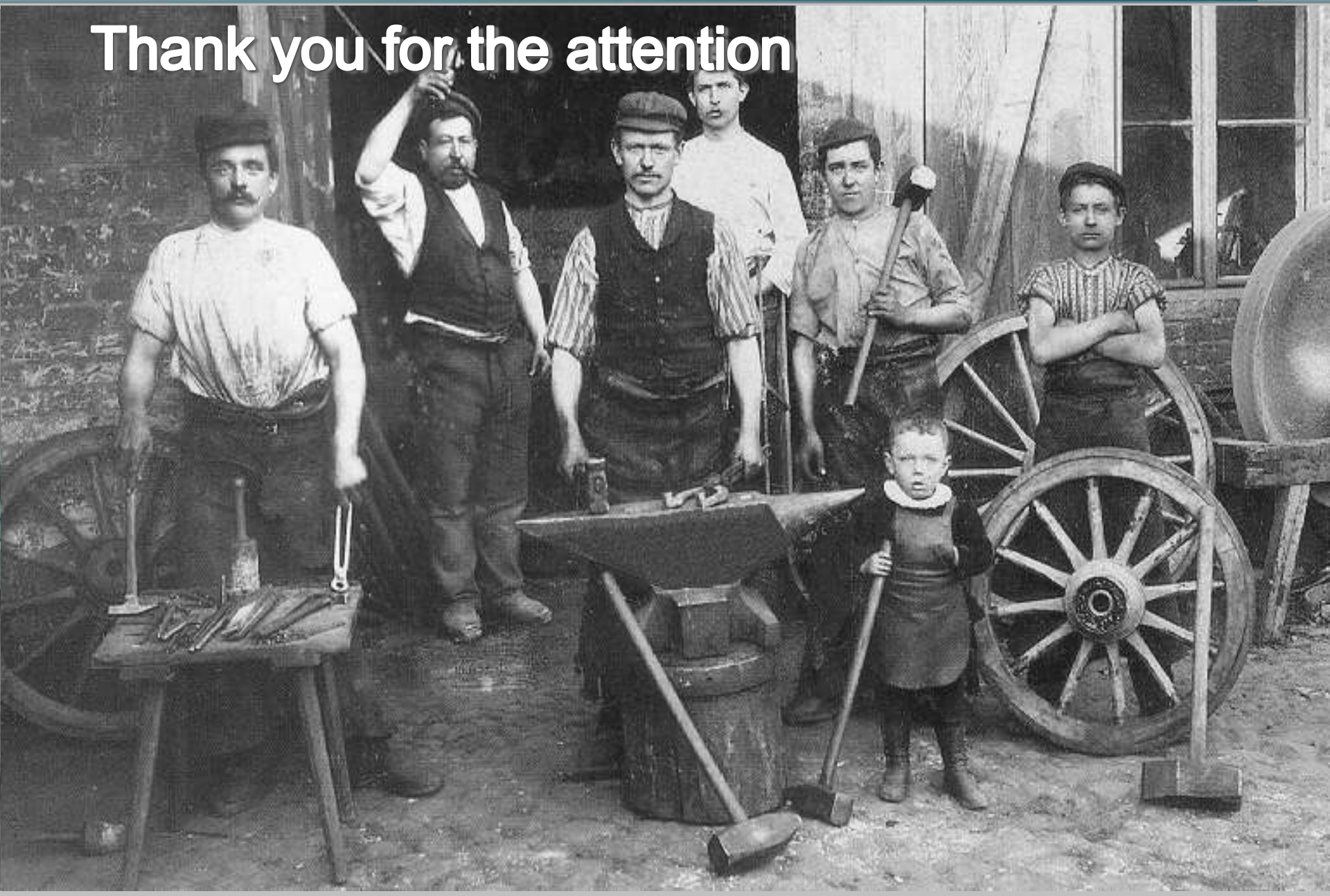
Inverse models

Time scale bridging

Scale hoping

More physics into continuum theory

Systematics of coarse graining: Renormalization group theory



Thank you for the attention