

Microstructure Mechanics of Complex Materials

Introduction

Dierk Raabe



**Max-Planck-Institut
für Eisenforschung GmbH**

Düsseldorf, Germany

WWW.MPIE.DE

d.raabe@mpie.de





class times

Friday, 12 am – 2 pm at IMM / RWTH

Course Lecturers:

**Prof. B. Svendsen, Prof. D. Raabe, Dr. H. Springer, Dr.
S.-L. Wong, Dr. S. Sandlöbes, Dr. M. Diehl**

Contact, website and class days

Date / Location	Topics	Lecturer
5. April 2019 IMM / RWTH	Introduction to materials micromechanics, multiscale problems in micromechanics, crystal structures and defects, relation to products and manufacturing	Raabe
12. April 2019 IMM / RWTH	Discrete and statistical dislocation dynamics, Crystal micromechanics, single crystal mechanics, yield surface, polycrystal models	Raabe
19. April 2019 IMM / RWTH	No classes	-
26. April 2019 IMM / RWTH	Micromechanics of polymers and biological materials	Raabe
3. May 2019 IMM / RWTH	Athermal phase transformations in micromechanics	Wong
10. May 2019 IMM / RWTH	Fatigue of materials	Sandlöbes
17. May 2019 IMM / RWTH	Dislocations and micromechanics in hexagonal materials	Sandlöbes
24. May 2019 IMM / RWTH	Mathematical micromechanics: Review of elasticity theory	Svendsen
31. May 2019 IMM / RWTH	No classes	-
7. June 2019 IMM / RWTH	Volterra dislocation theory, Peierls-Nabarro dislocation theory and dislocation core modeling	Svendsen
14. June 2019 IMM / RWTH	No classes	-
21. June 2019 IMM / RWTH	Dislocation interaction modeling, Partial and extended dislocations	Svendsen
28. June 2019 MPIE Düsseldorf	Fracture Mechanics & MPI Lab Tour	Diehl, Raabe

Further reading

Gottstein: Physical Metallurgy

Reed-Hill: Physical Metallurgy Principles

Hull and Bacon: Introduction to Dislocations, Butterworth-Heinemann

Hirth and Lothe: Theory of Dislocations

Hosford: The Mechanics of Crystals and Textured Polycrystals, Oxford University Press

Kocks, Tomé and Wenk: Texture and Anisotropy. Preferred Orientations in Polycrystals and Their Effect on Material Properties. Cambridge University Press

Raabe, Roters, Barlat and L.-Q. Chen: Weinheim, Continuum Scale Simulation of Engineering Materials - Fundamentals - Microstructures - Process Applications. Wiley-VCH

Roters, Eisenlohr, Bieler, Raabe: Crystal plasticity finite element methods: in materials science and engineering 2011, John Wiley & Sons

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

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

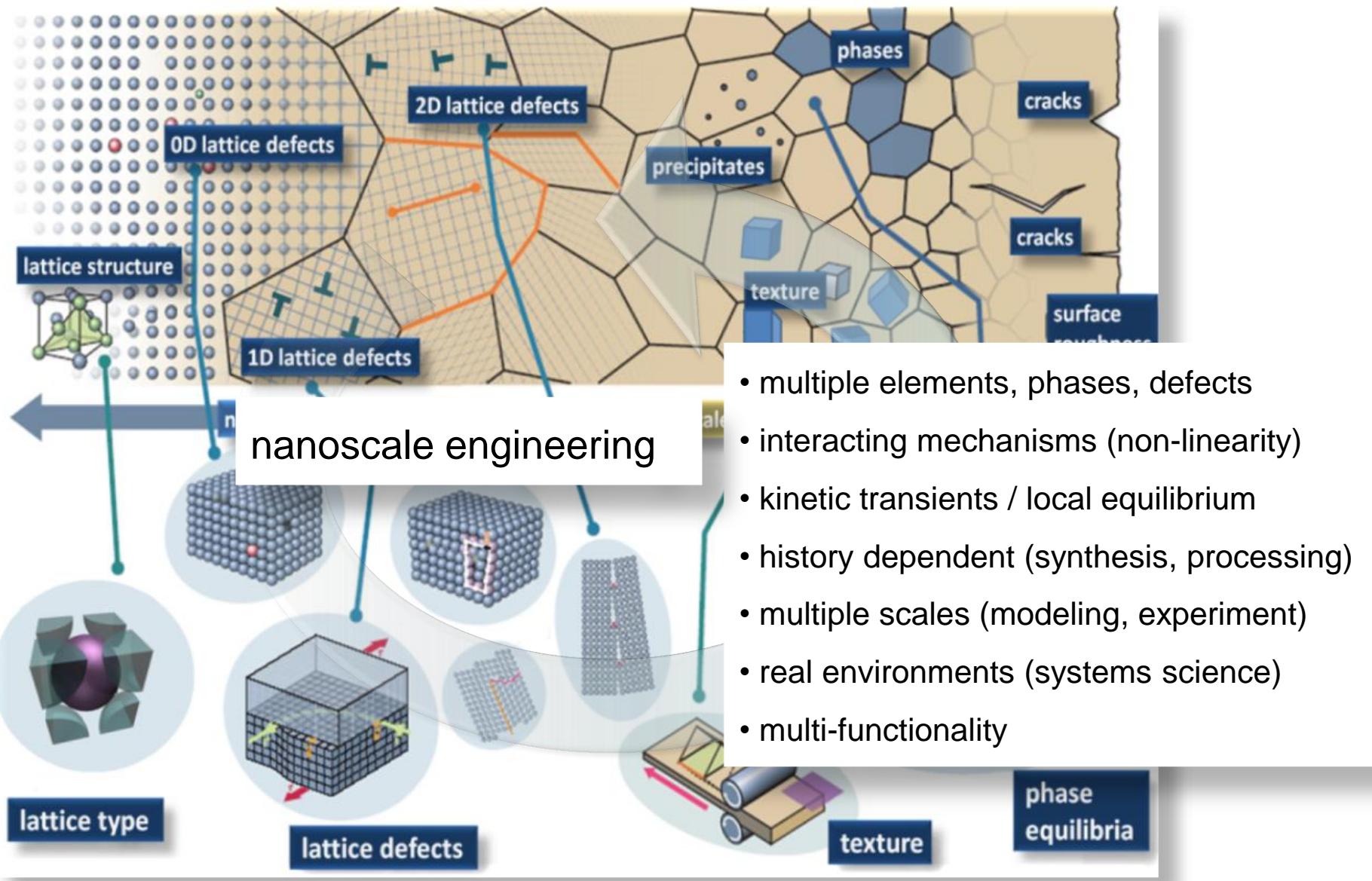
Materials-related industries account for 46% of all EU manufacturing value and
11% of the EU's total domestic product

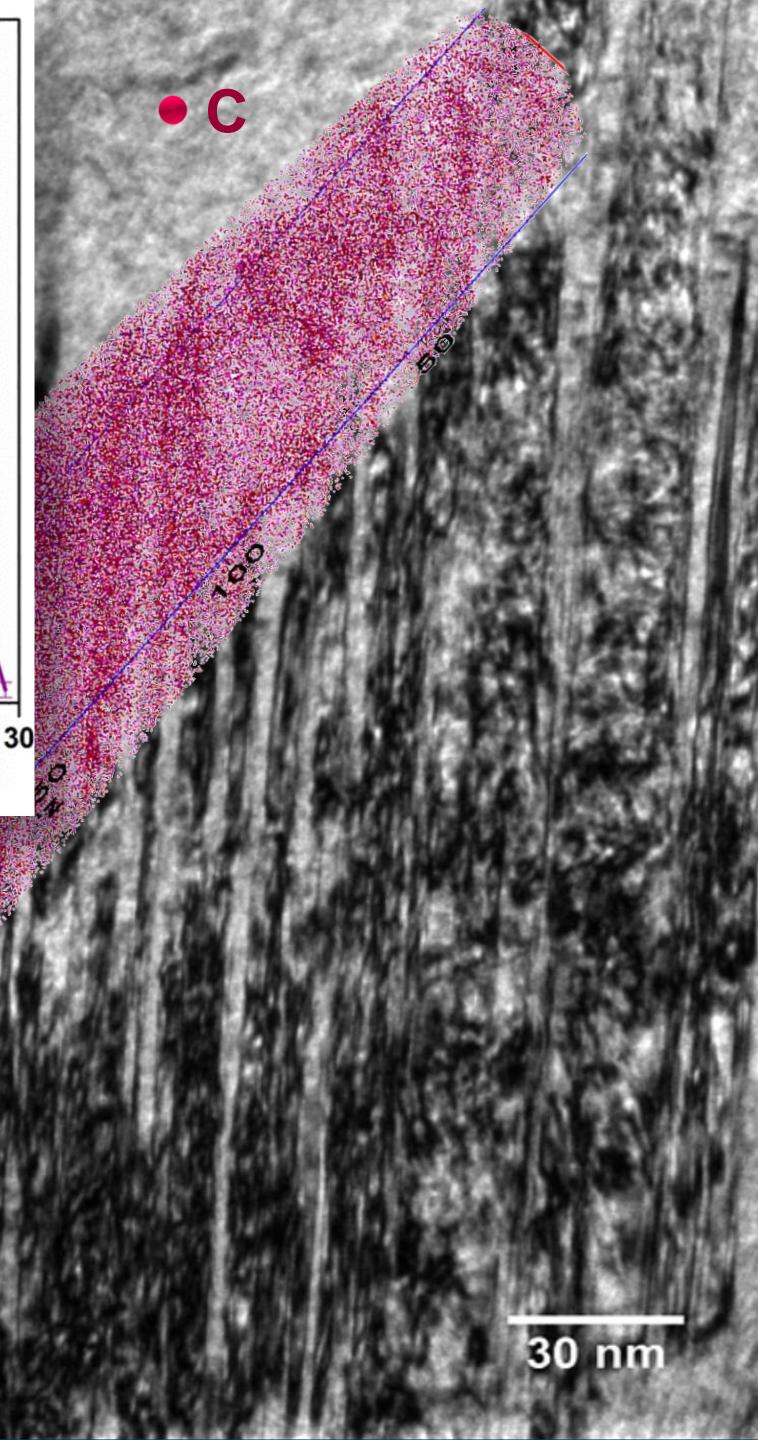
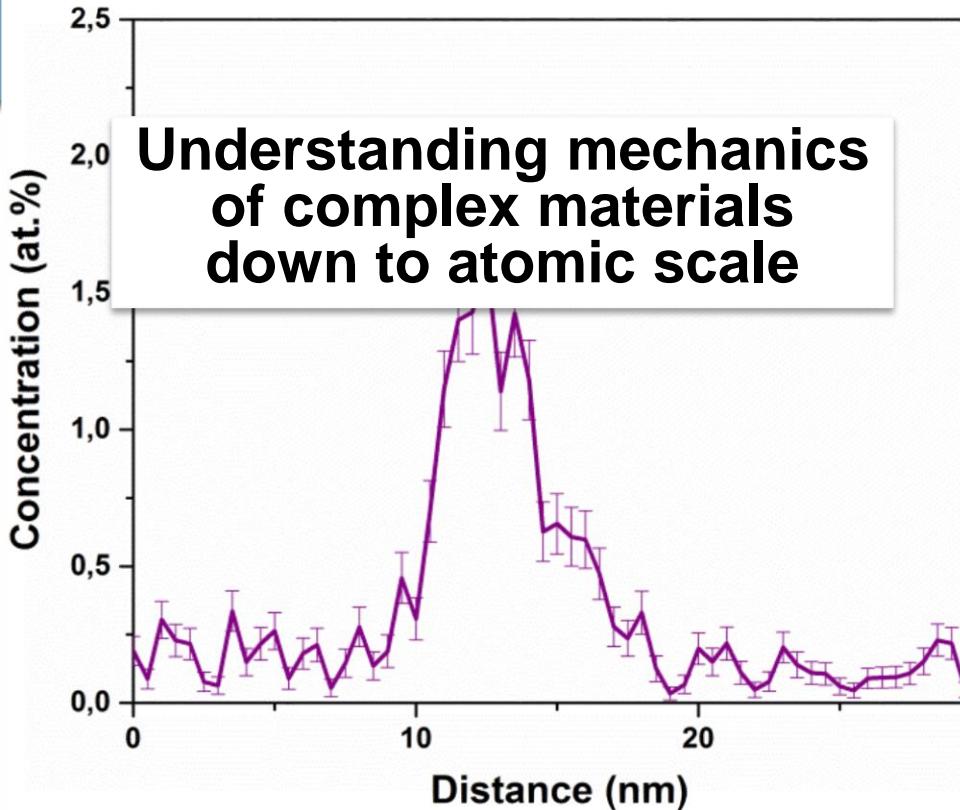
3.5 billion € per day in the EU
World Trade Organisation

Mission: Understanding micromechanics of complex
materials from first principles and the defect level upwards

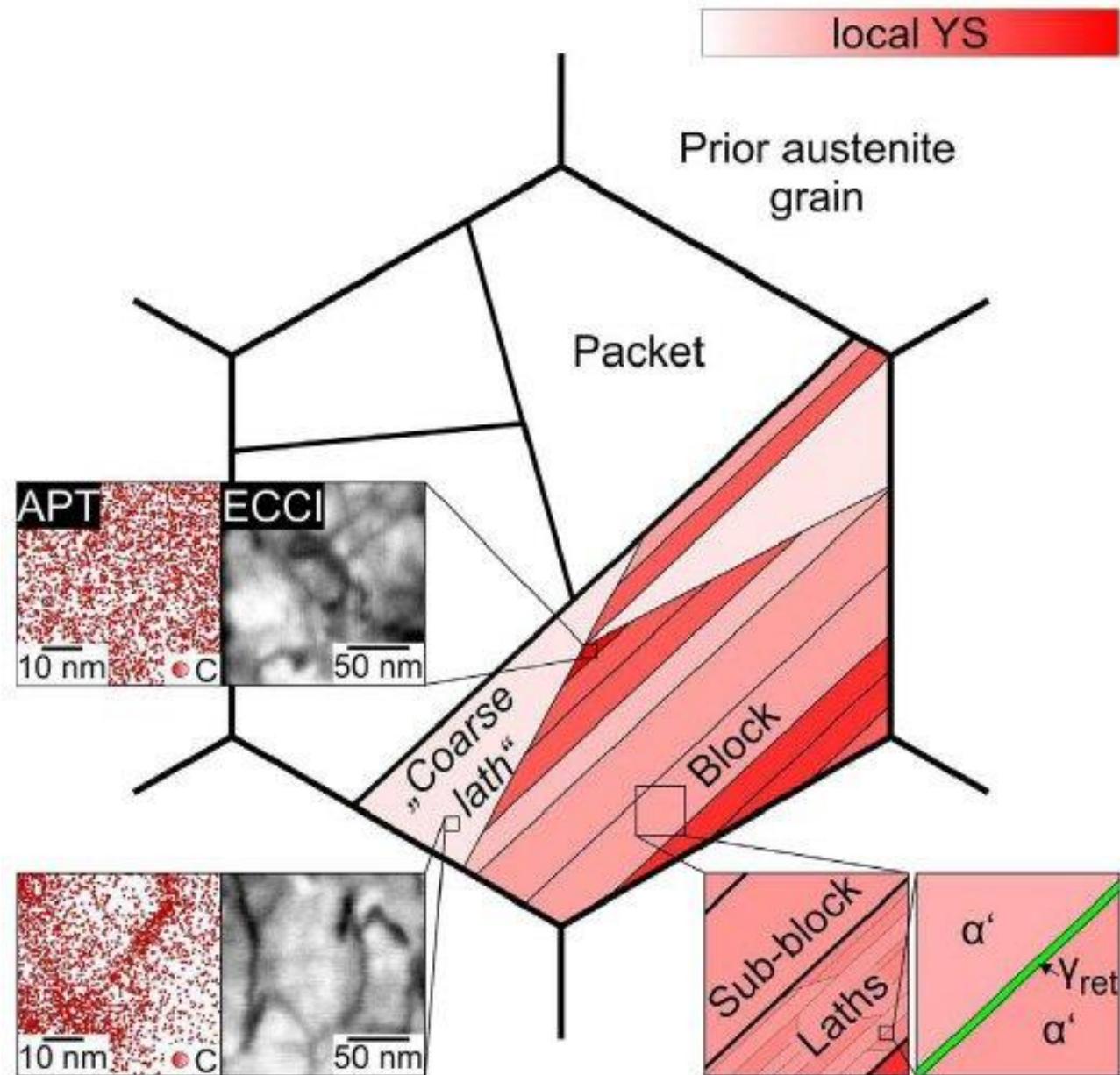


- **Introduction to the scales**
- **Introduction to the engineering background**
- **Quantum mechanics primer**
- **Examples**

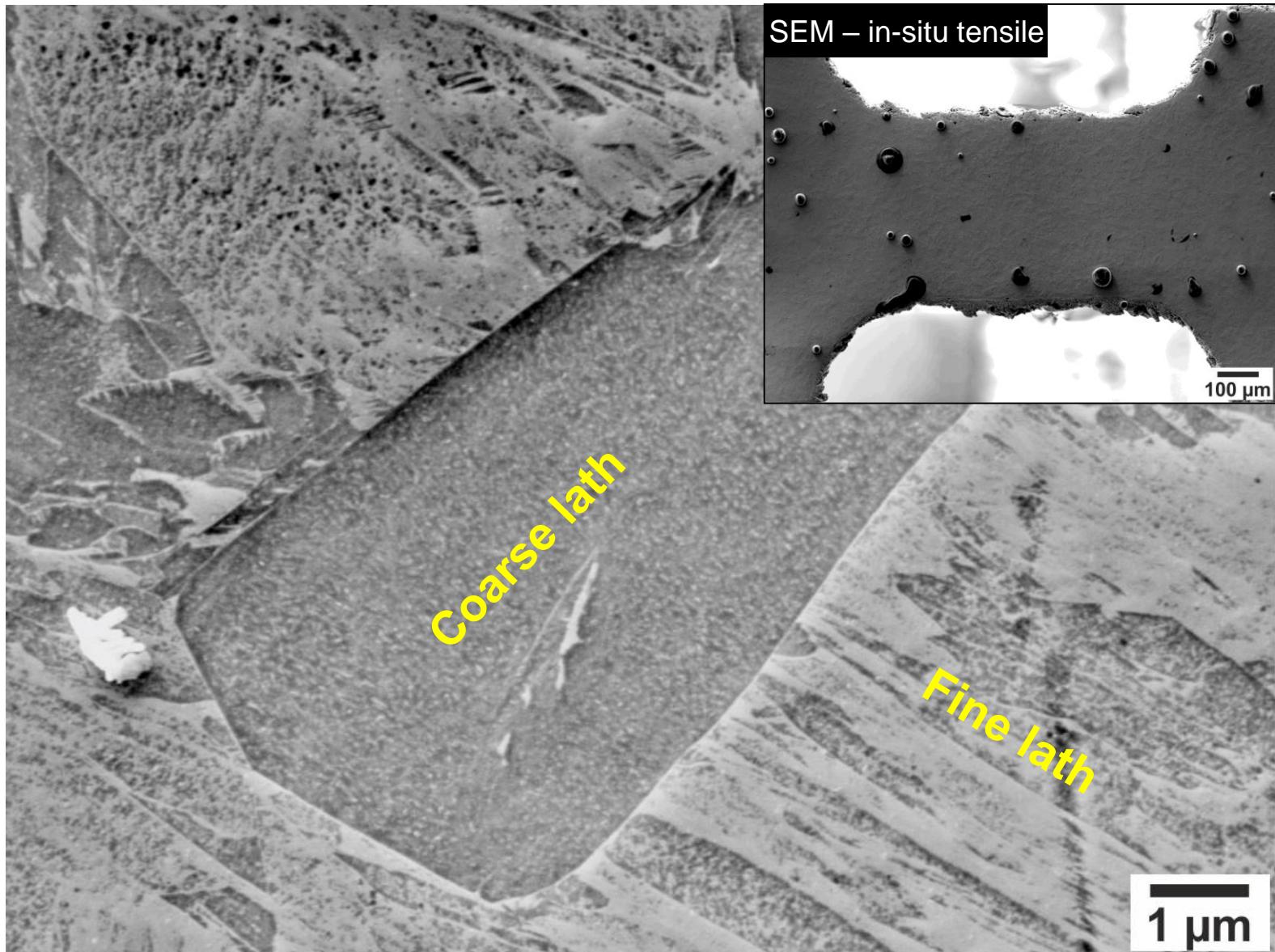




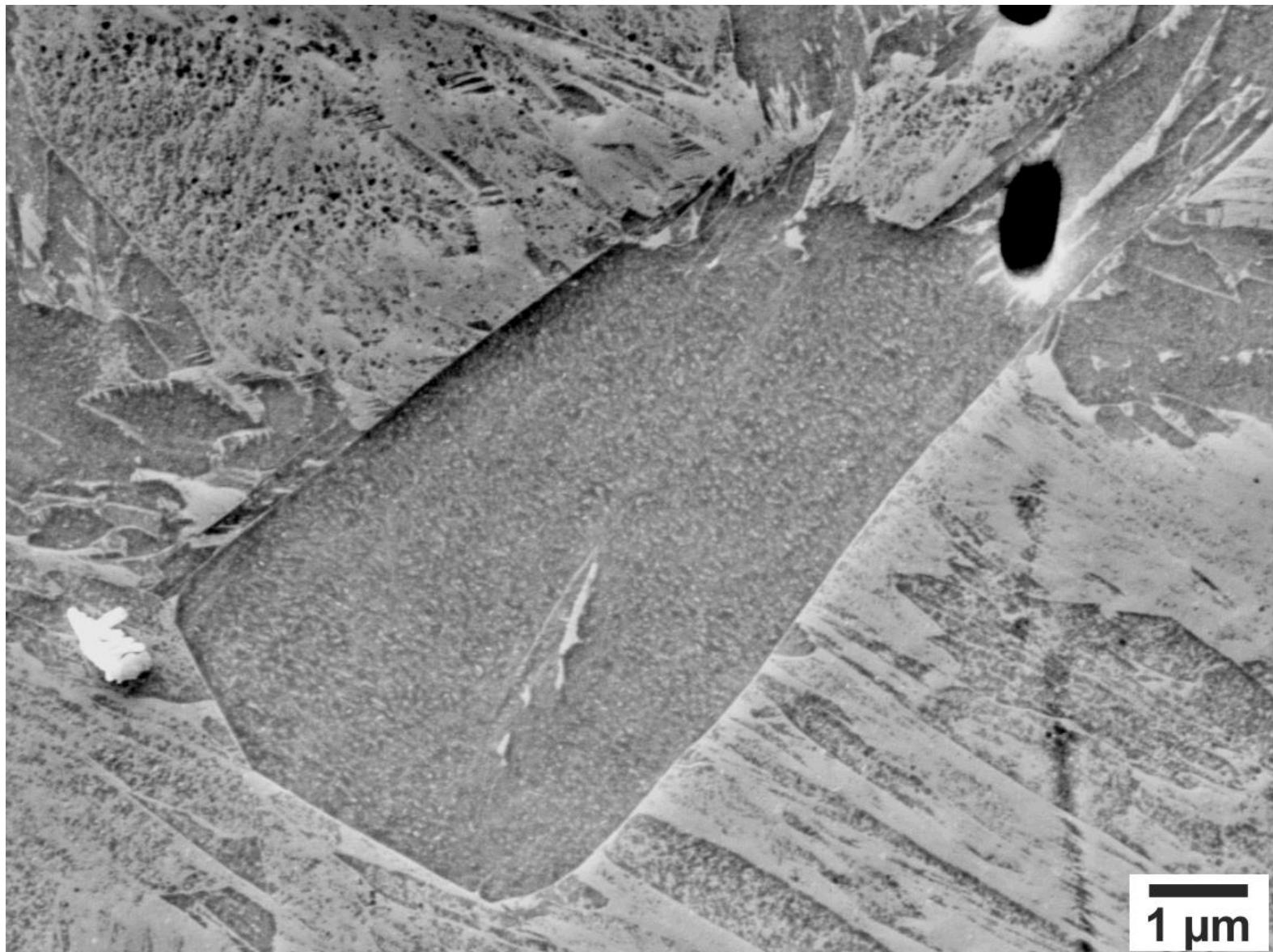
Martensite: Microstructure scales

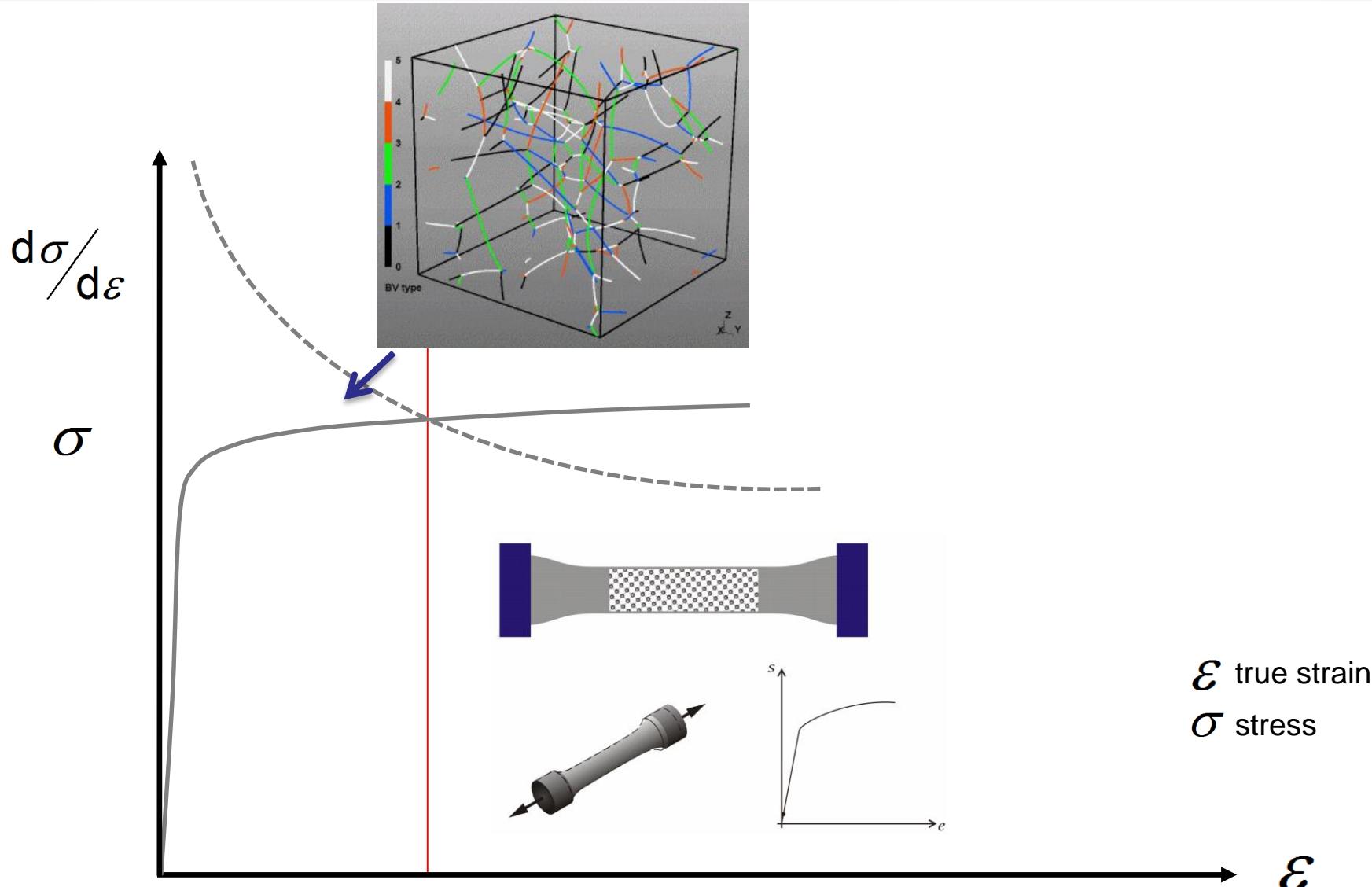


In-situ tensile testing: role of coarse lath in martensite fracture

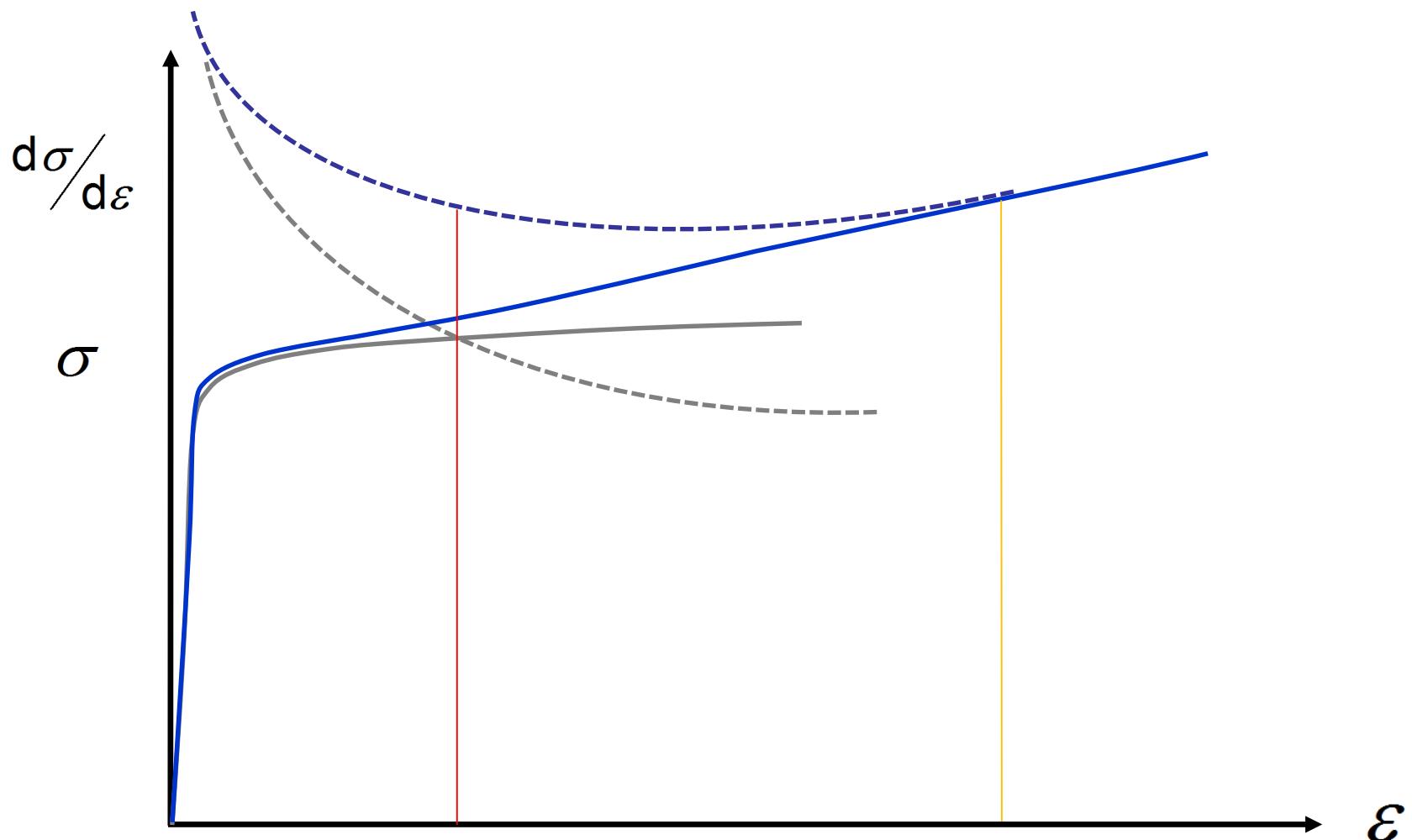


In-situ tensile testing: role of coarse lath in martensite fracture

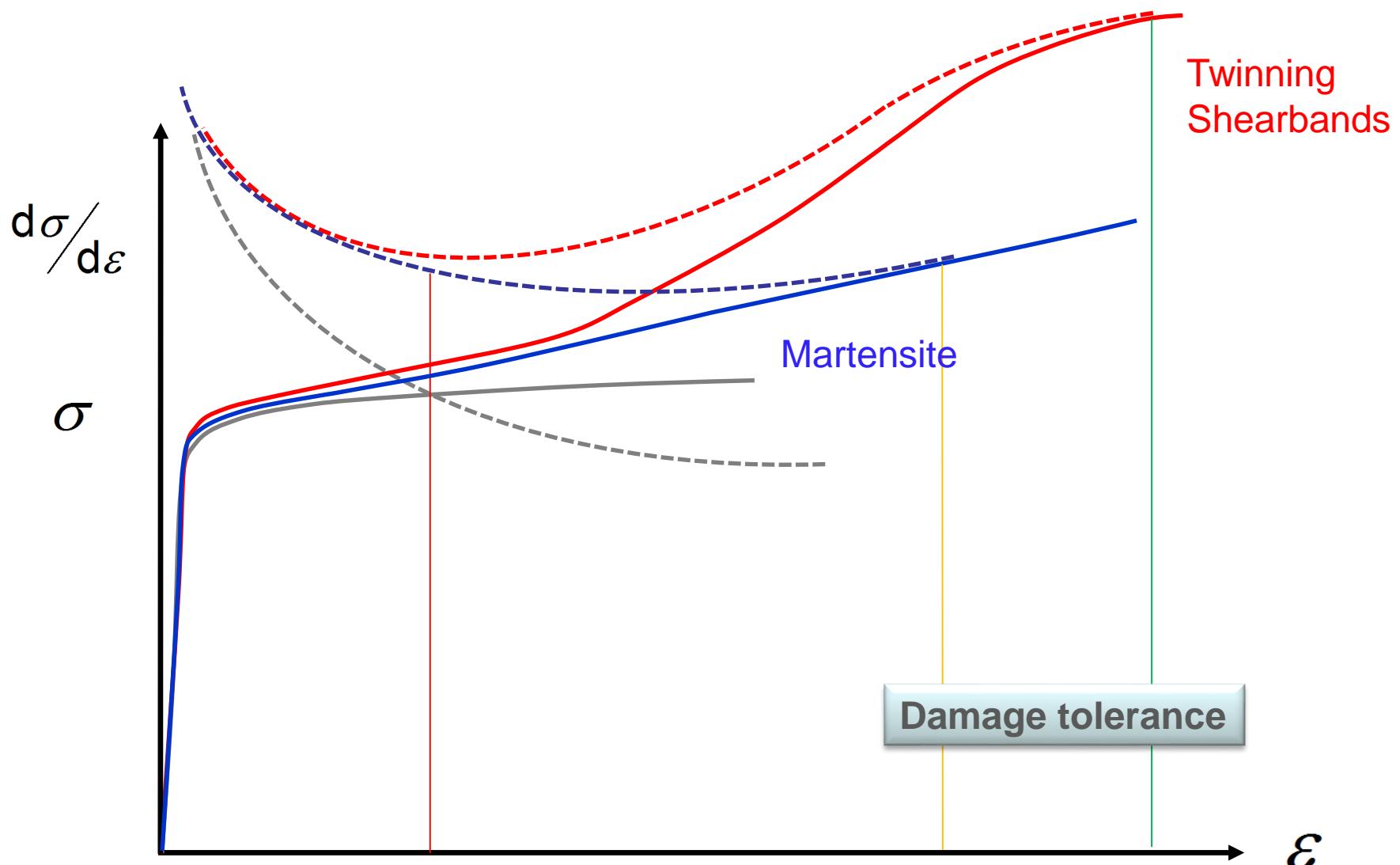


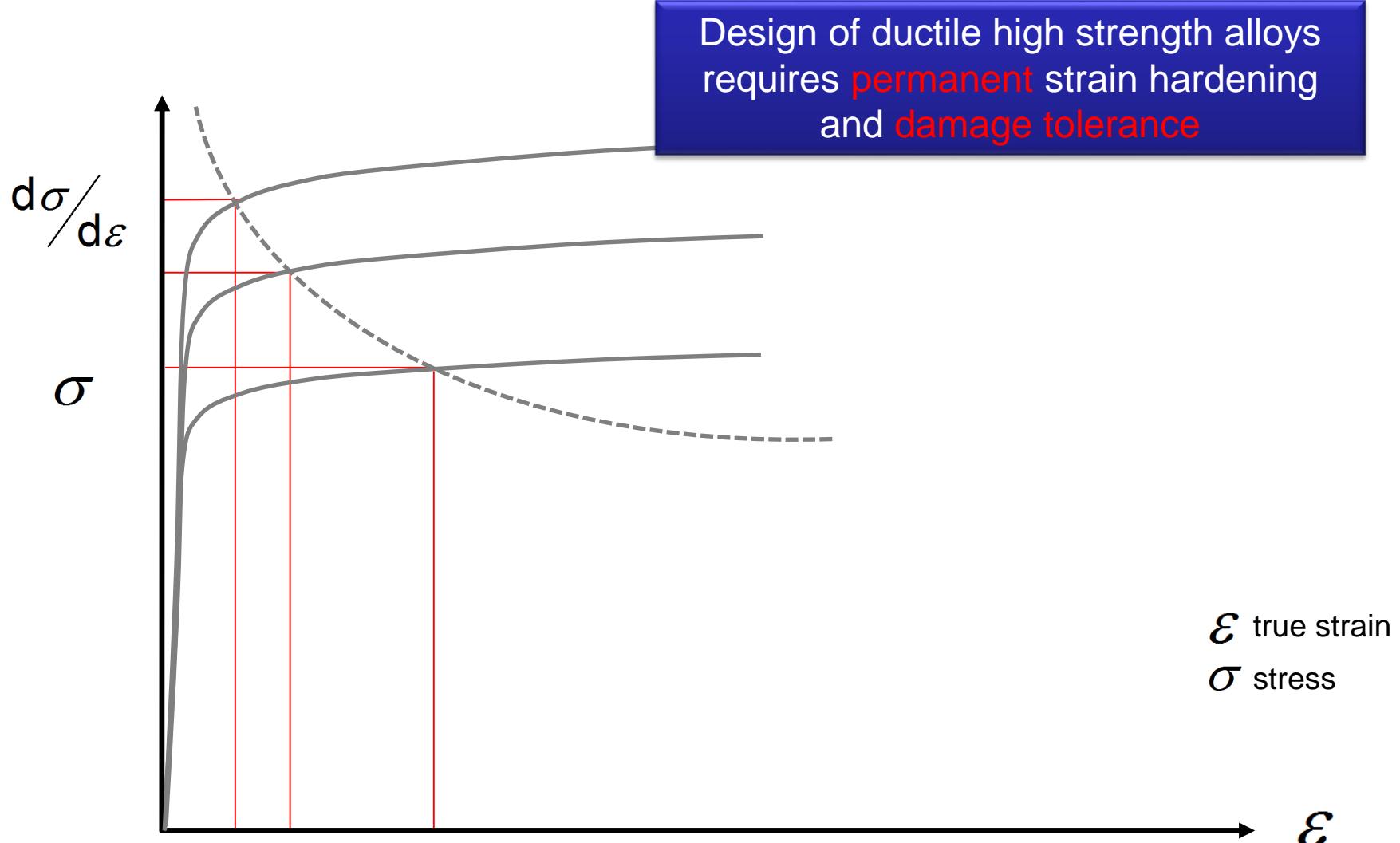


Inverse strength-ductility: phenomenological analysis



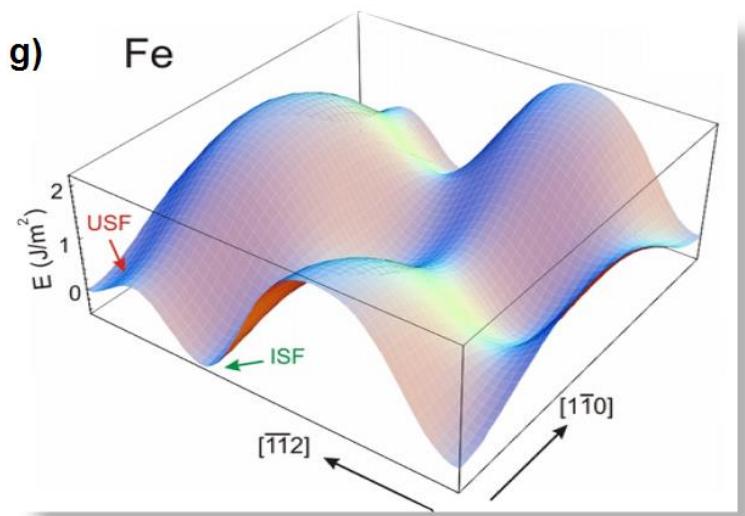
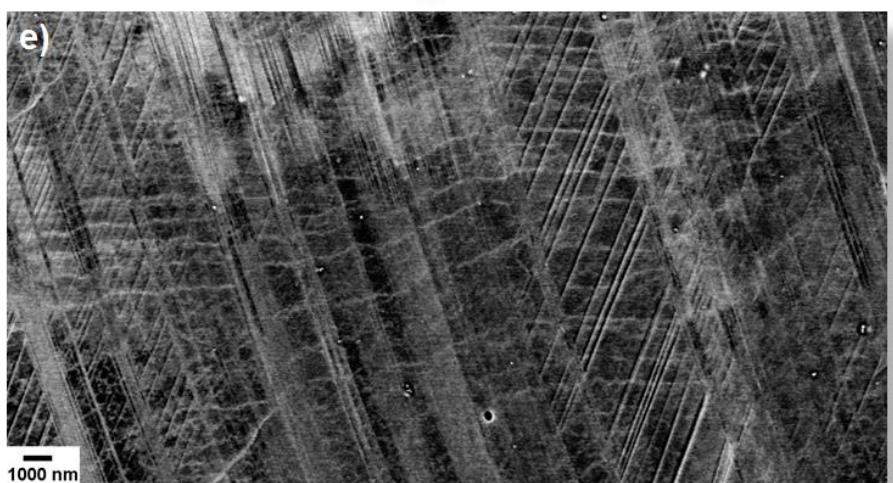
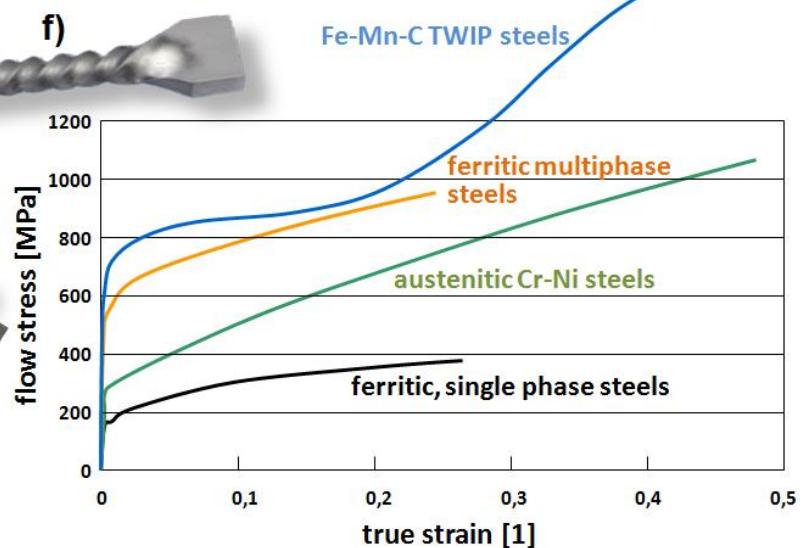
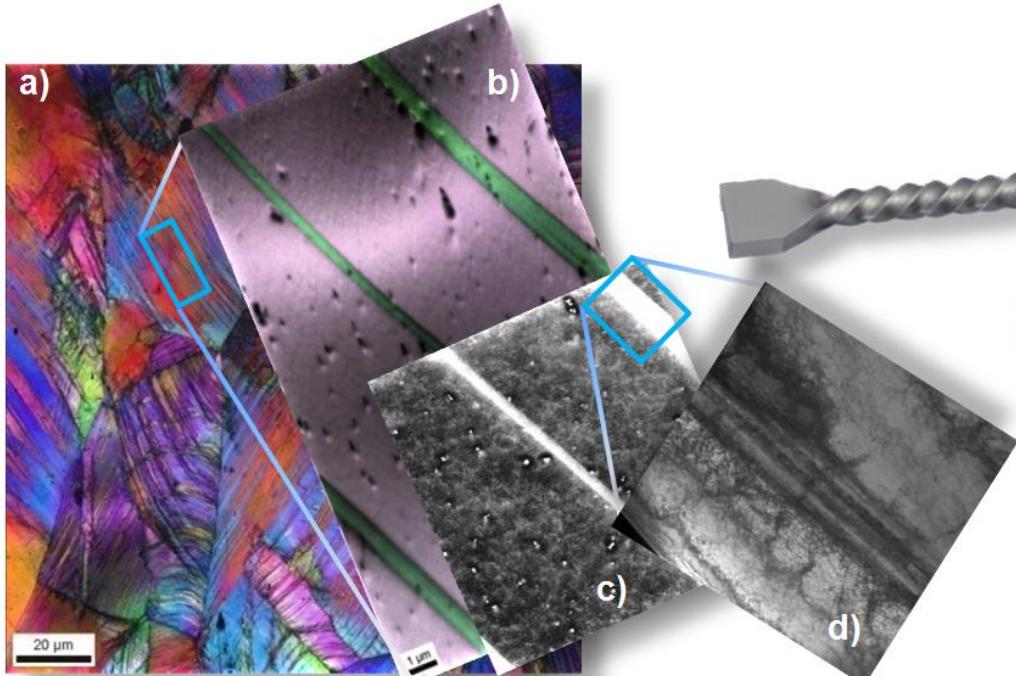
Inverse strength-ductility: phenomenological analysis



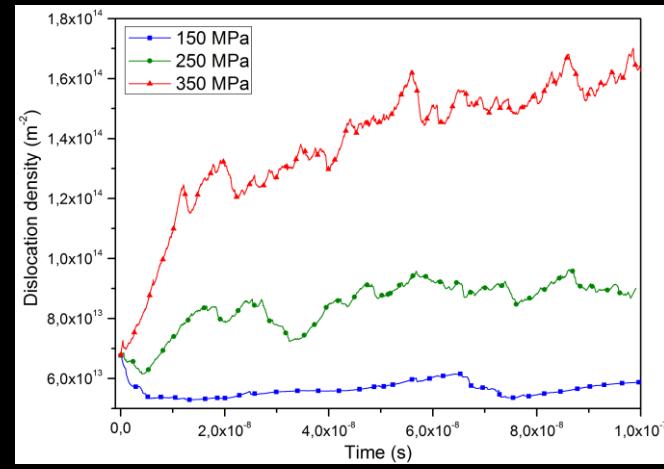


- **Introduction to the scales**
- **Introduction to the engineering background**
- **Quantum mechanics primer**
- **Examples**

Ab initio-based development of new alloys



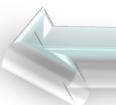
Example: 4th generation superalloys for turbine blades (SFB / TR 103)

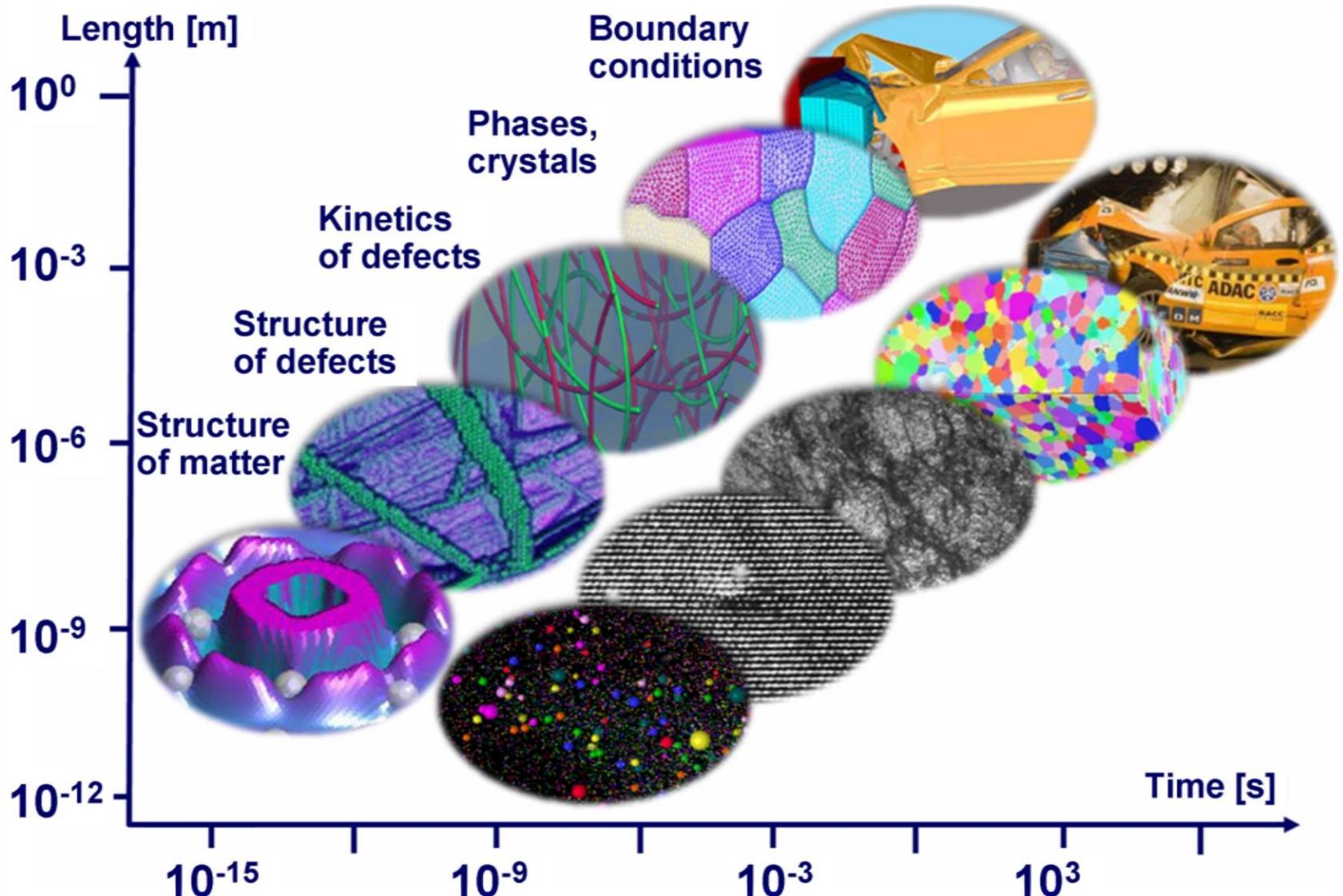


sources GE; FAU Erlangen Nürnberg und RU Bochum

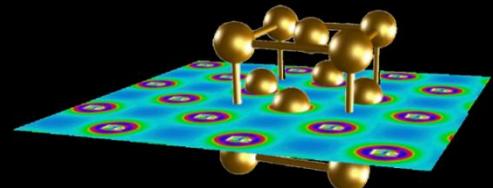


- **Introduction to the scales**
- **Introduction to the engineering background**
- **Quantum mechanics primer**
- **Examples**





- **MOST EXACT KNOWN MATERIALS THEORY**
- **COMBINE TO ATOMIC SCALE EXPERIMENTS**
- **OBTAIN DATA NOT ACCESSIBLE OTHERWISE**
- **CAN BE USED AT CONTINUUM SCALE**
- **ELECTRONIC RULES FOR ALLOY DESIGN:
ADD ELECTRONS RATHER THAN ATOMS**



$$-\frac{\hbar^2}{2m} \nabla^2 \psi(r) + U(r) \psi(r) = E \psi(r)$$

$\hbar/(2\pi)$

square $|\psi(\underline{r})|^2$ of the wave function $\psi(\underline{r})$ at position $\underline{r} = (x, y, z)$
is a measure of the probability (Aufenthaltswahrscheinlichkeit)

many particles

$$\left(-\frac{\hbar^2}{2} \sum_i \frac{1}{m_i} \nabla_i^2 + U(r_i) \right) \psi(r_i) = E \psi(r_i)$$

i Electrons: Mass m_e ; Charge $q_e = -e$; Coordinates r_{ei}
j Cores: Mass m_n ; Charge $q_n = ze$; Coordinates r_{nj}

$$\left(-\frac{\hbar^2}{2m_e} \sum_i \nabla_i^2 - \frac{\hbar^2}{2m_n} \sum_j \nabla_j^2 + \right. \\ \left. \sum_{\substack{il, i2 \\ il \neq i2}} \frac{e^2}{4\pi\epsilon_0 |r_{e_{i1}} - r_{e_{i2}}|} + \sum_{\substack{j1, j2 \\ jl \neq j2}} \frac{z_{jl} z_{j2} e^2}{4\pi\epsilon_0 |r_{n_{j1}} - r_{n_{j2}}|} + \sum_{i,j} \frac{z_j e^2}{4\pi\epsilon_0 |r_{e_i} - r_{n_j}|} \right) \psi(r_{e_i}, r_{n_j}) \\ = E \psi(r_{e_i}, r_{n_j})$$

Decoupling of cores and electrons

$$\psi(\mathbf{r}_e, \mathbf{r}_n) = \varphi(\mathbf{r}_e)\phi(\mathbf{r}_n)$$

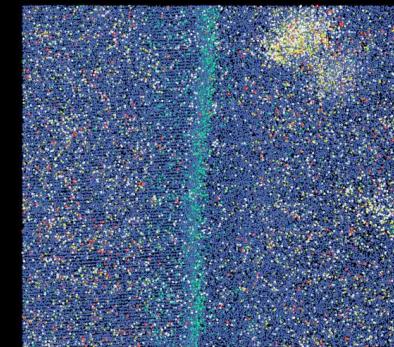
Electrons

$$\left(-\frac{\hbar}{2m_e} \sum_i \nabla_i^2 + \sum_{\substack{i1,i2 \\ i1 \neq i2}} \frac{e^2}{4\pi\epsilon_0 |r_{e_{i1}} - r_{e_{i2}}|} + \sum_{i,j} \frac{z_j e^2}{4\pi\epsilon_0 |r_{e_i} - r_{n_j}|} \right) \varphi(r_{e_i}) = E \varphi(r_{e_i})$$

Atom cores

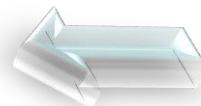
$$\left(-\frac{\hbar}{2m_n} \sum_j \nabla_j^2 + \sum_{\substack{j1,j2 \\ j1 \neq j2}} \frac{z_{j1} z_{j2} e^2}{4\pi\epsilon_0 |r_{n_{j1}} - r_{n_{j2}}|} + \sum_{i,j} \frac{z_j e^2}{4\pi\epsilon_0 |r_{e_i} - r_{n_j}|} \right) \phi(r_{n_j}) = E \phi(r_{n_j})$$

Atom Probe: atomic species Some crystallographic features



Al  Ga  Cu  Zn  Mg 

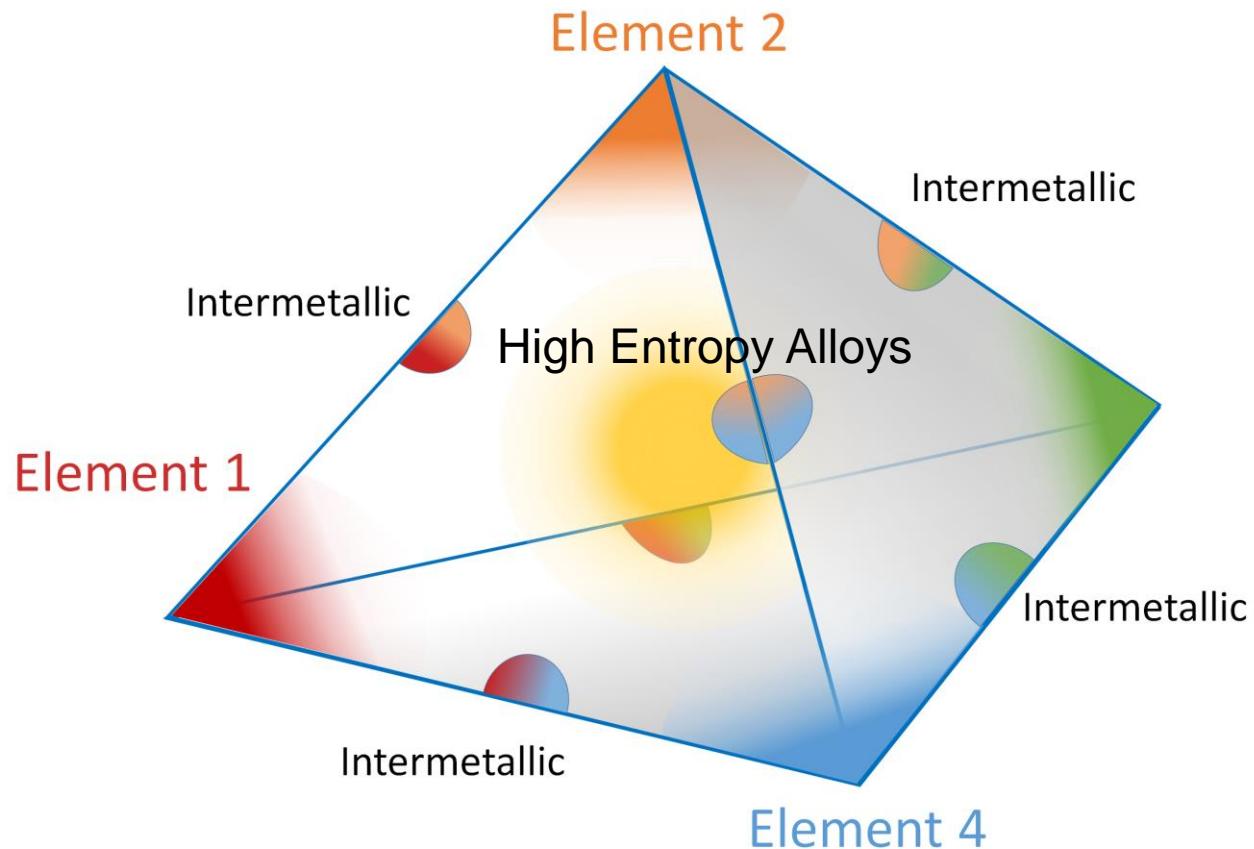
- **Introduction to the scales**
- **Introduction to the engineering background**
- **Quantum mechanics primer**
- **Examples**



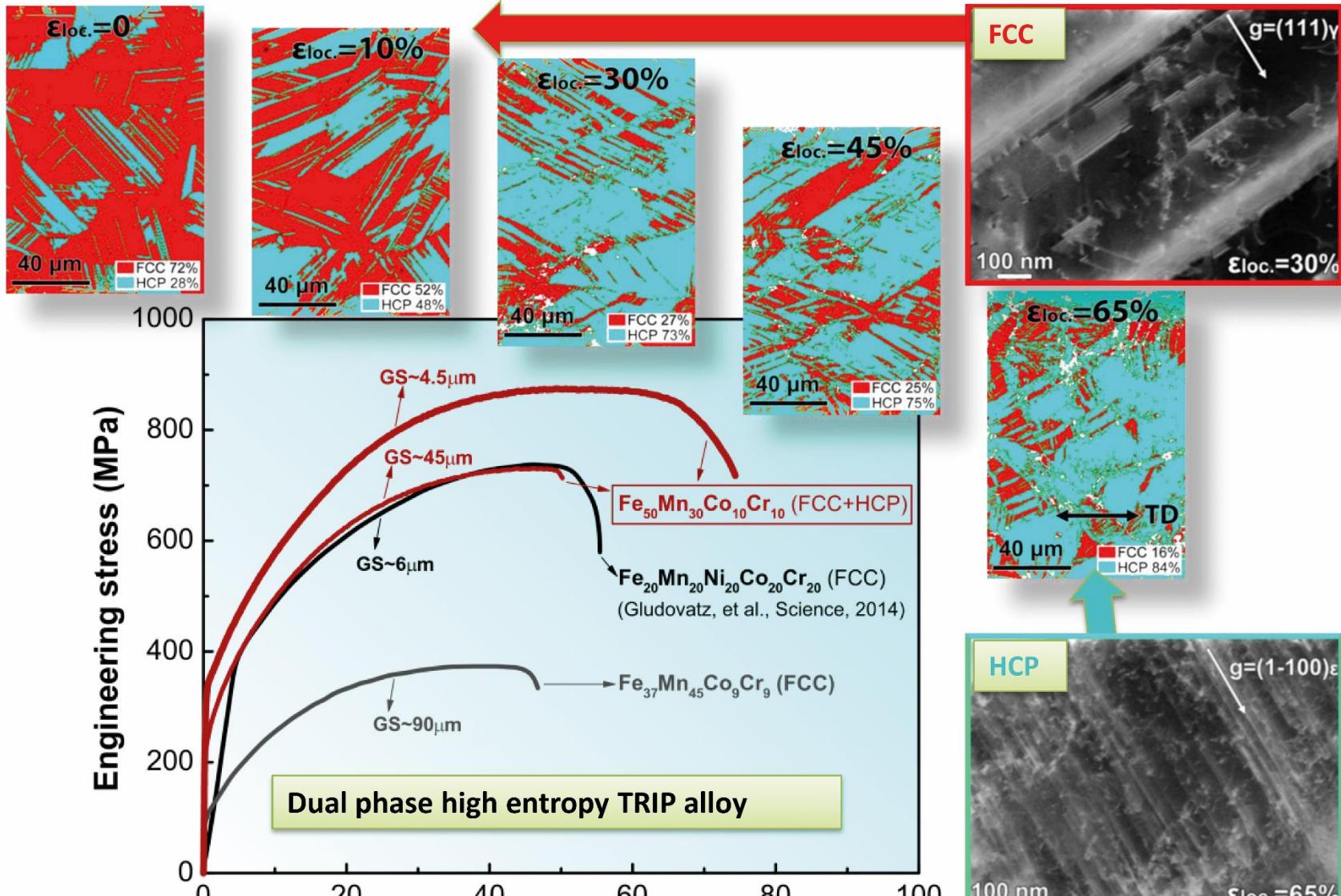
Interdepartmental collaboration example



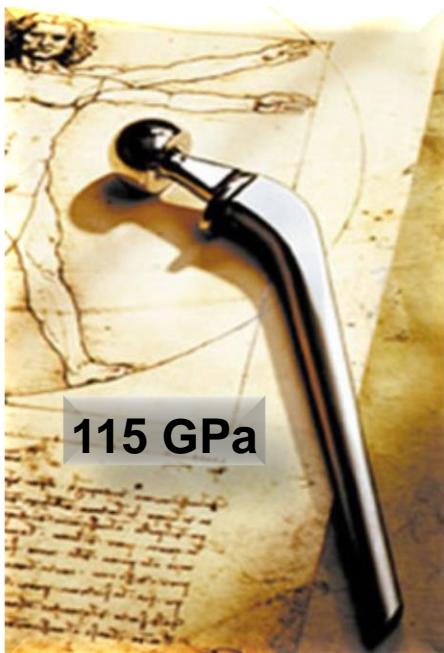
YEARS 1917–2017



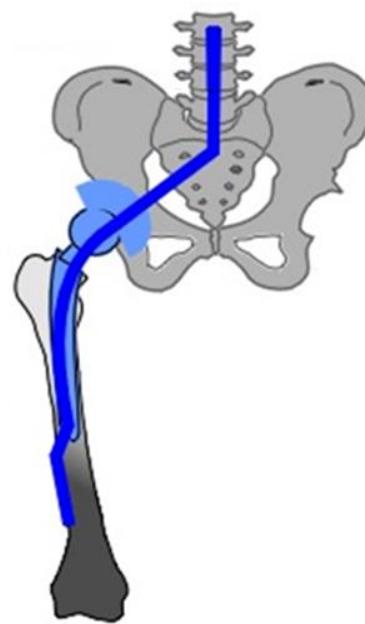
Interdepartmental collaboration example



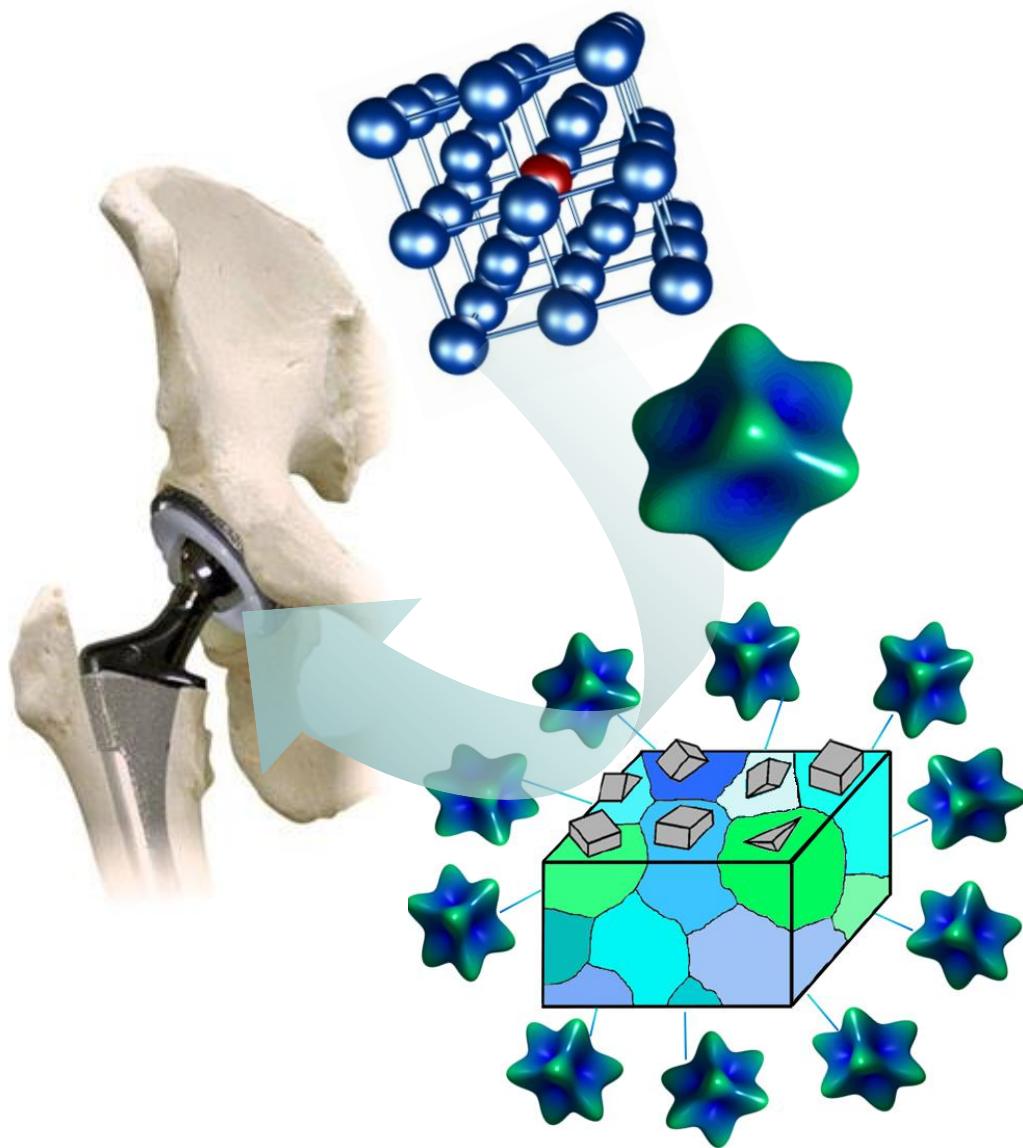
Z. Li et al. Nature 2016



Spannungs-Abschattung (Stress shielding)
Elastische Fehlpassung:
Knochenuflösung, Abrasion, Entzündung

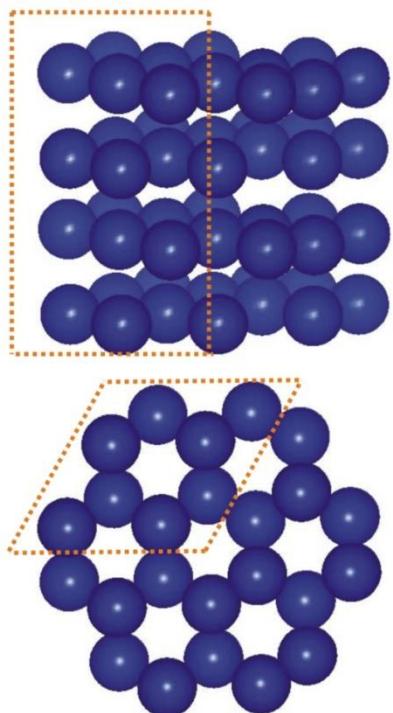


ab-initio Simulation of elastic stiffness



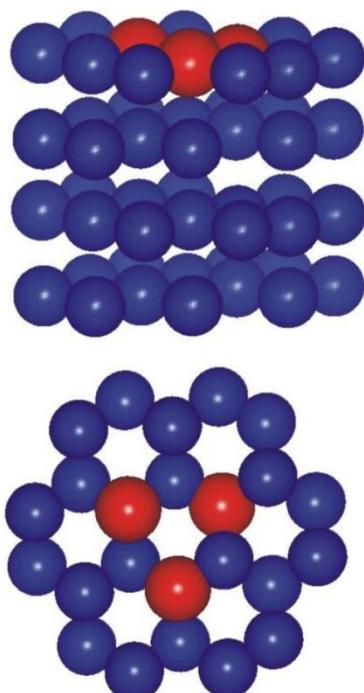
Construct binary alloys in the hexagonal phase

Ti hcp phase



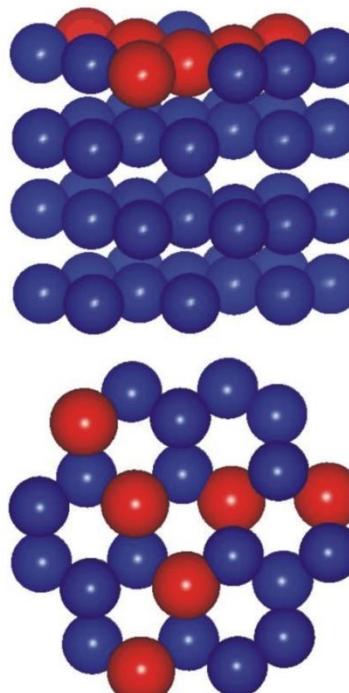
Ti atoms

15/1 Ti:X ratio



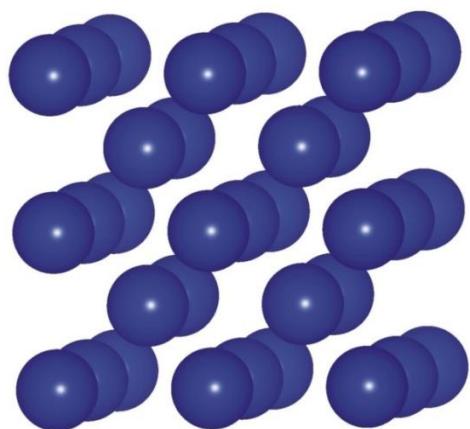
substituent X

14/2 Ti:X ratio



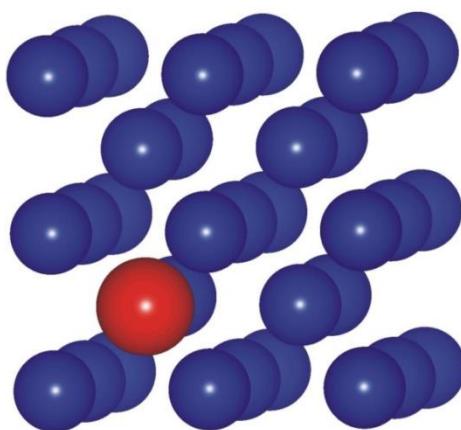
Construct binary alloys in the cubic phase

Ti bcc phase



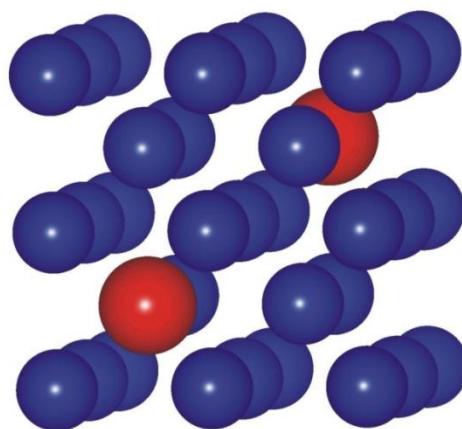
Ti atoms

15/1 Ti:X ratio



substituent X

14/2 Ti:X ratio



Young's modulus surface plots

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

