

Microstructure Mechanics of Complex Materials

Introduction

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class times

Friday, 10:15 am – 2 pm at IMM / RWTH

Course Lecturers:

**Dr. S. Sandlöbes, Dr. P. Shanthraj,
Dr. S.-L. Wong, Prof. Svendsen, Prof. D. Raabe**



Contact, website and class days

Date / Location	Topics	Lecturer
21. April 2017 IMM / RWTH	Introduction to materials micromechanics, multiscale problems in micromechanics, case studies, crystal structures and defects, relation to products and manufacturing	Raabe
28. April 2017 IMM / RWTH	Discrete and statistical dislocation dynamics, Crystal micromechanics, single crystal mechanics, yield surface mechanics, polycrystal models, Taylor model	Raabe
5. May 2017 IMM / RWTH	Athermal phase transformations in micromechanics	Wong
12. May 2017 IMM / RWTH	Fracture mechanics, Introduction to FEM	Shanthraj
19. May 2017 MPI / Düsseldorf	Micromechanics of polymers and biological (natural) composites and MPI Lab tour	Raabe
26. May 2017 IMM / RWTH	Fatigue of materials	Sandlöbes
2. June 2017 IMM / RWTH	Mathematical micromechanics: Review of elasticity theory	Svendsen
9. June 2017 IMM / RWTH	Volterra dislocation theory	Svendsen
16. June 2017 IMM / RWTH	Dislocations and micromechanics in hexagonal materials	Sandlöbes
23. June 2017 IMM / RWTH	Dislocation interaction modeling	Svendsen
30. June 2017 IMM / RWTH	Partial and extended dislocations	Svendsen
7. July 2017 IMM / RWTH	Peierls-Nabarro dislocation theory and dislocation core modeling	Svendsen



- **Introduction**
- **Quantum mechanics primer**
- **Crystal structures and why they matter for micromechanics**
- **Dislocation statics**
- **Dislocation dynamics**
- **Single crystal mechanics**
- **Polycrystal mechanics (Taylor model, single crystal yield surface)**
- **Polymer crystal mechanics**
- **Mechanics of biological (natural) materials**
- **Introduction to fracture mechanics**
- **Introduction to the FEM method**
- **Integrated micromechanical experimentation and simulation**
- **High-throughput testing and materials development**
- **Case study: Hydrogen embrittlement**



Gottstein: Physical Metallurgy

Reed-Hill: Physical Metallurgy Principles

Hull and Bacon: Introduction to Dislocations, Butterworth-Heinemann

Hirth and Lothe: Theory of Dislocations

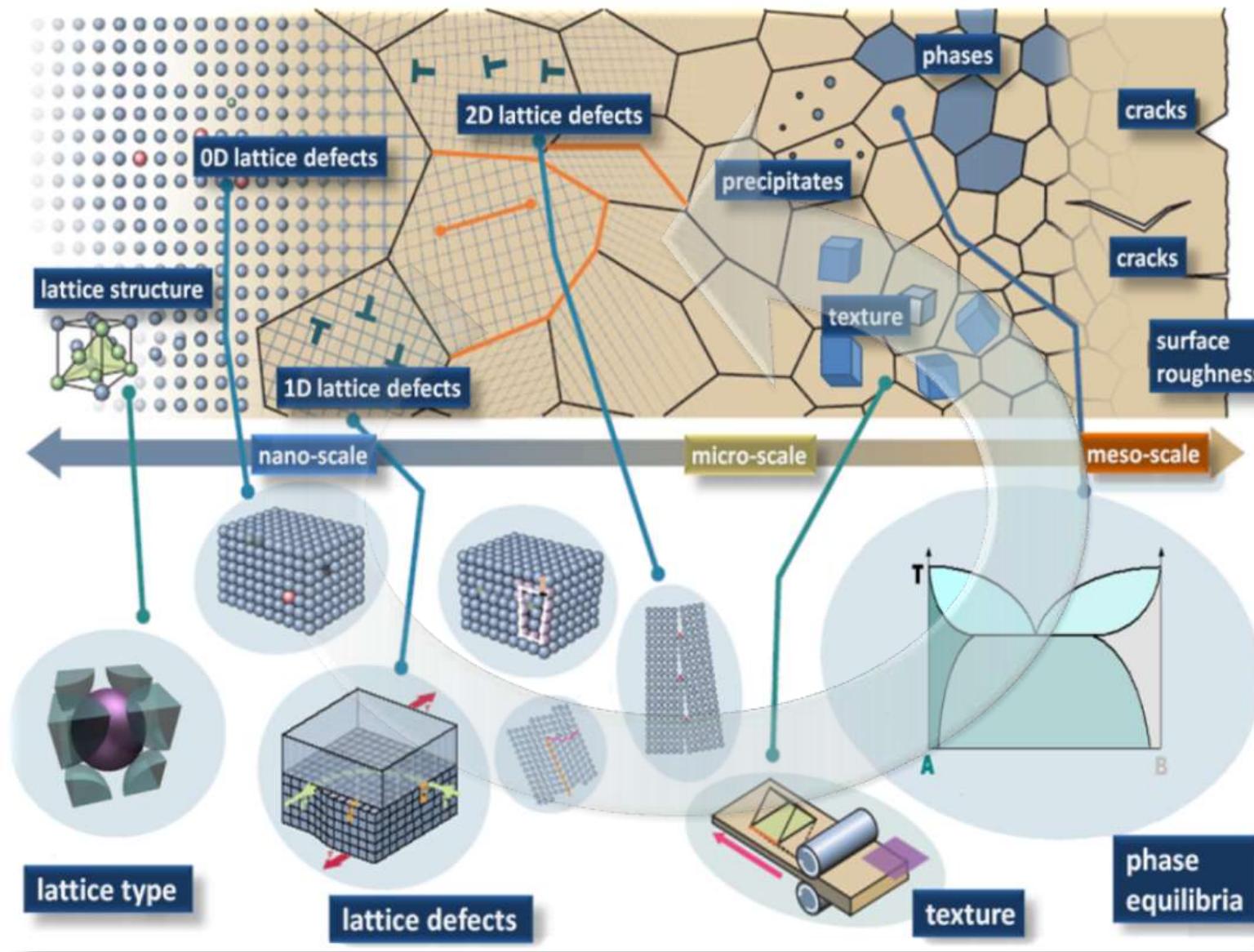
Hosford: The Mechanics of Crystals and Textured Polycrystals, Oxford University Press

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

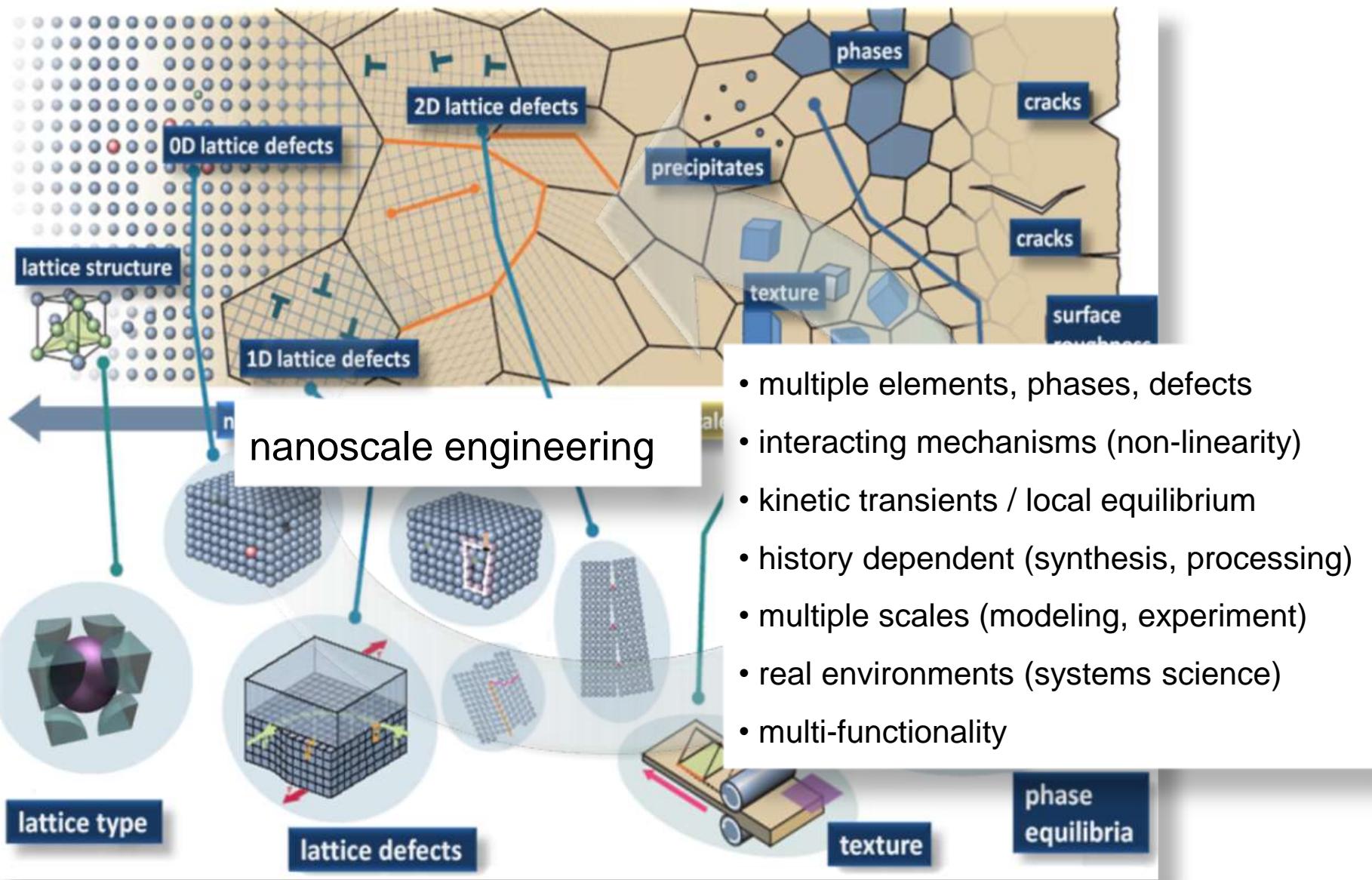
Raabe, Roters, Barlat and L.-Q. Chen: Weinheim, Continuum Scale Simulation of Engineering Materials - Fundamentals - Microstructures - Process Applications. Wiley-VCH

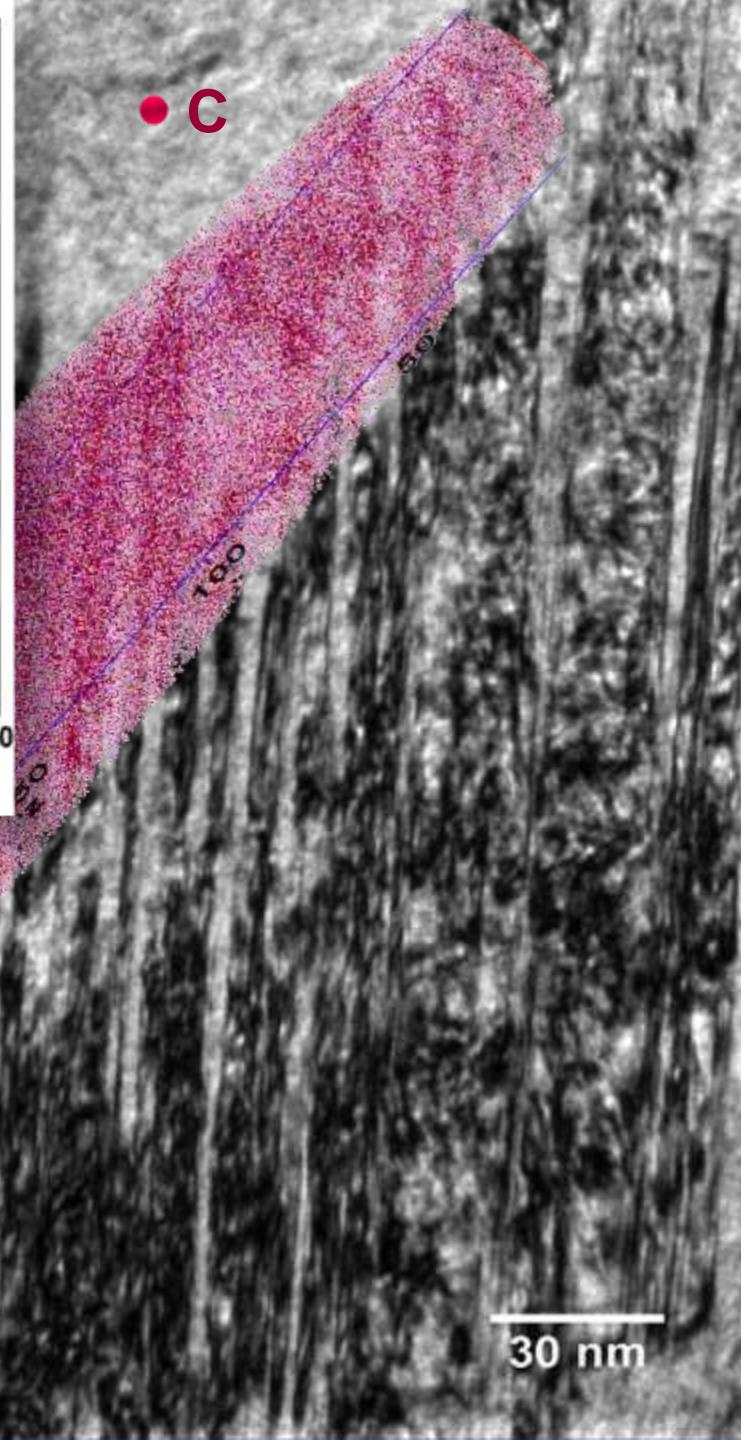
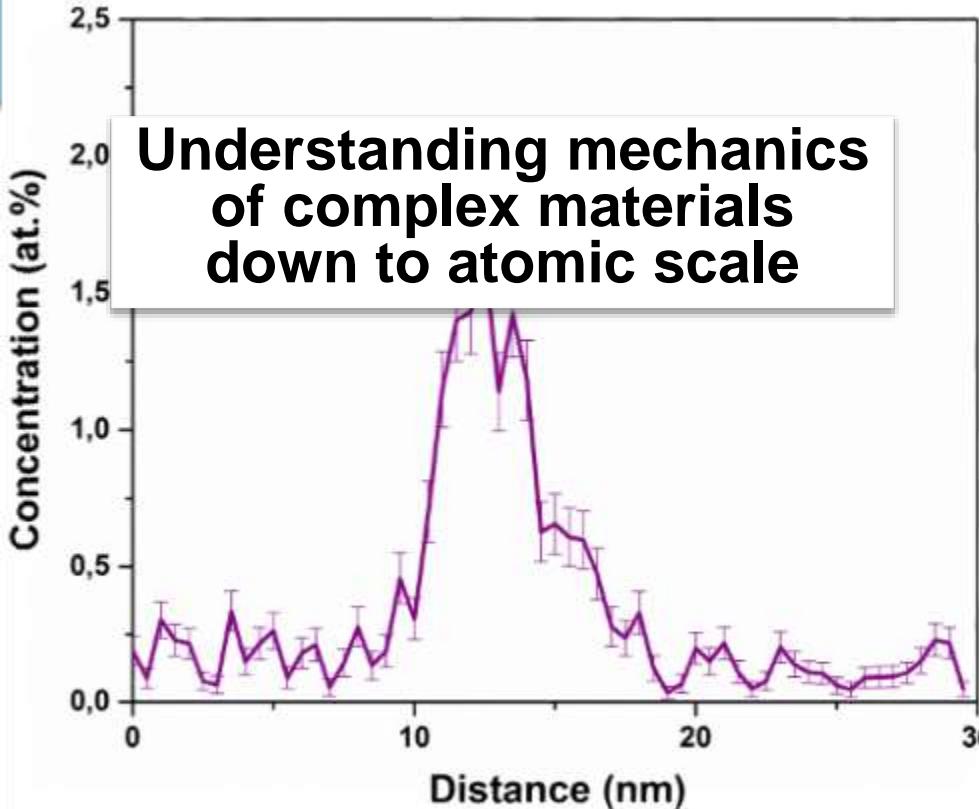
- **Introduction to the scales**
- **Introduction to the engineering background**
- **Quantum mechanics primer**

Scientific mission: complex materials in real environments



Scientific mission: complex materials in real environments



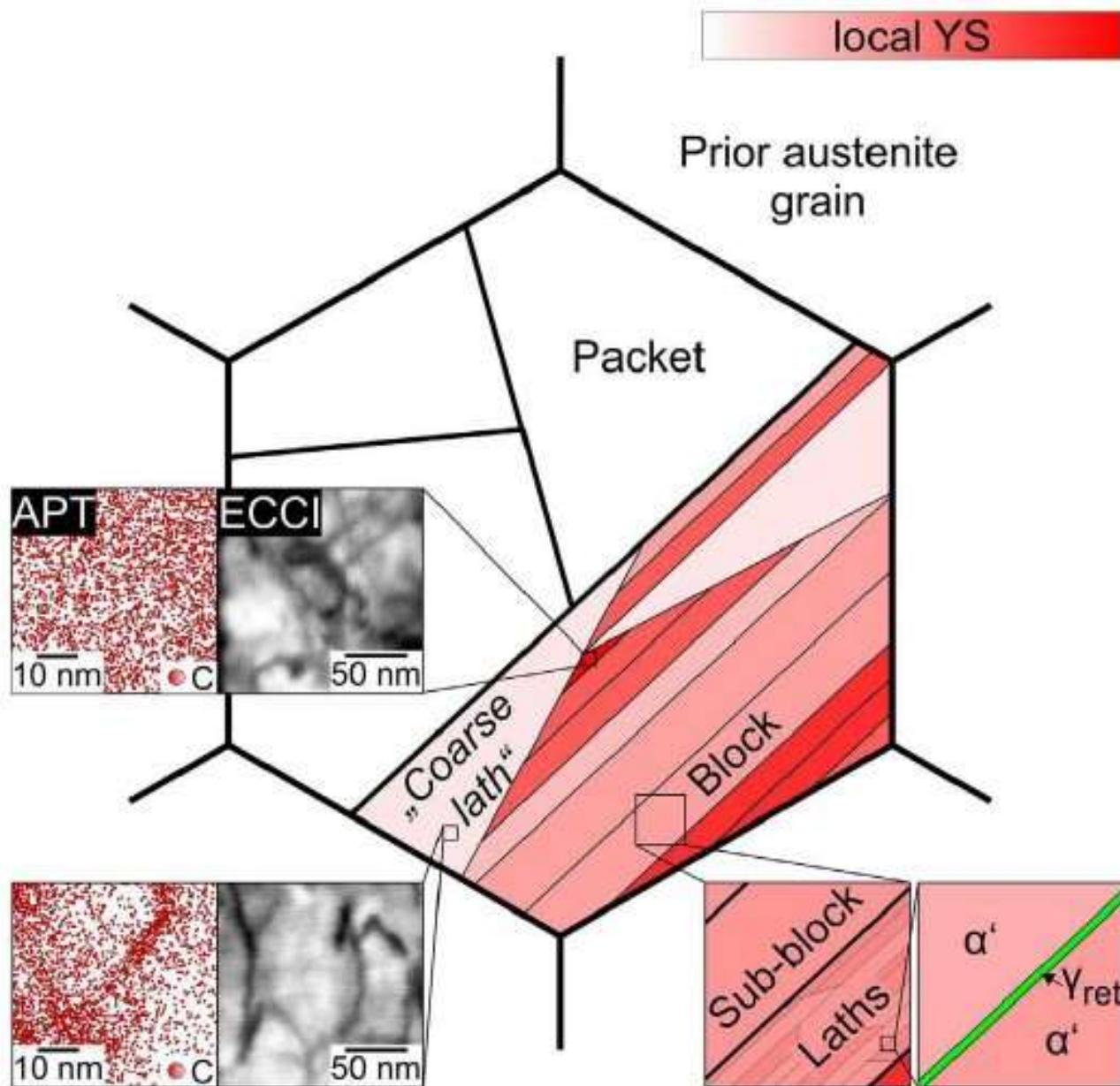


30 nm

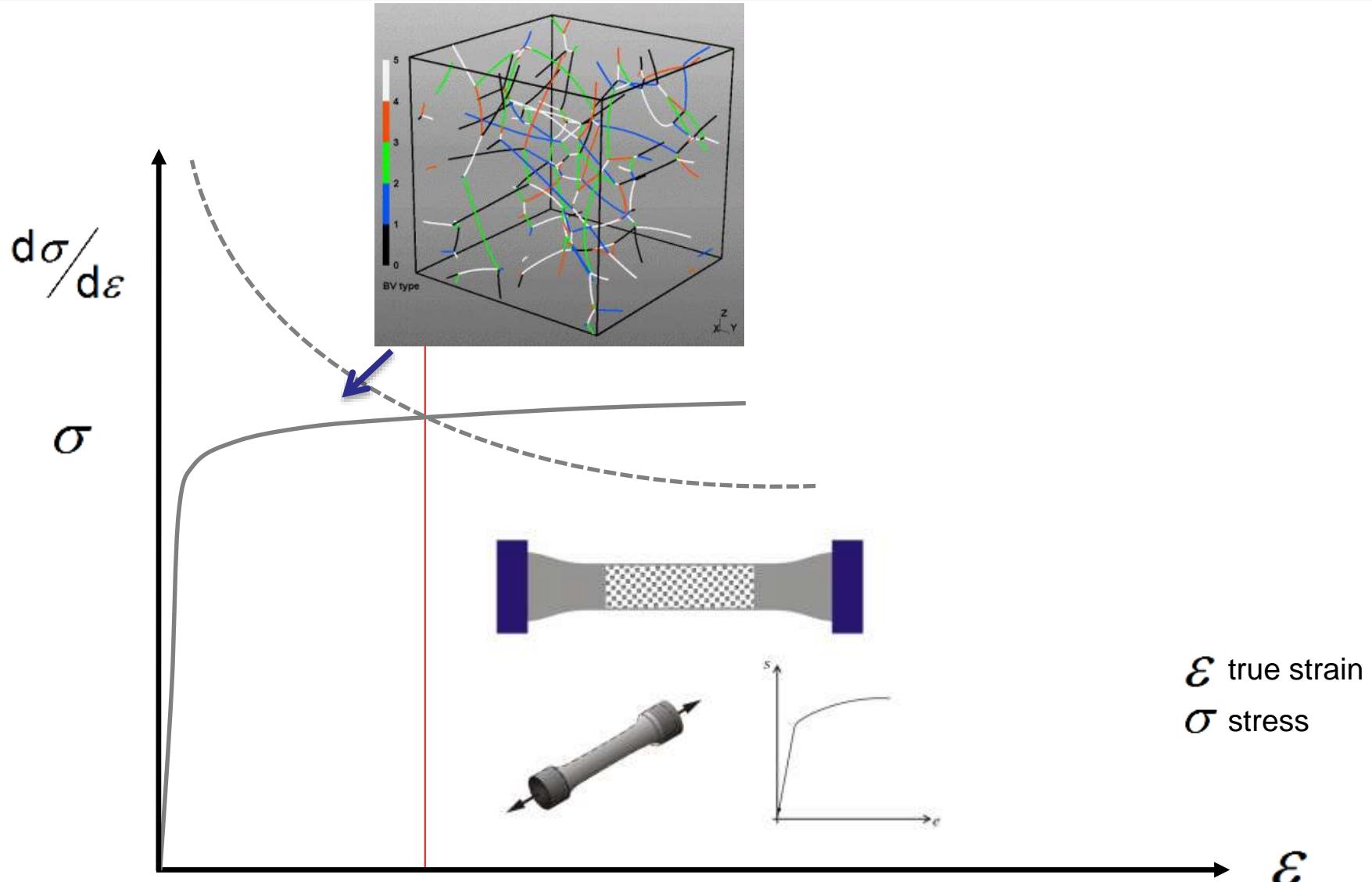
95 (2015) 366

P steel 8

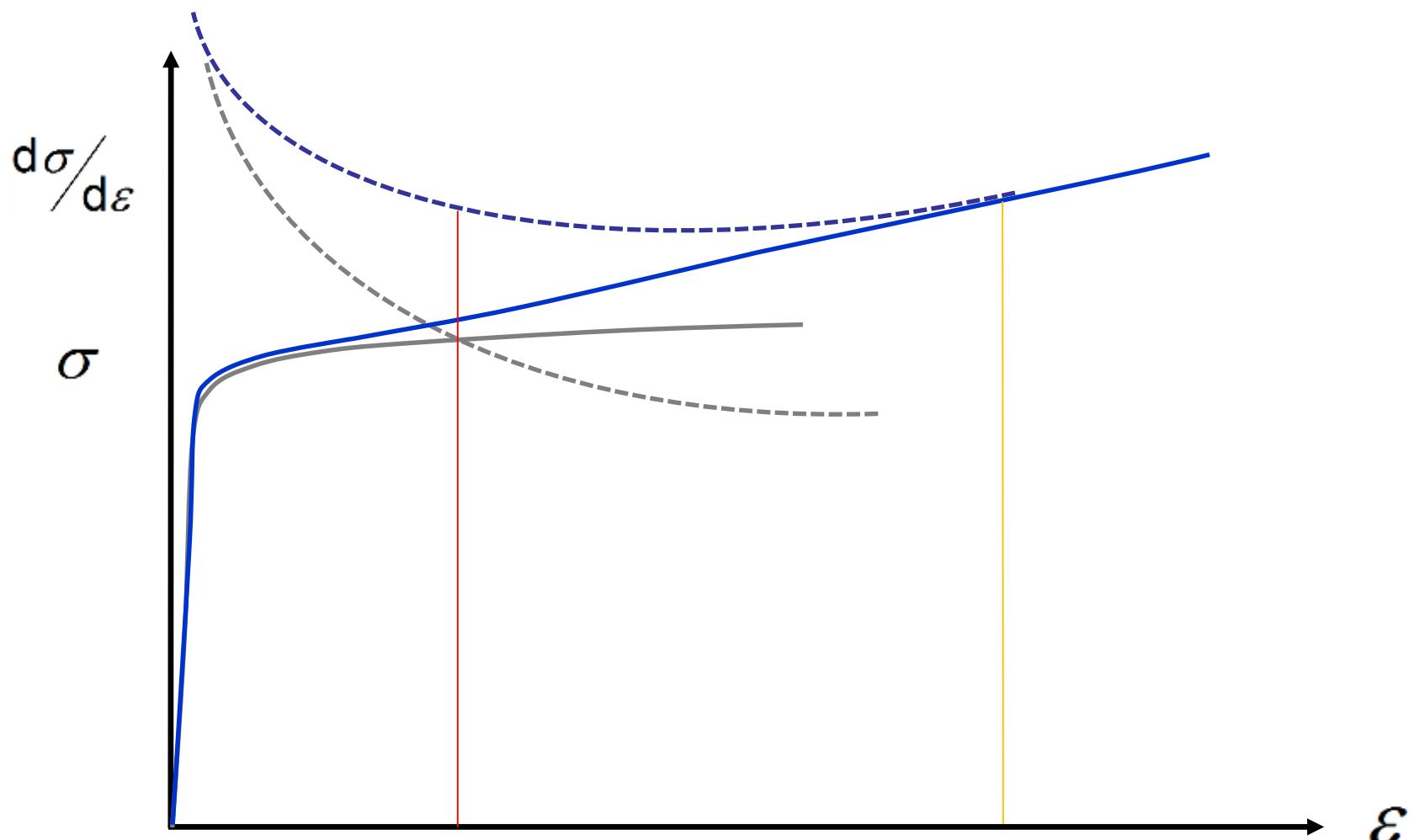
Martensite: Microstructure scales



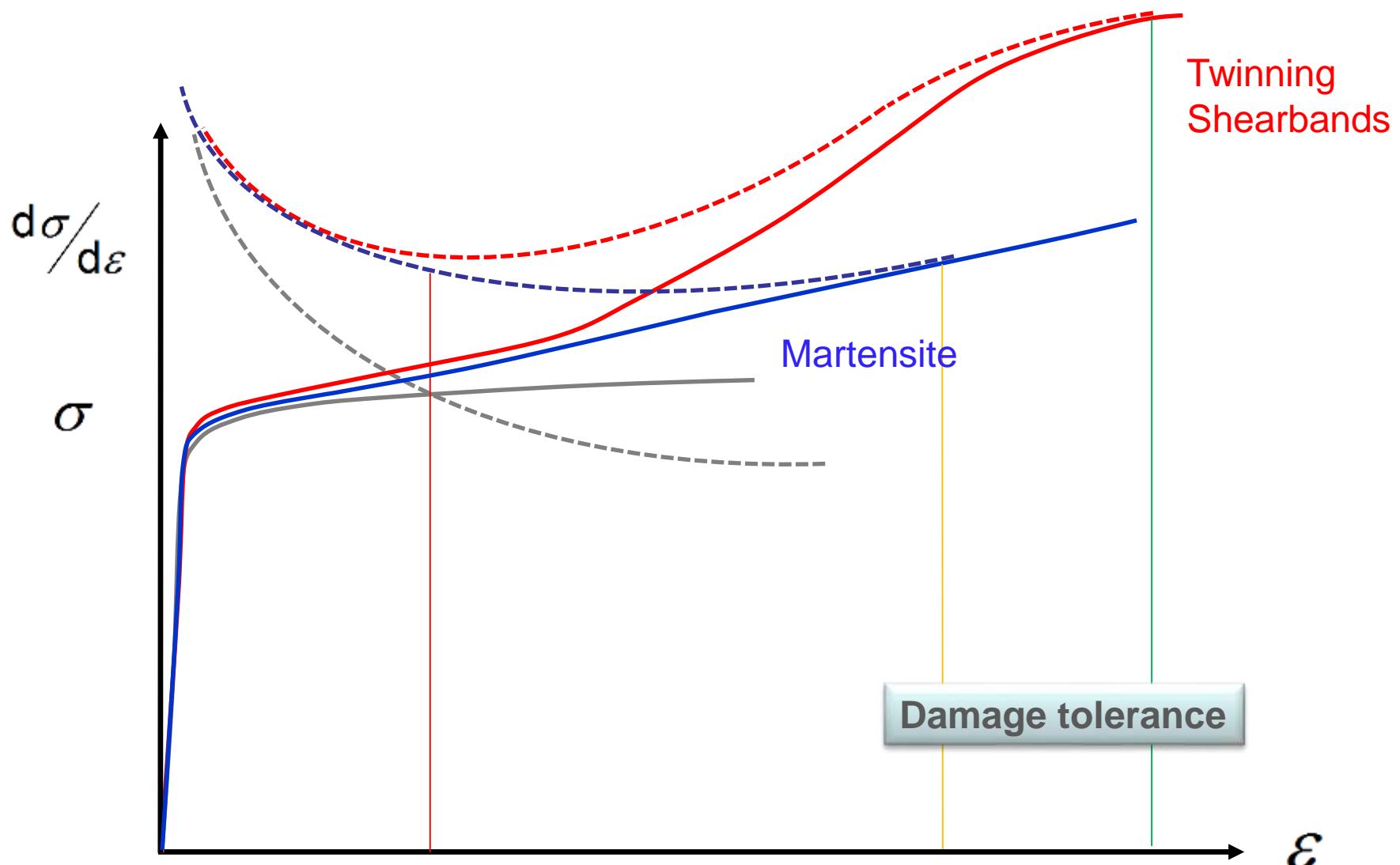
Inverse strength-ductility: phenomenological analysis

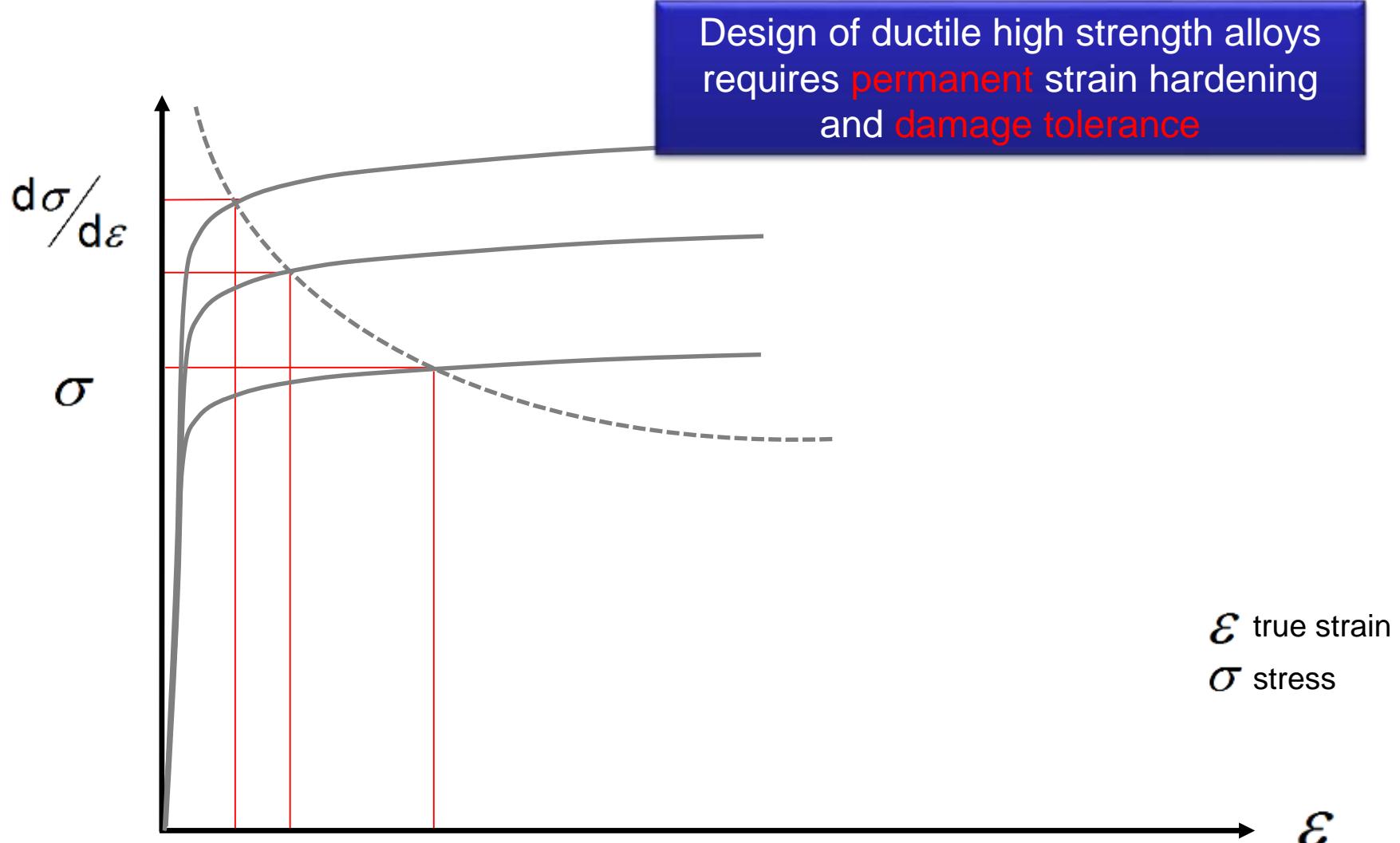


Inverse strength-ductility: phenomenological analysis

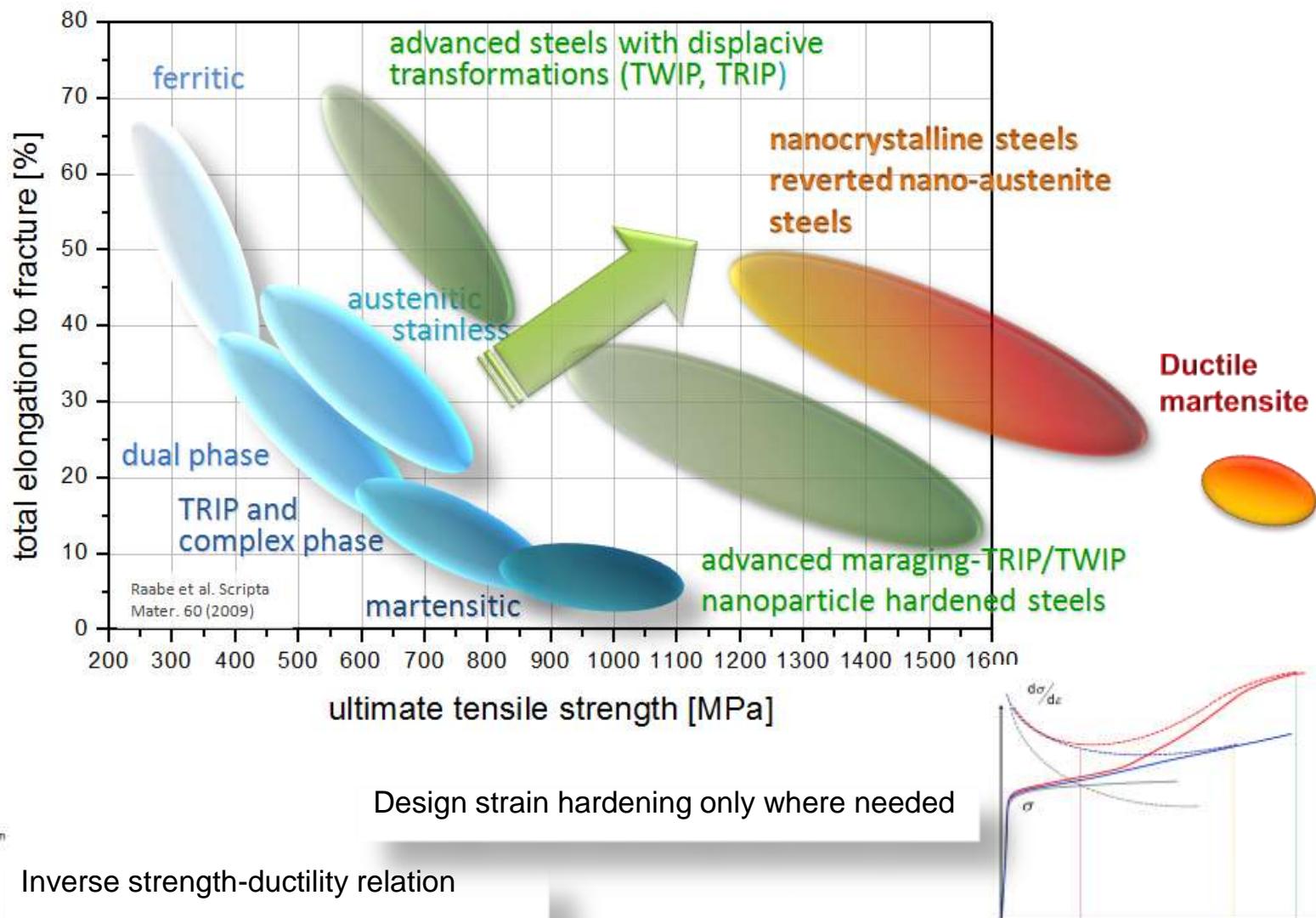


Inverse strength-ductility: phenomenological analysis

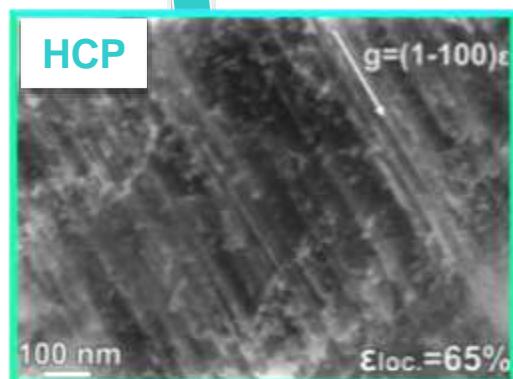
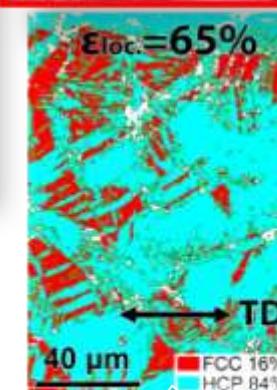
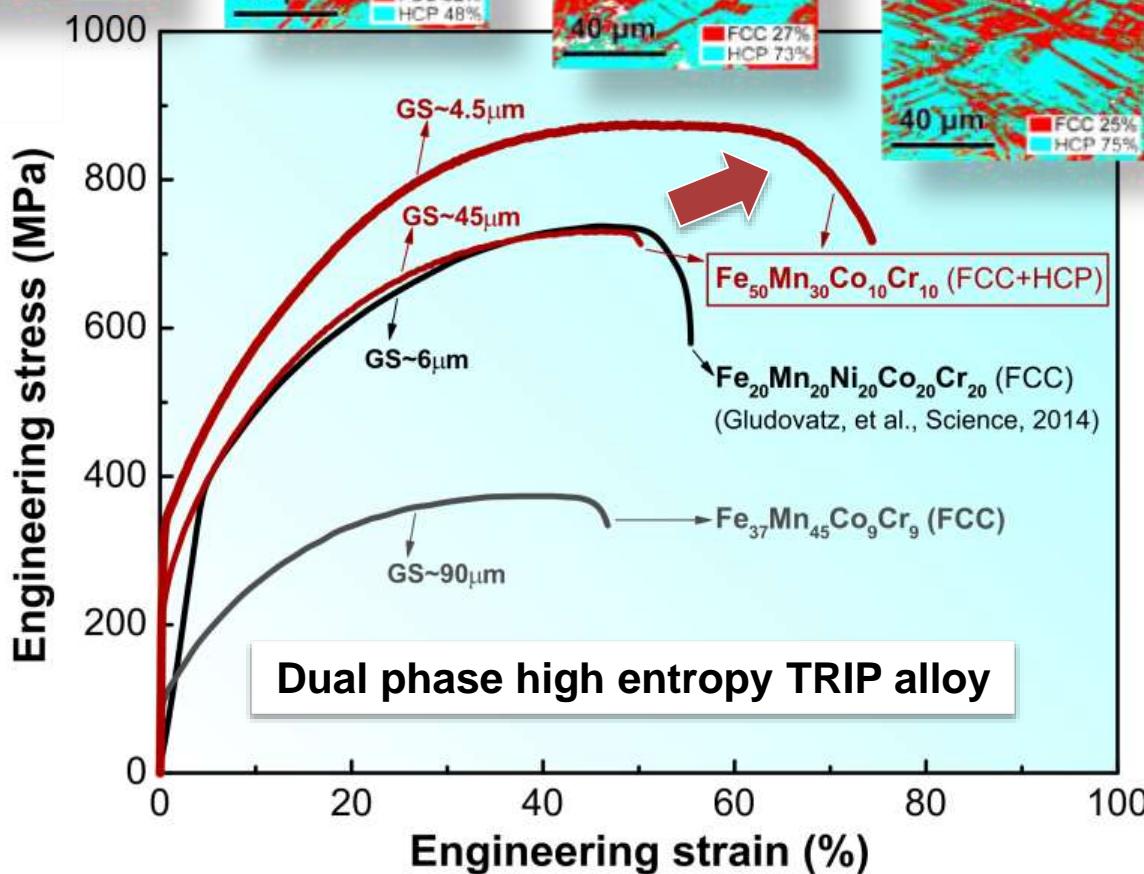
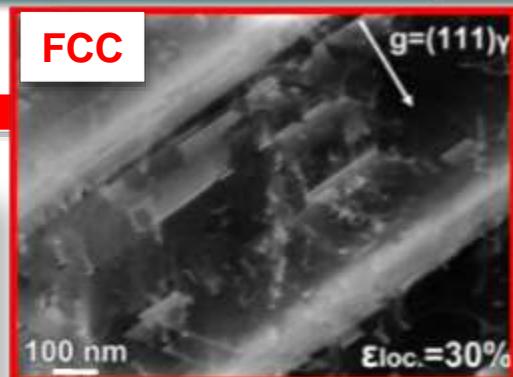
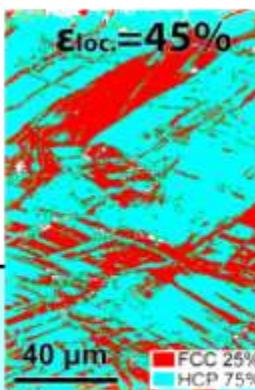
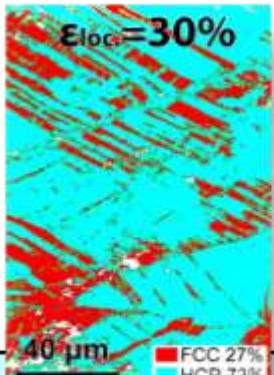




Local phase transformations enable high strength of bulk metals



Theory-guided design: non-iso concentration high entropy alloys

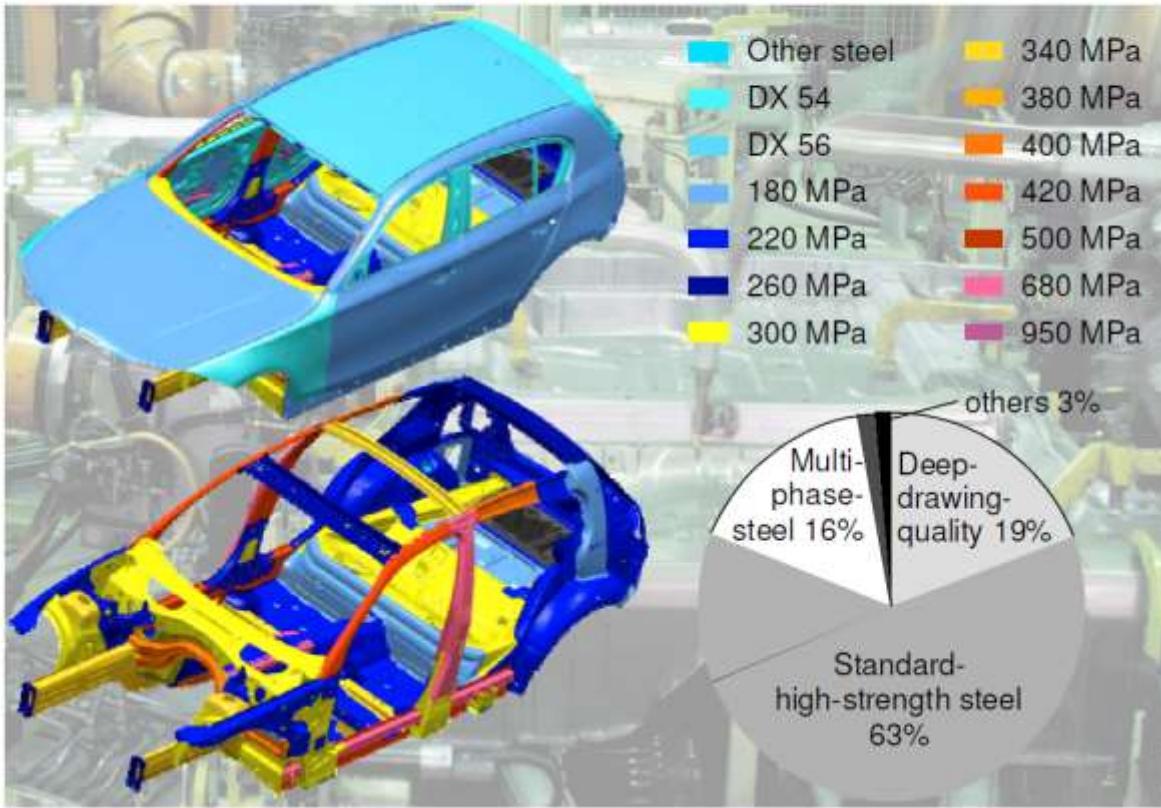


Z. Li et al. Nature

- **Introduction to the scales**
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Car Body Structure. High Strength Steel. BMW 1 Series.





Der neue Audi A8

Audi Space Frame in Multimaterialbauweise

The new Audi A8

Multimaterial Audi space frame

04/17



Aluminium-Blech
Aluminum sheet

Aluminium-Profil
Aluminum section

Aluminium-Guss
Aluminum castings

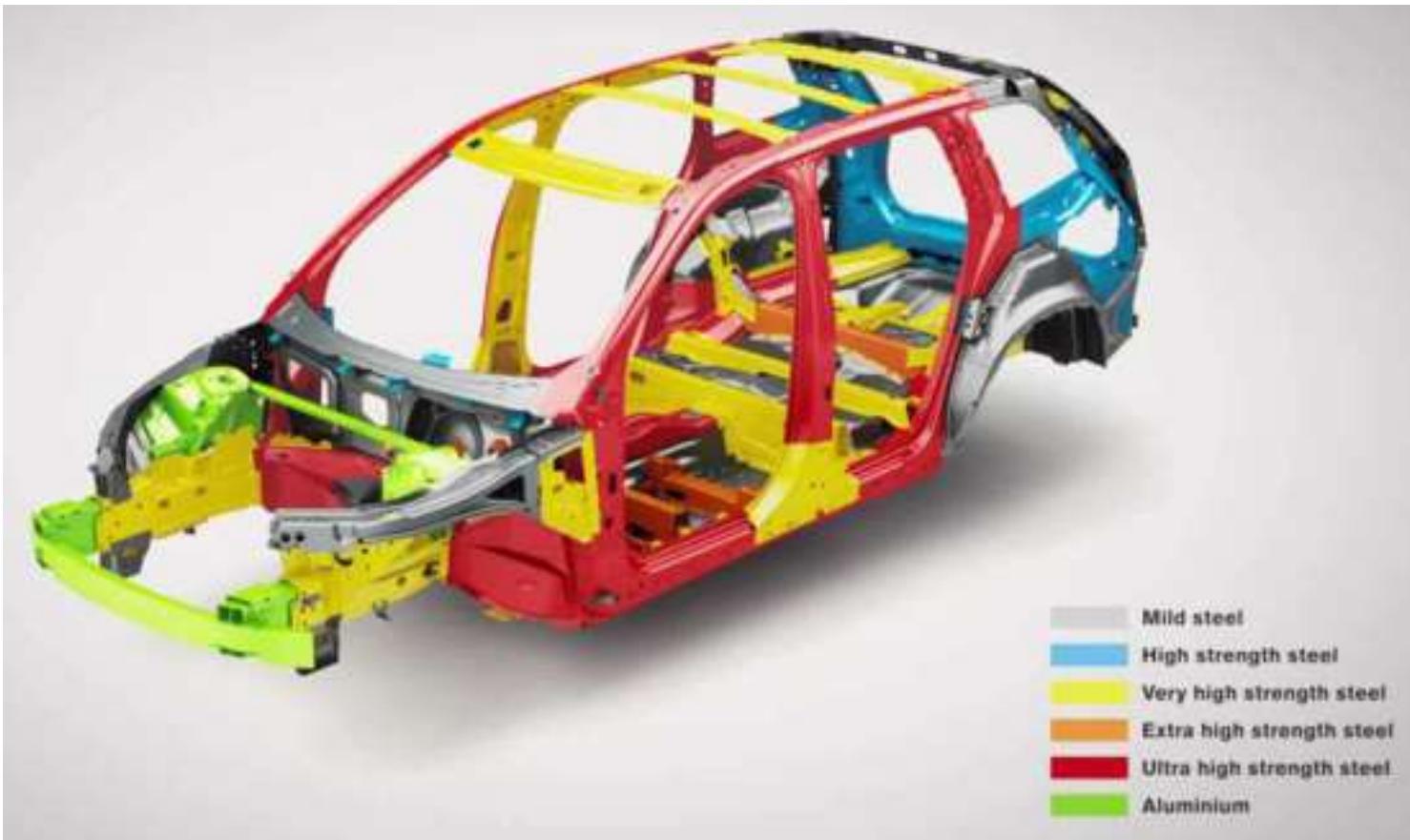
Ultrahochfester Stahl (warmumgeformt)
Ultra-high strength steel (hot-formed)

Konventioneller Stahl
Conventional steel

Kohlenstofffaserverstärkter Kunststoff (CFK)
Carbon fiber-reinforced plastic (CFRP)

Magnesium

New materials automotive (courtesy Volvo)



New materials for key technologies: health

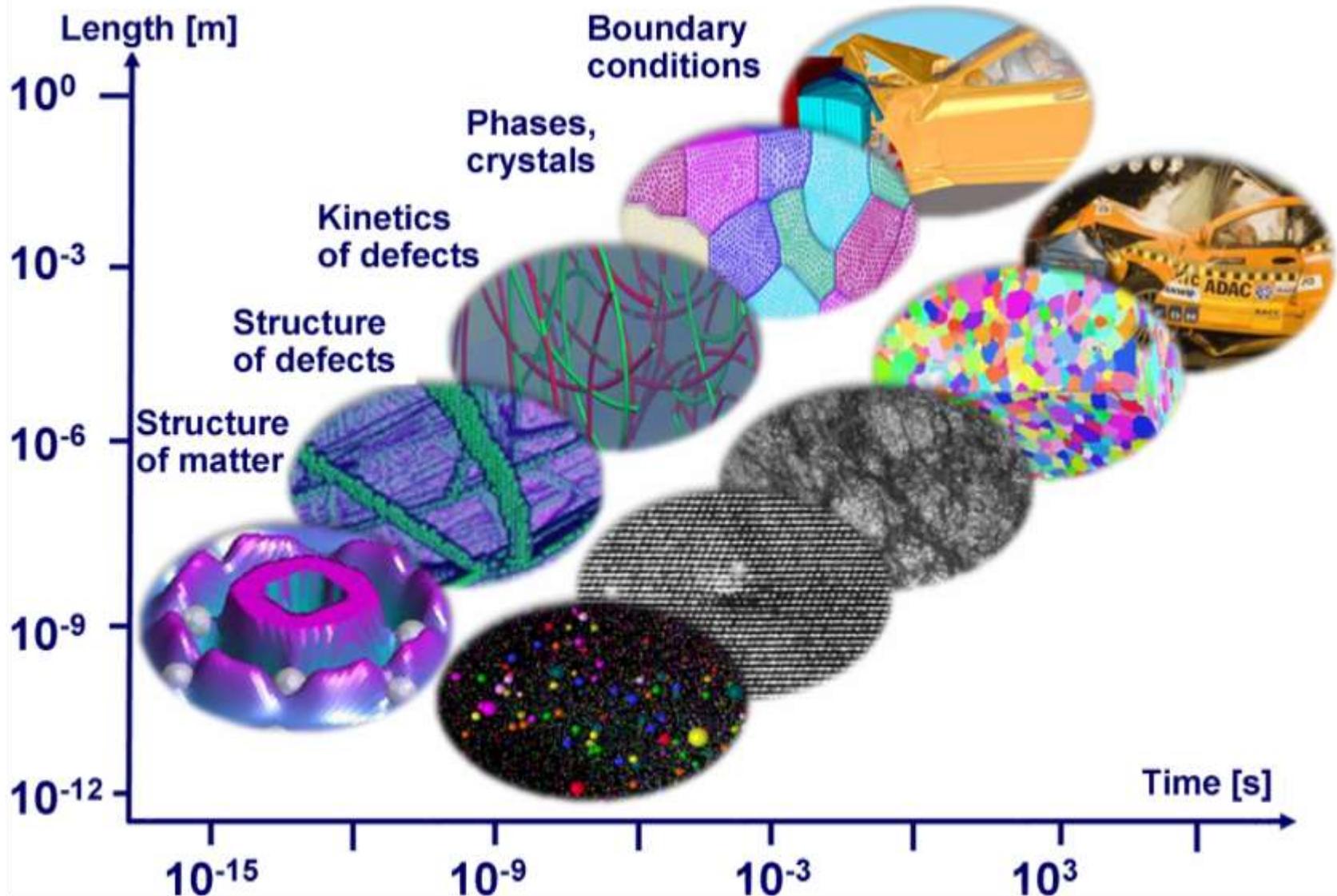
**TITANIUM
MAGNESIUM
COPPER
STEELS**



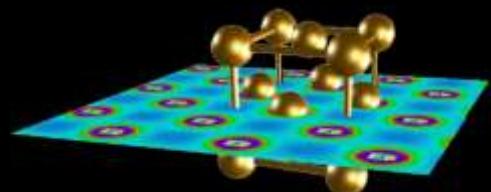


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- **MOST EXACT KNOWN MATERIALS THEORY**
- **COMBINE TO ATOMIC SCALE EXPERIMENTS**
- **OBTAIN DATA NOT ACCESSIBLE OTHERWISE**
- **CAN BE USED AT CONTINUUM SCALE**
- **ELECTRONIC RULES FOR ALLOY DESIGN:
ADD ELECTRONS RATHER THAN ATOMS**



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

$\hbar/(2\pi)$

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

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

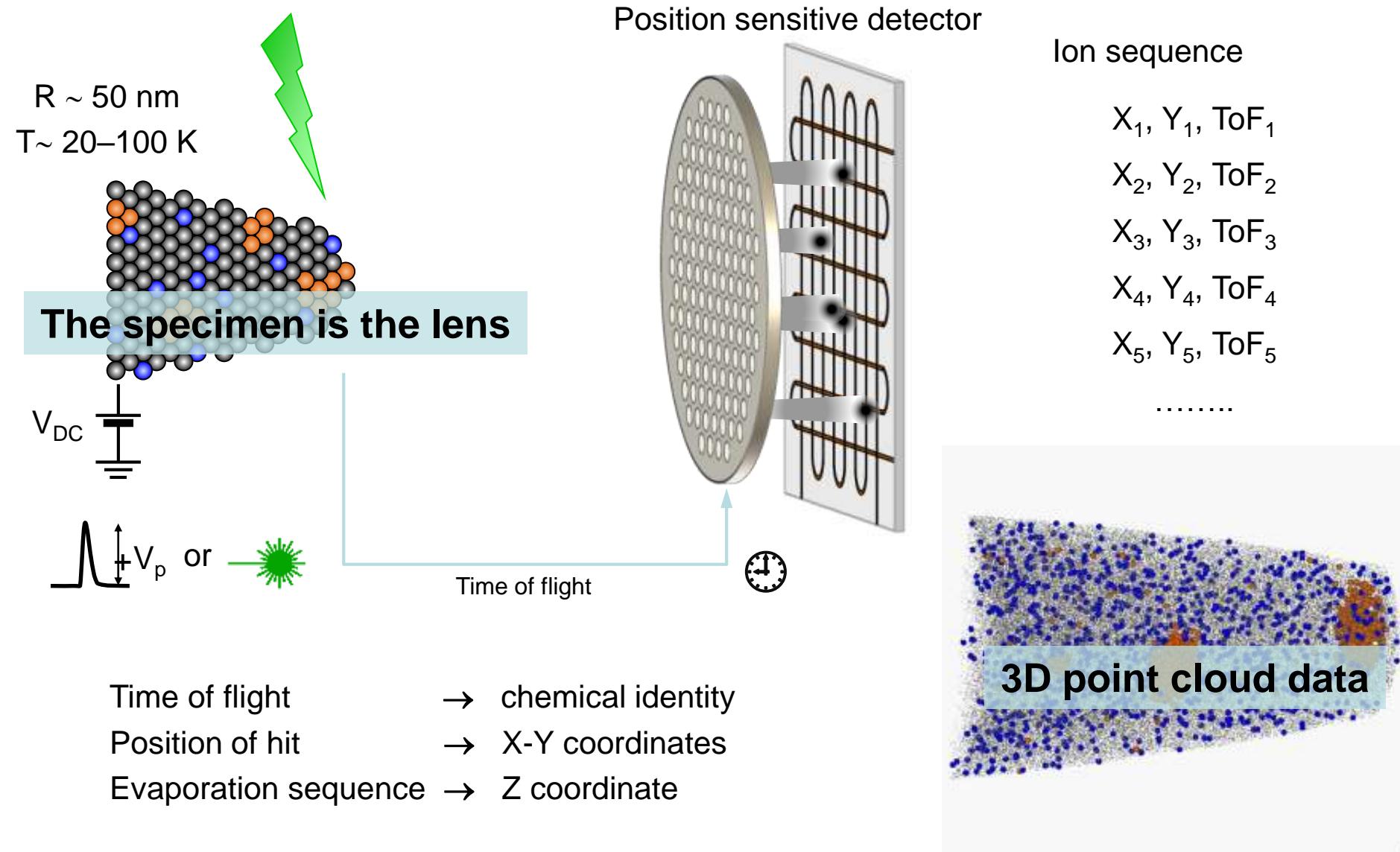
Electrons

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

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 Tomography (APT)



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- **Some examples**

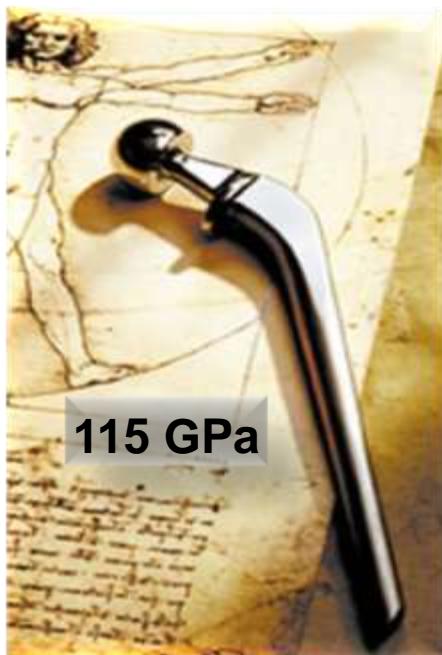
Health: Titanium

Mobility: Steel



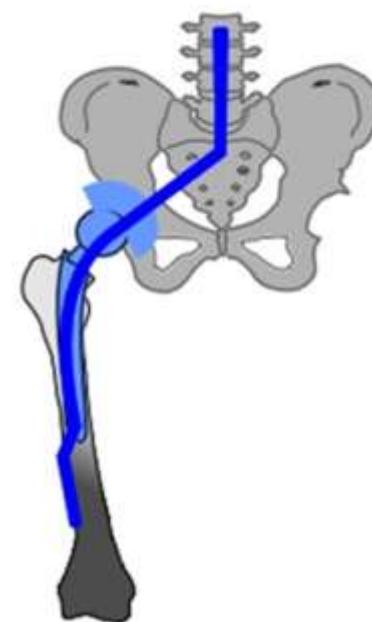


20-25 GPa



Medscape®

<http://www.medscape.com>

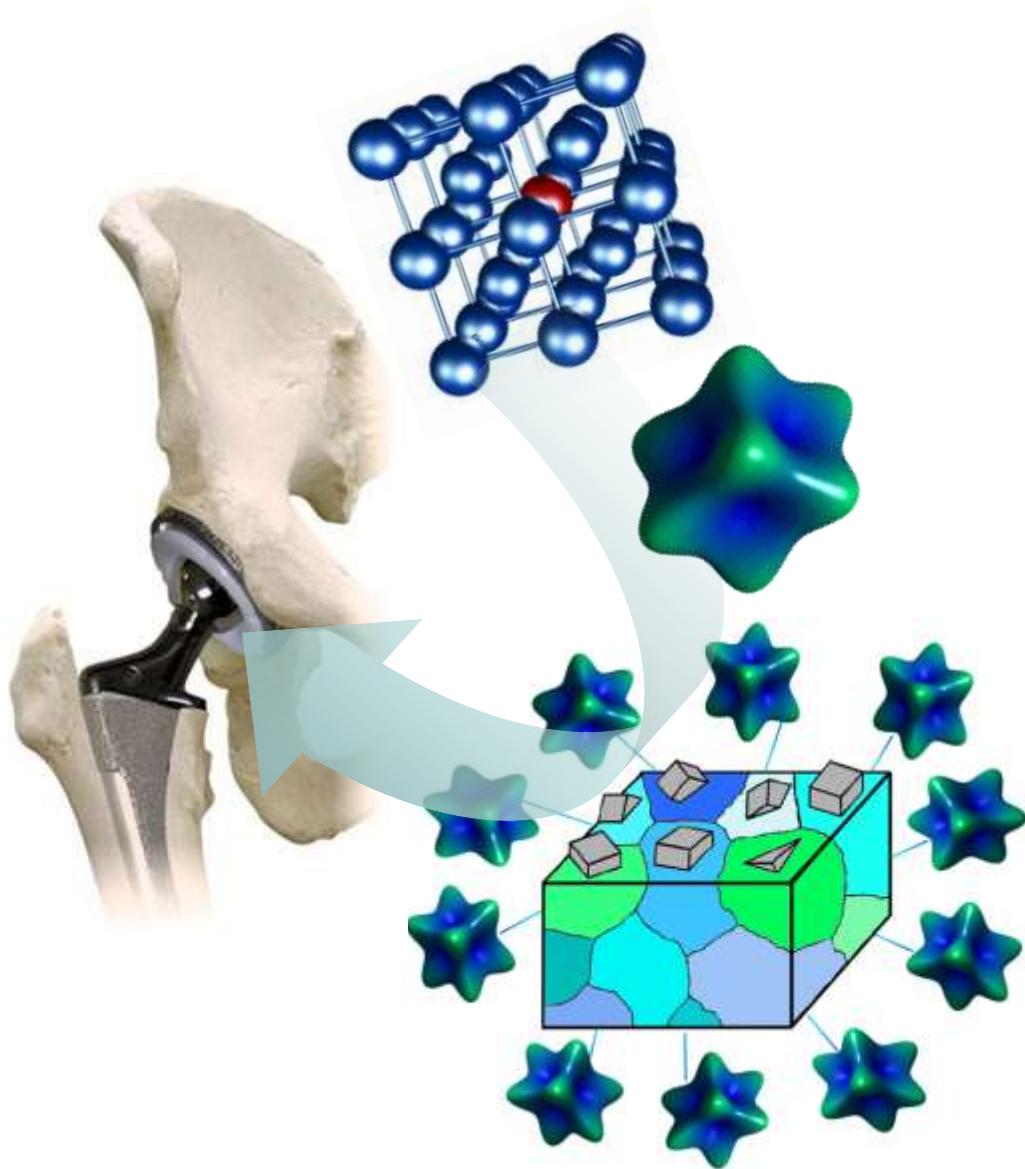


Spannungs-Abschattung (Stress shielding)

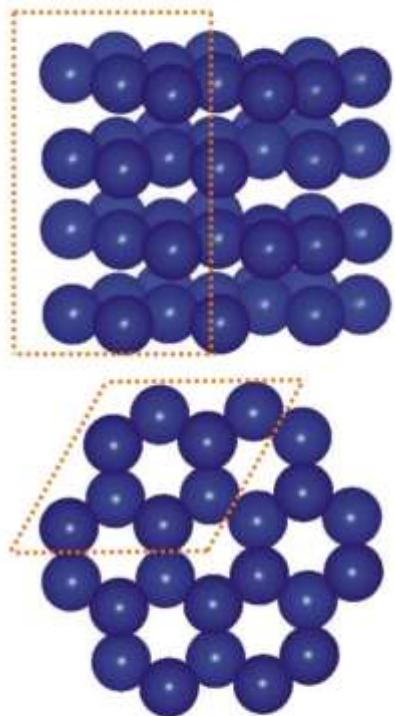
Elastische Fehlpassung:

Knochenaulösung, Abrasion, Entzündung

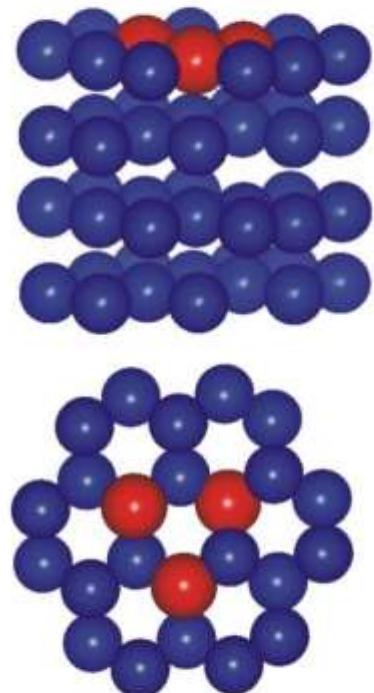
ab-initio Simulation of elastic stiffness



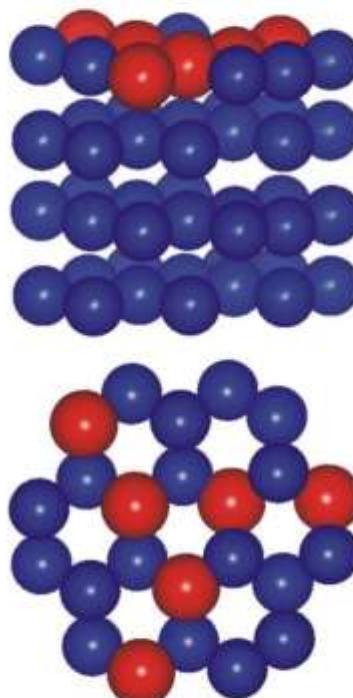
Ti hcp phase



15/1 Ti:X ratio

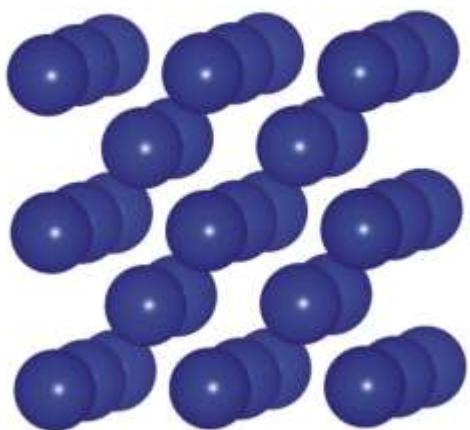


14/2 Ti:X ratio



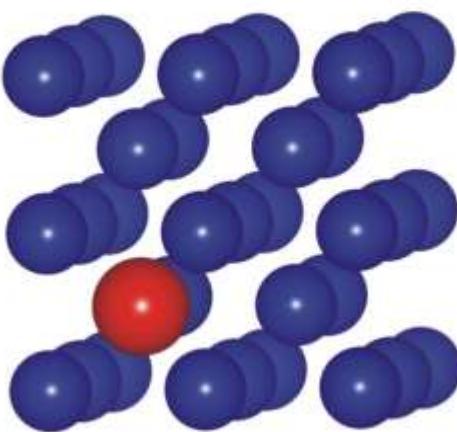
Construct binary alloys in the cubic phase

Ti bcc phase



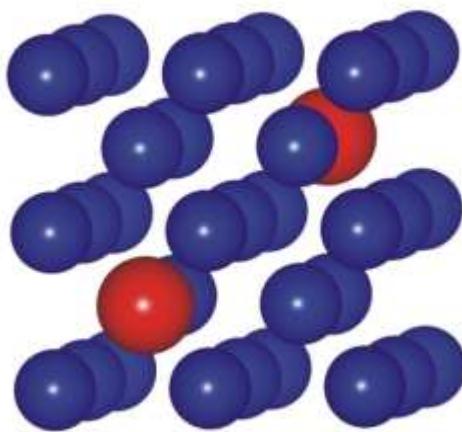
Ti atoms

15/1 Ti:X ratio

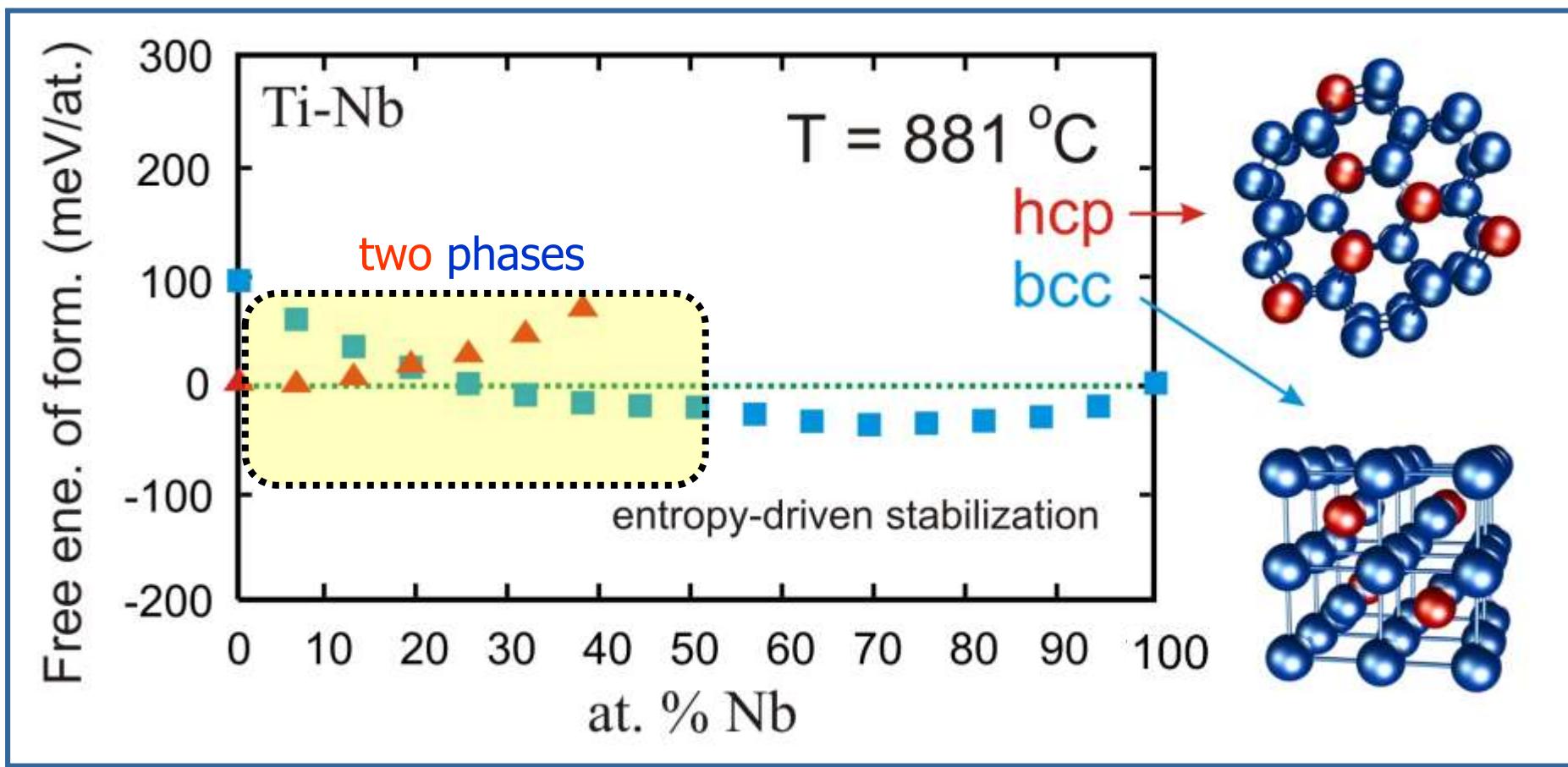


substituent X

14/2 Ti:X ratio



$$\text{Free energy } F(x,c,T) = U - T \cdot S$$



Young's modulus surface plots

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

