

# Microstructure Mechanics of Complex Materials

## Introduction

Dierk Raabe



Max-Planck-Institut  
für Eisenforschung GmbH

Düsseldorf, Germany

WWW.MPIE.DE

d.raabe@mpie.de

**This class:  
Understanding mechanics of complex  
materials down to atomic scale**



## **class times**

Friday, 10 am – 2 pm at IMM / RWTH  
(last class at MPI Düsseldorf)

### **Course Lecturers:**

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



# Contact, website and class days

Date / Location	Topics	Lecturer
<b>15. April 2016 IMM / RWTH</b>	Introduction to materials micromechanics, multiscale problems in micromechanics, case studies, crystal structures and defects, relation to products and manufacturing	Raabe
<b>22. April 2015 IMM / RWTH</b>	Crystal structures, dislocation statics, crystal dislocations, dislocation dynamics	Raabe
<b>29. April 2015 IMM / RWTH</b>	Dislocations, crystalline anisotropy and crystal mechanics in hexagonal metals	Sandlöbes
<b>6. May 2015 IMM / RWTH</b>	No classes	-
<b>13. May 2015 IMM / RWTH</b>	Fracture mechanics Introduction to FEM	Shanthraj
<b>20. May 2015 IMM / RWTH</b>	Athermal phase transformations in micromechanics	Wong
<b>27. May 2015 IMM / RWTH</b>	No classes	-
<b>3. June 2015 IMM / RWTH</b>	Crystal micromechanics, single crystal mechanics, yield surface mechanics, polycrystal models, Taylor model, Integrated micromechanical experimentation and simulation for complex alloys, hydrogen embrittlement	Raabe
<b>10. June 2015 IMM / RWTH</b>	Micromechanics of polymers and biological (natural) composites	Raabe
<b>17. June 2015 MPI / Düsseldorf</b>	!! Class at MPI !! Applied micromechanics: multiphase and composite material design MPI Lab tour	Springer



- **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

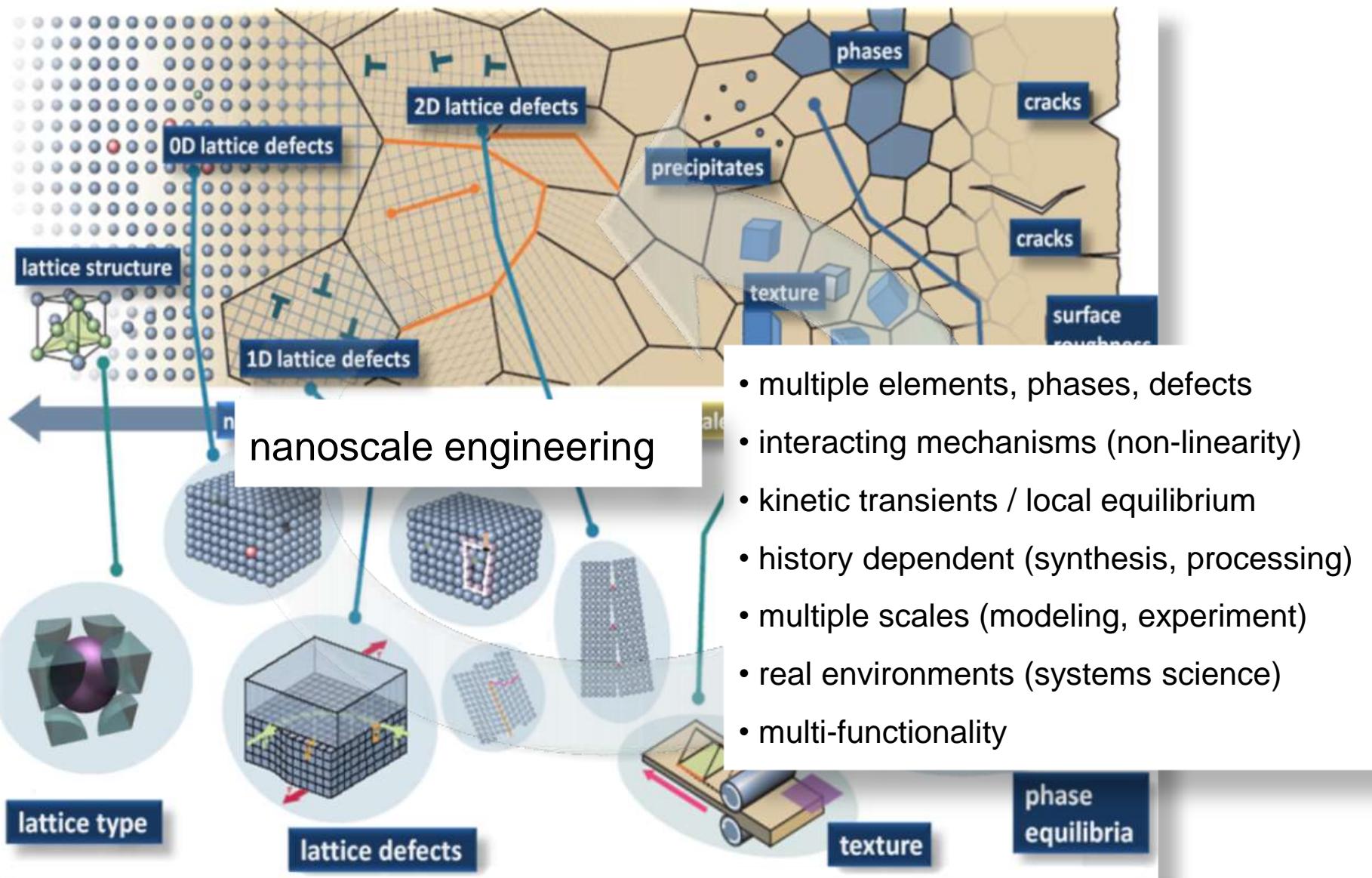
Hosford: The Mechanics of Crystals and Textured Polycrystals, Oxford University Press

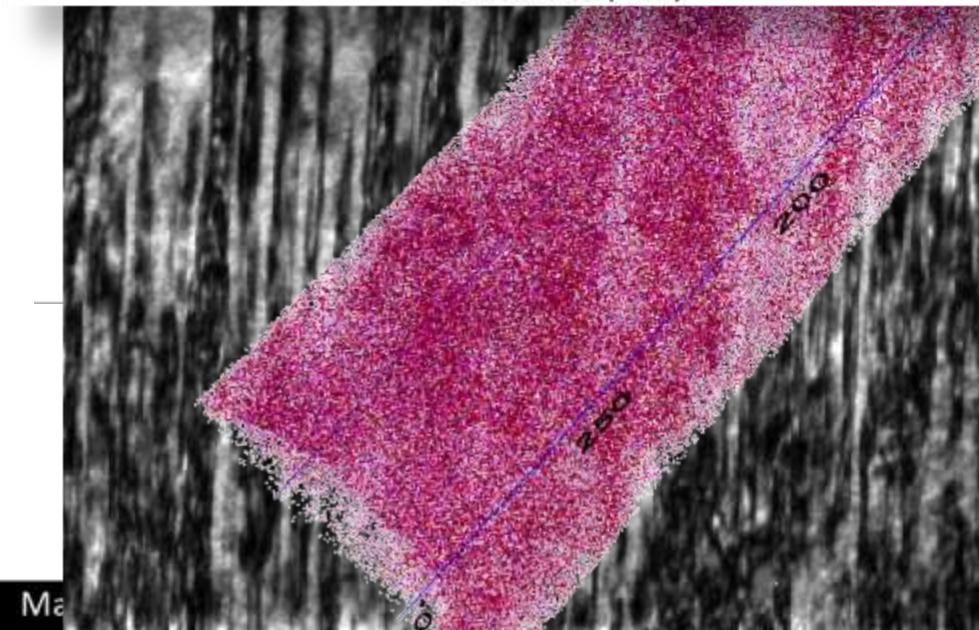
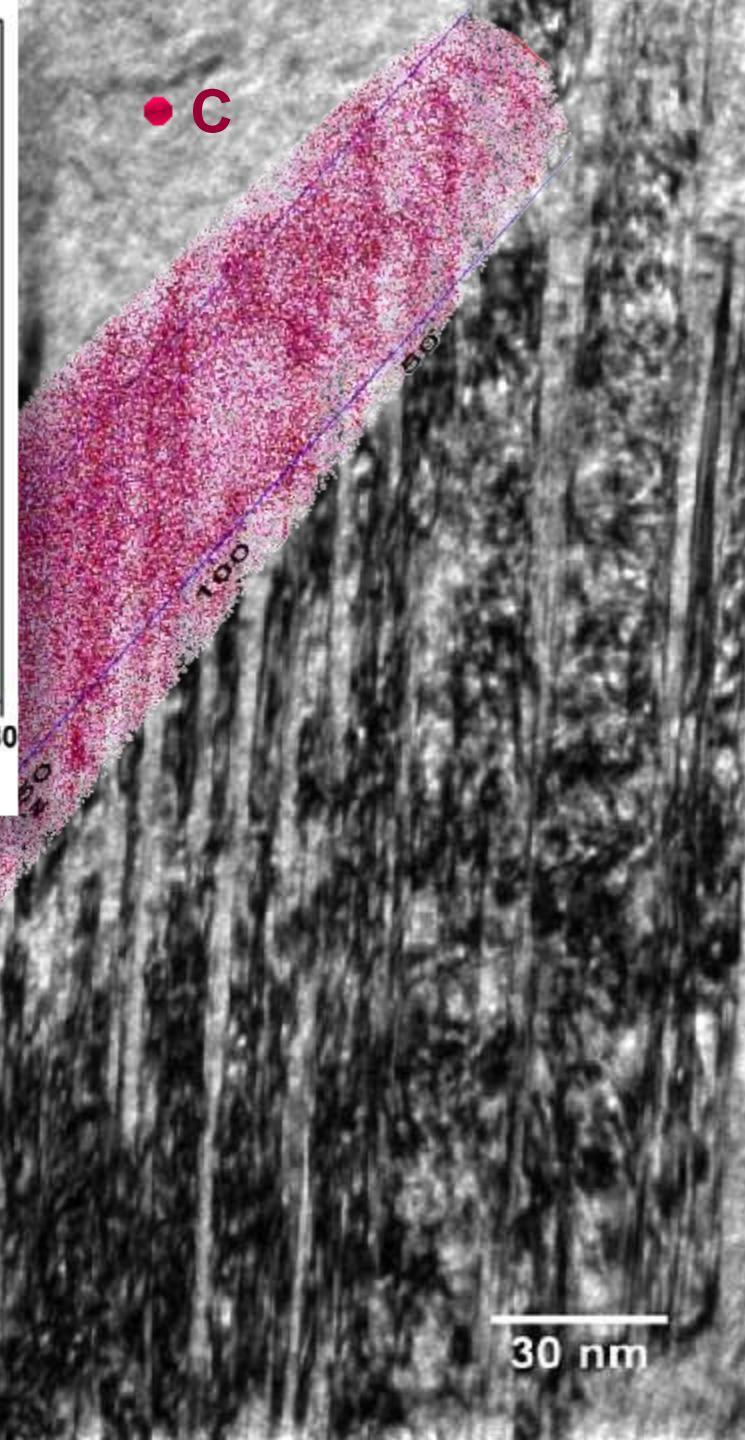
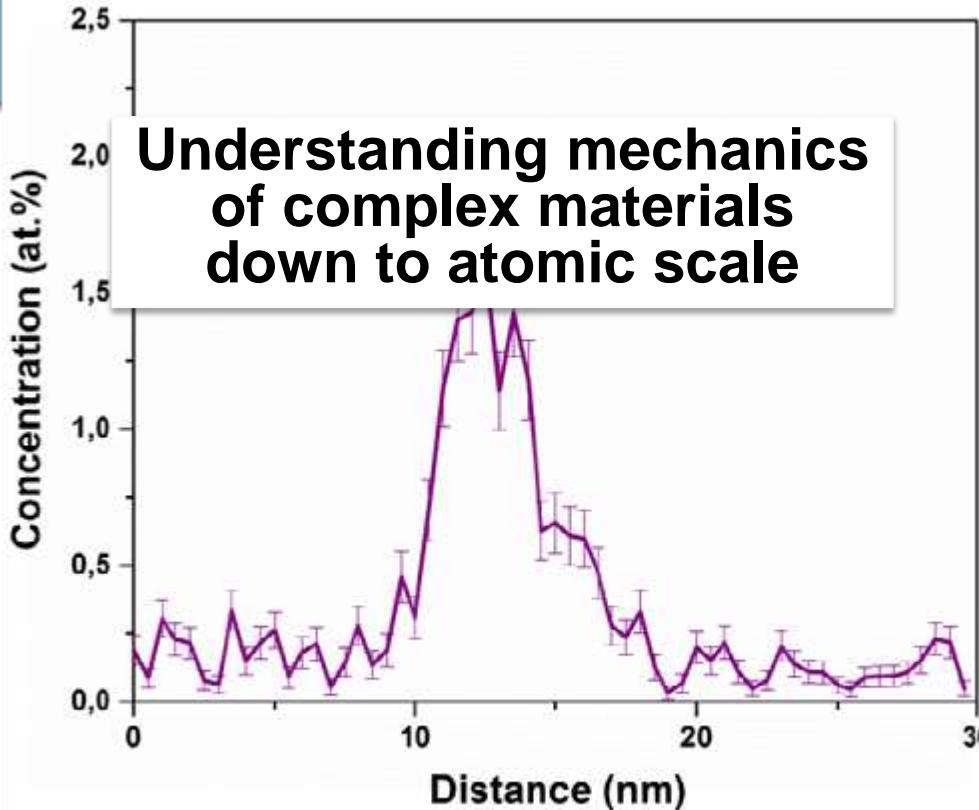
Kocks, Tomé and Wenk: Texture and Anisotropy. Preferred Orientations in Polycrystals and Their Effect on Material Properties. Cambridge University Press

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

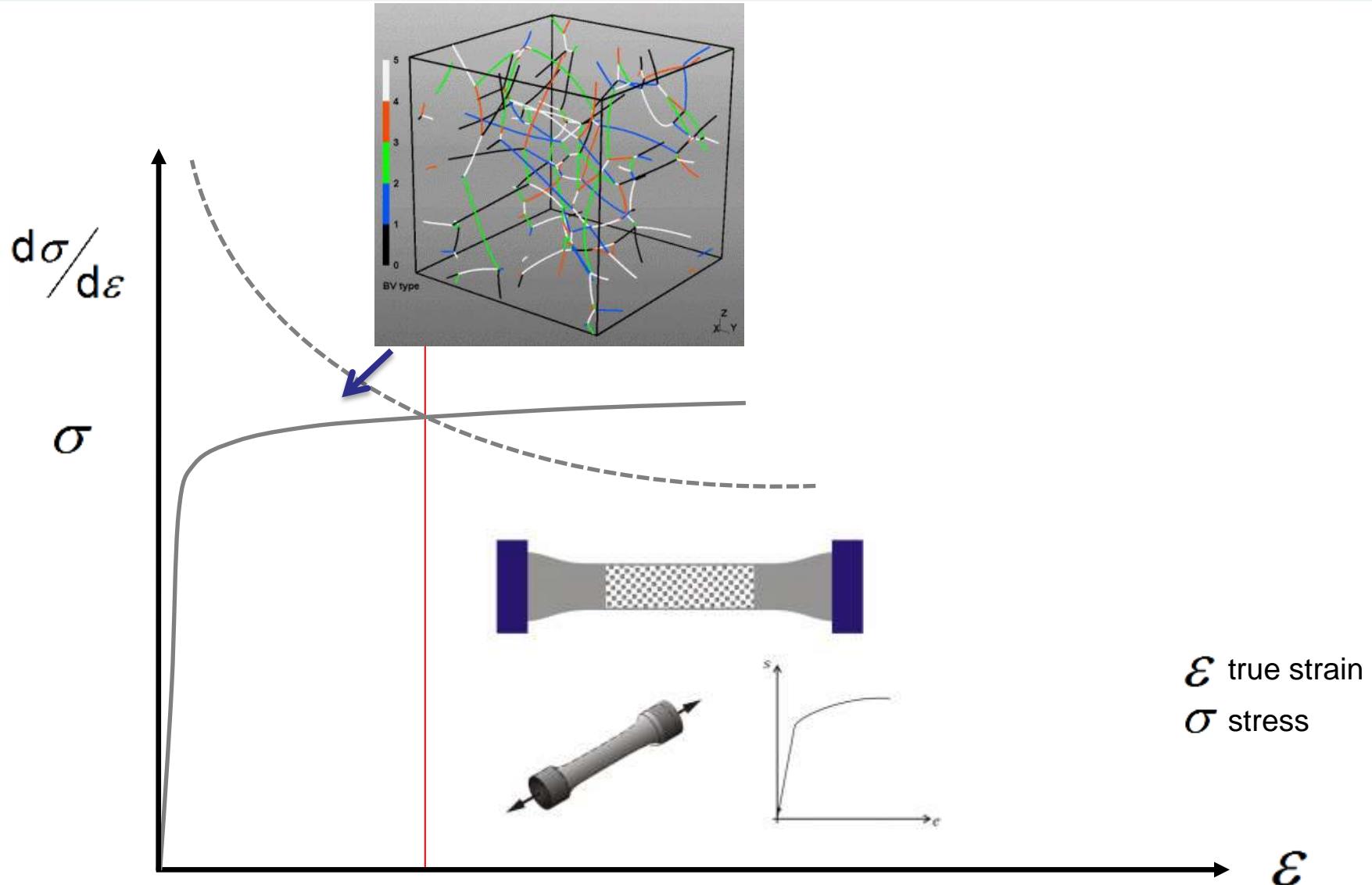


- **Introduction to the scales**
- **Introduction to the engineering background**
- **Quantum mechanics primer**

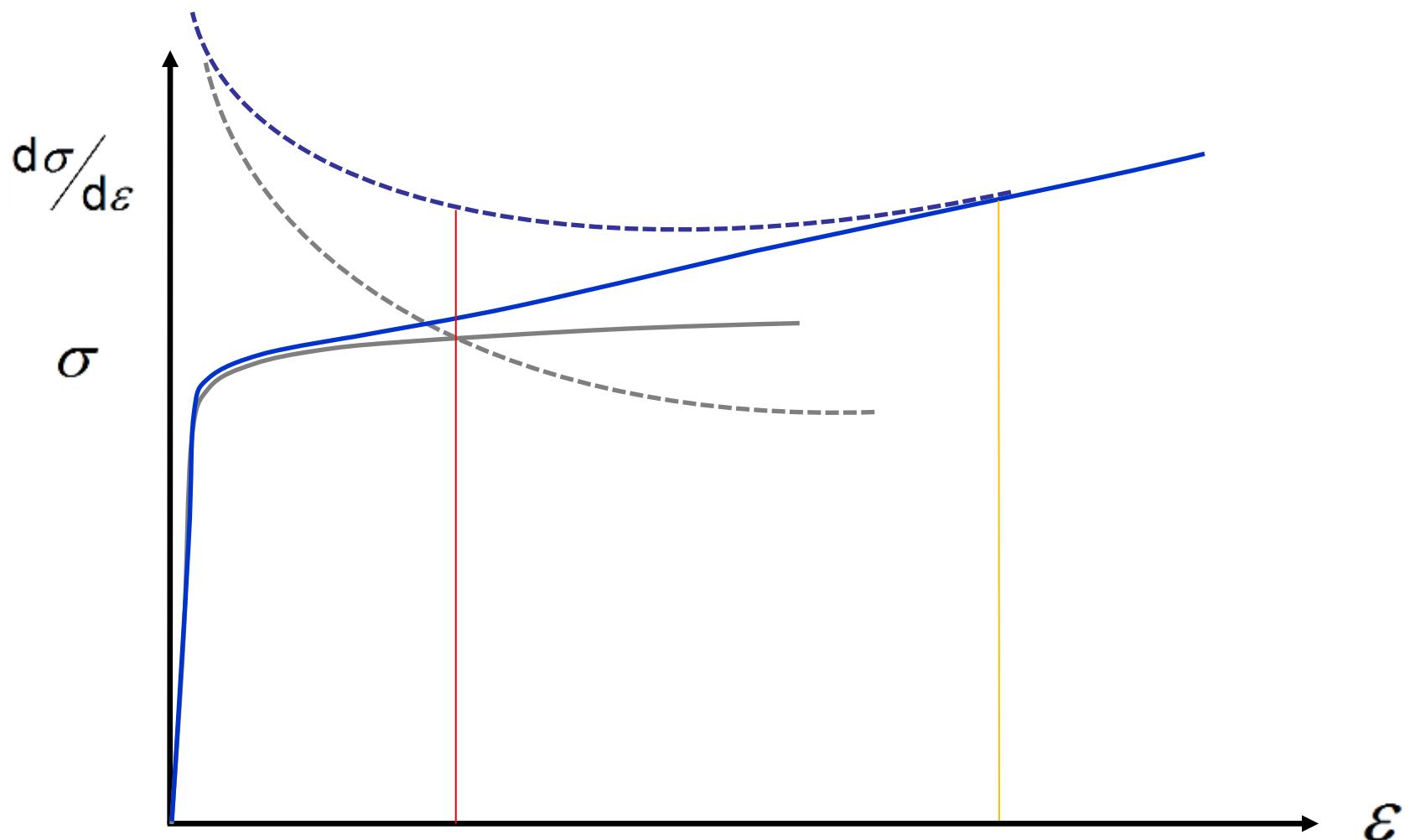




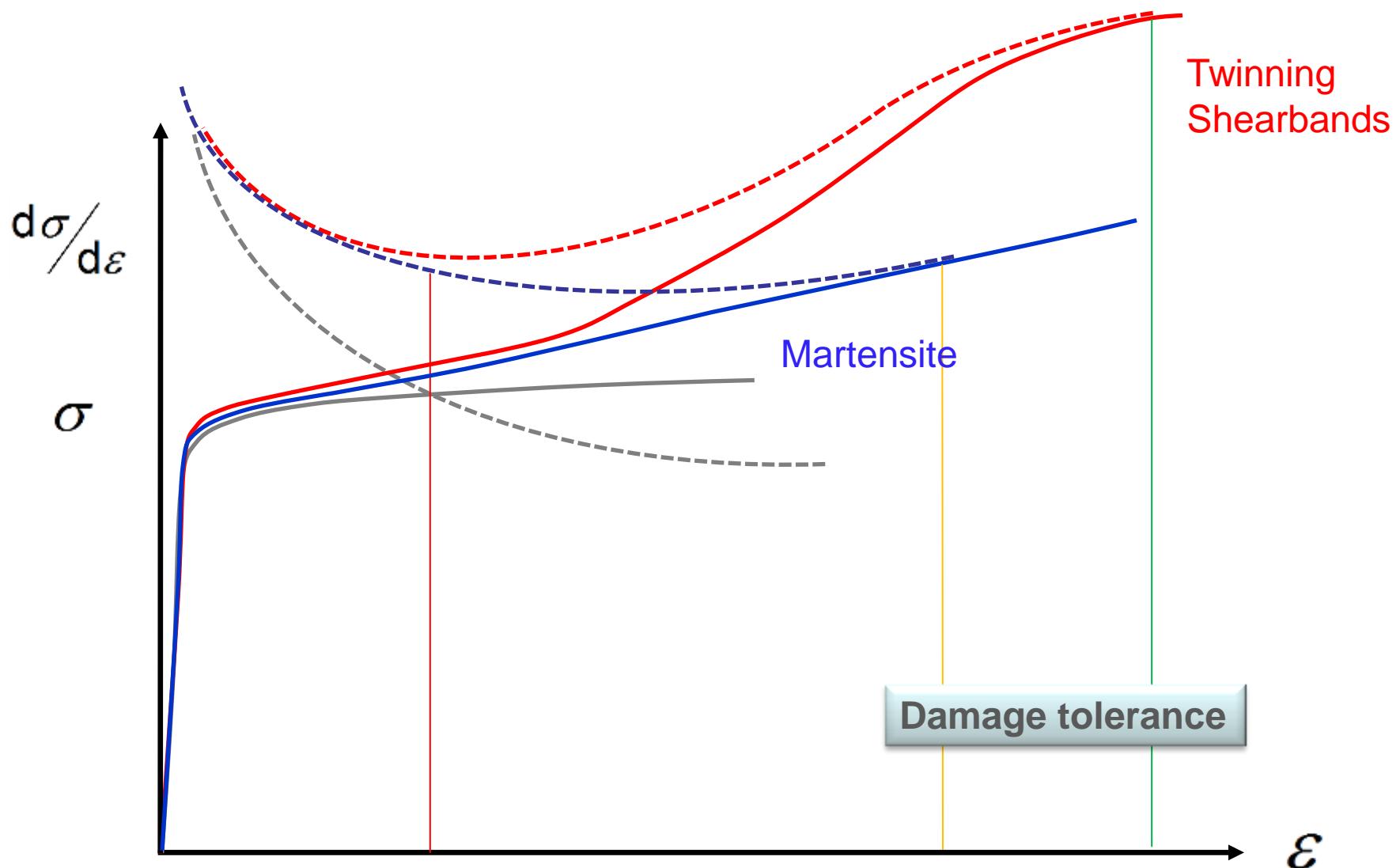
# Inverse strength-ductility: phenomenological analysis

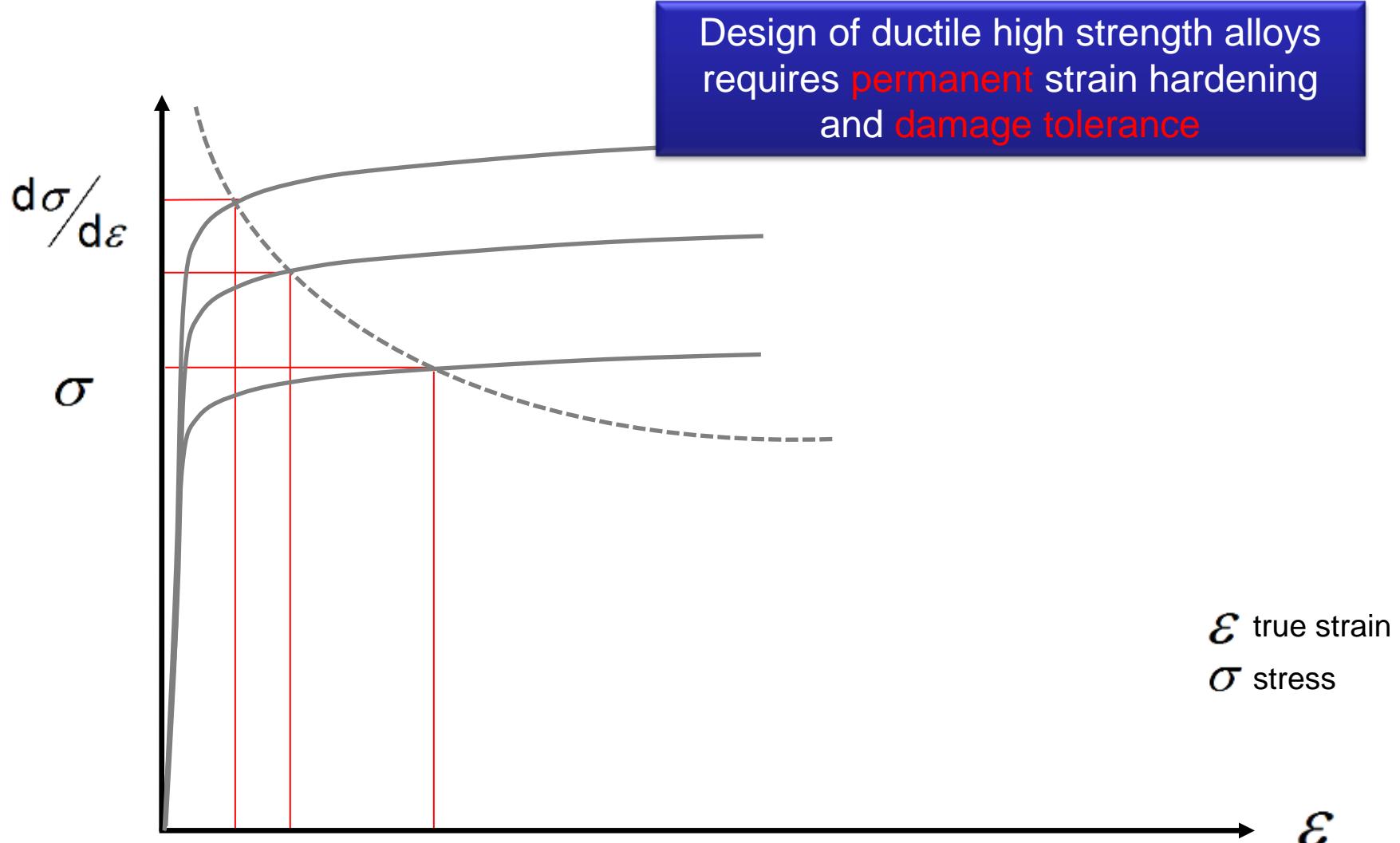


# Inverse strength-ductility: phenomenological analysis

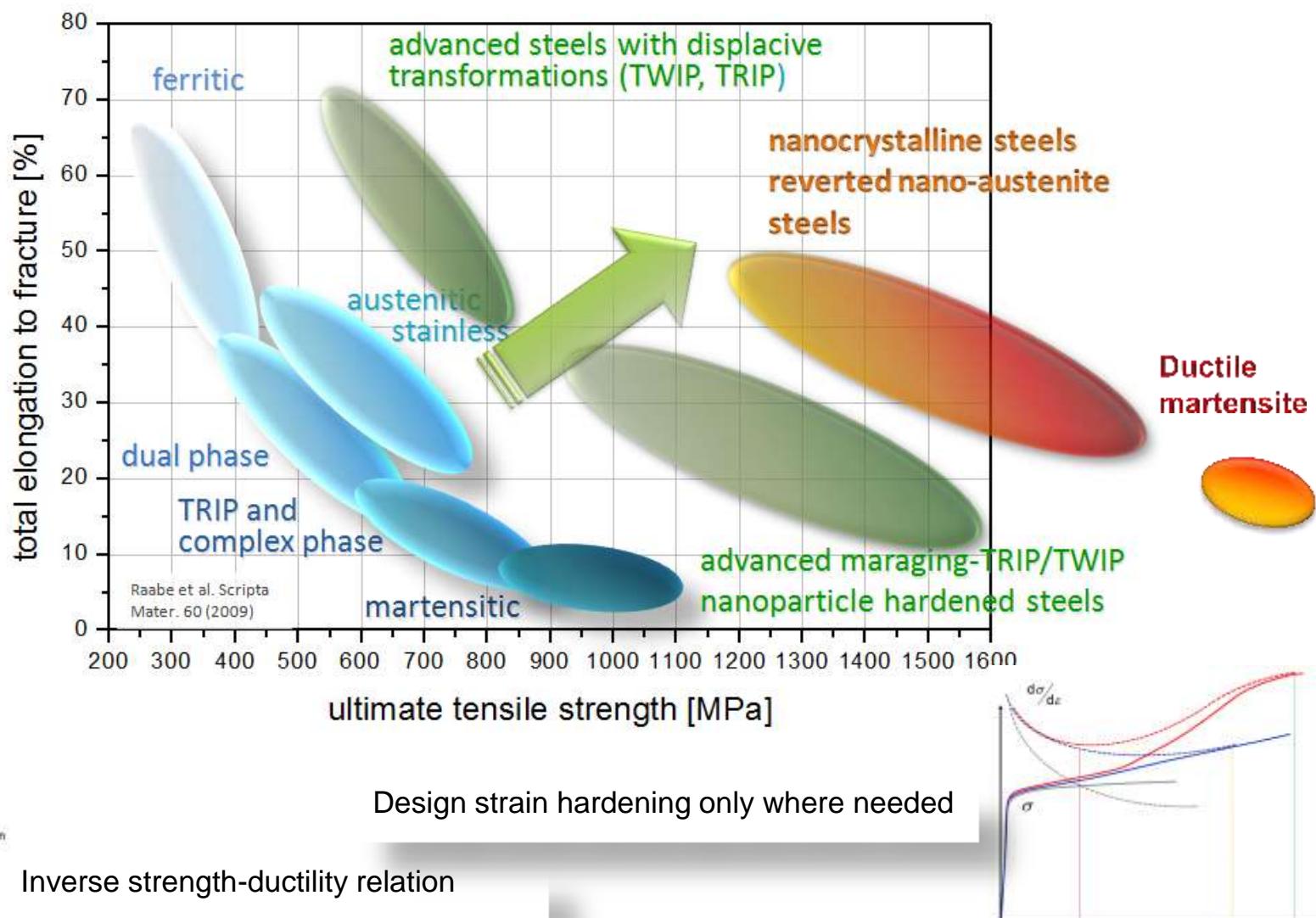


# Inverse strength-ductility: phenomenological analysis





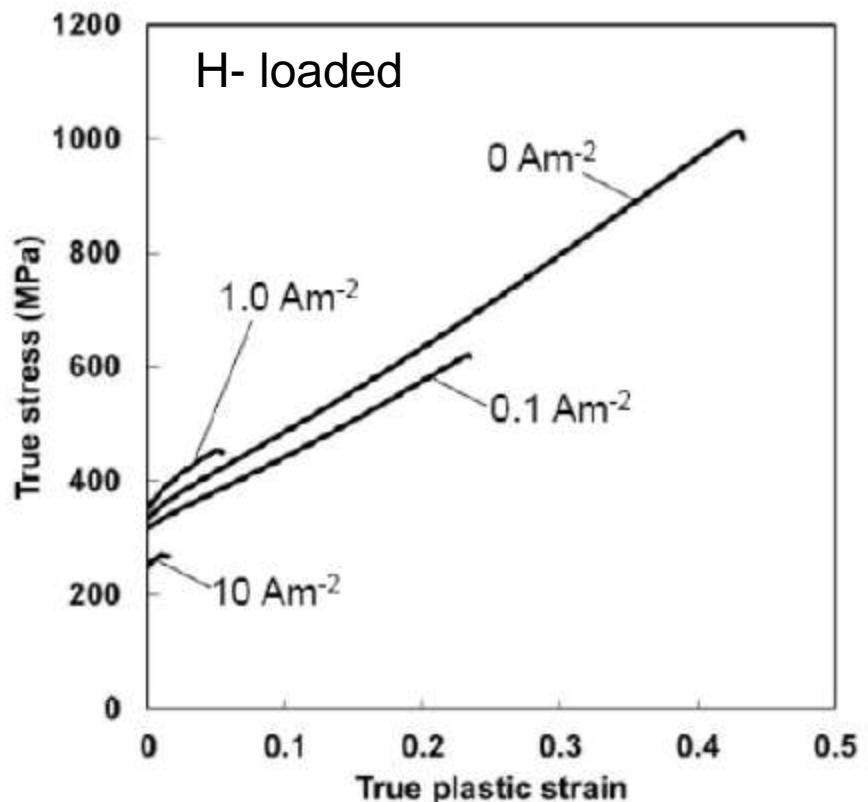
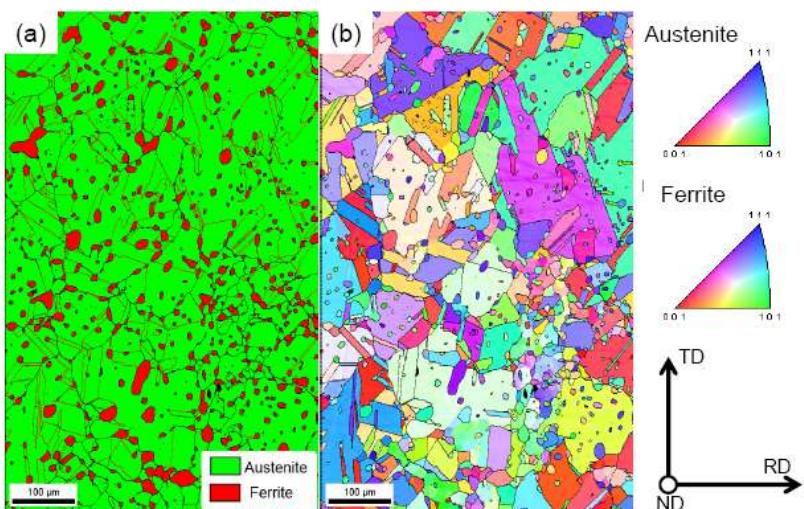
# Local phase transformations enable high strength of bulk metals



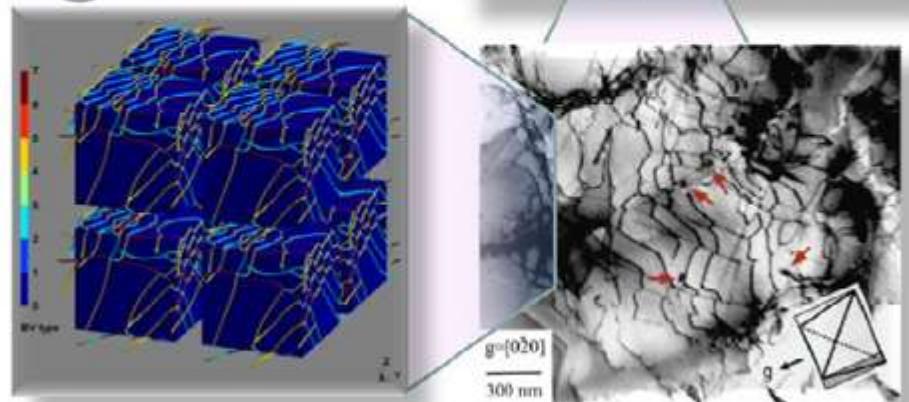
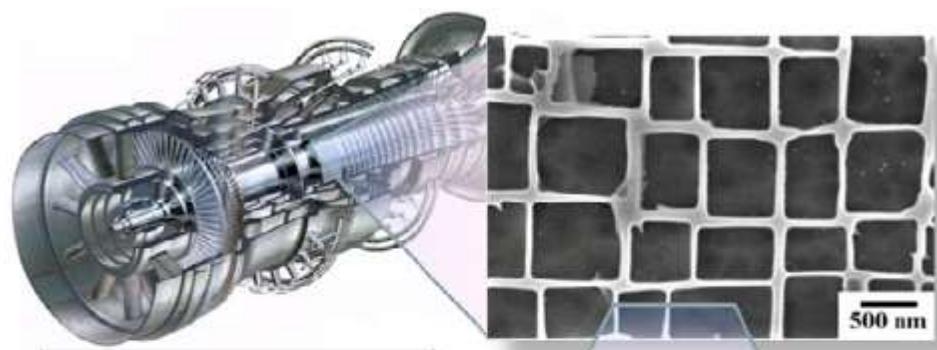
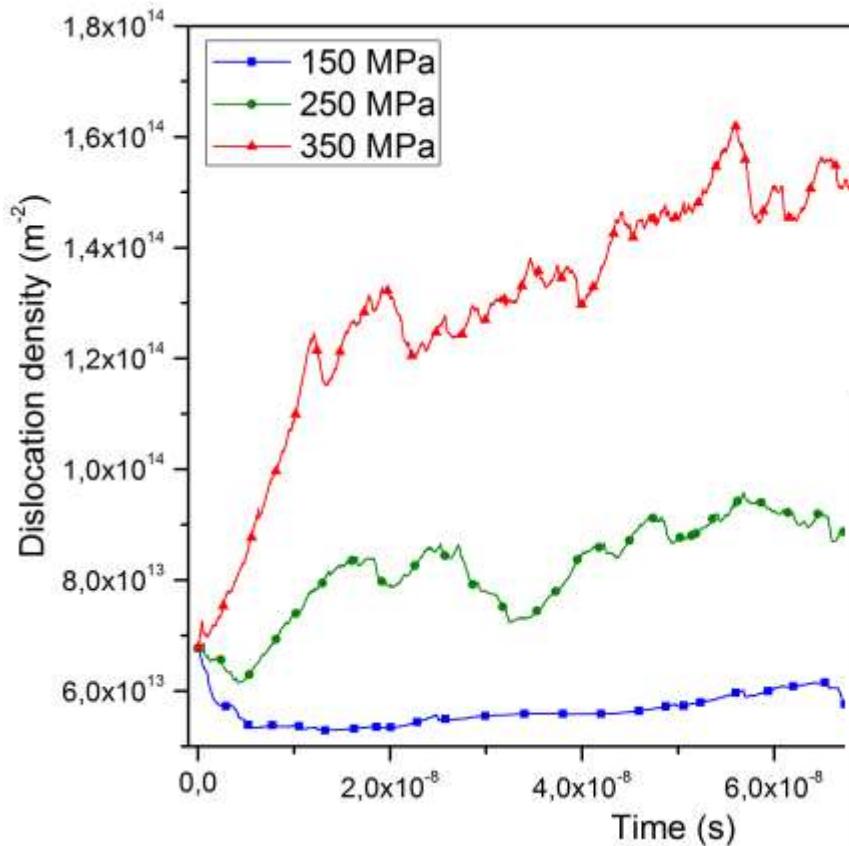


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## Fe-24Mn-0.5C-8.6Al (wt%)



# Example of Discrete Dislocation Dynamics in 3D: superalloys



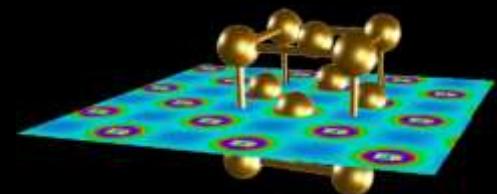


- **Introduction to the scales**
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- **Quantum mechanics primer**





- **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

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

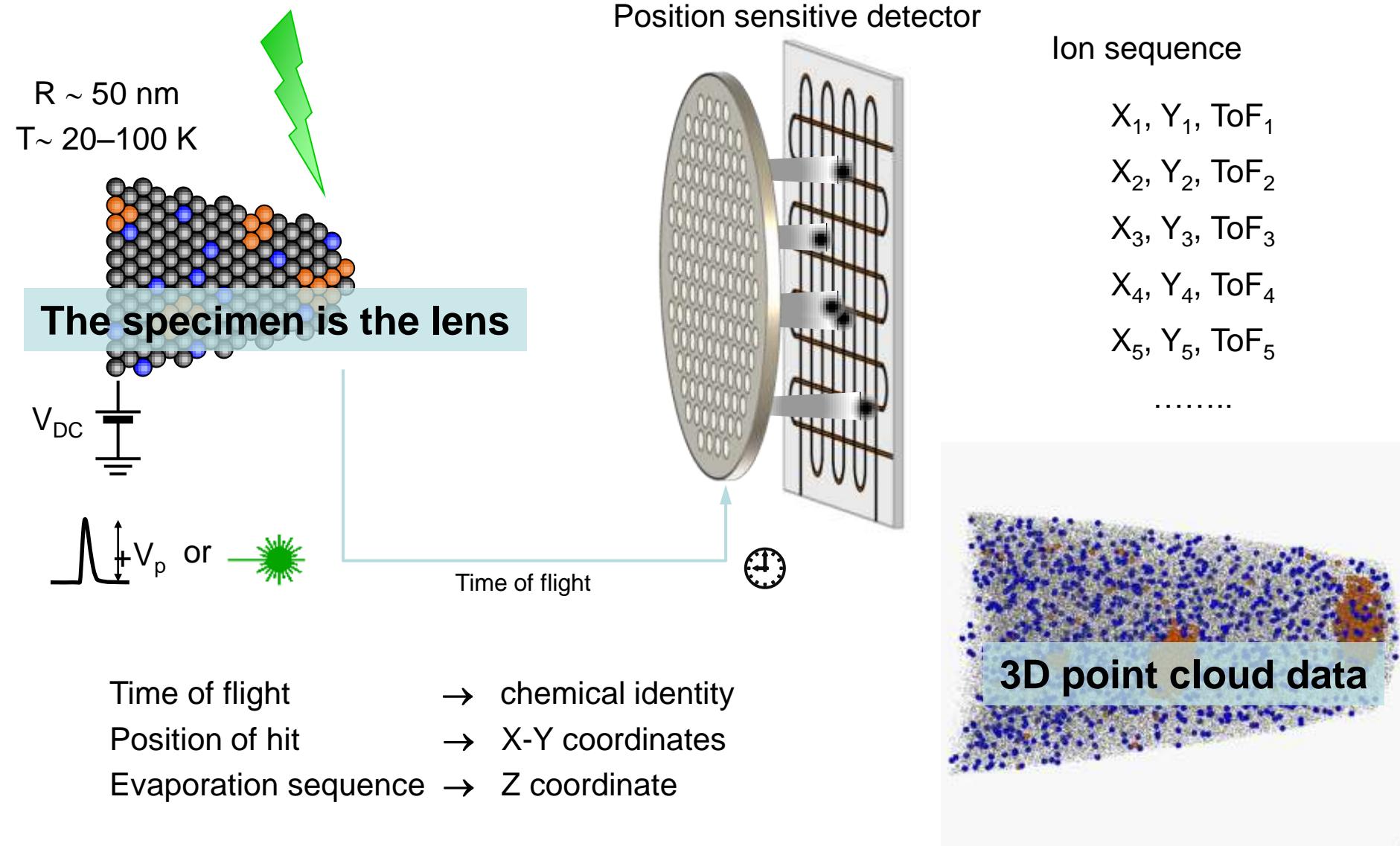
Electrons

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

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)

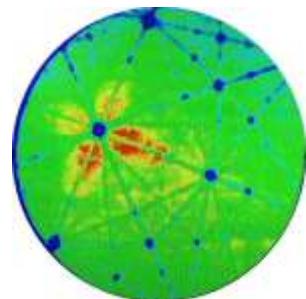
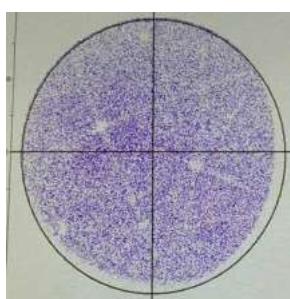
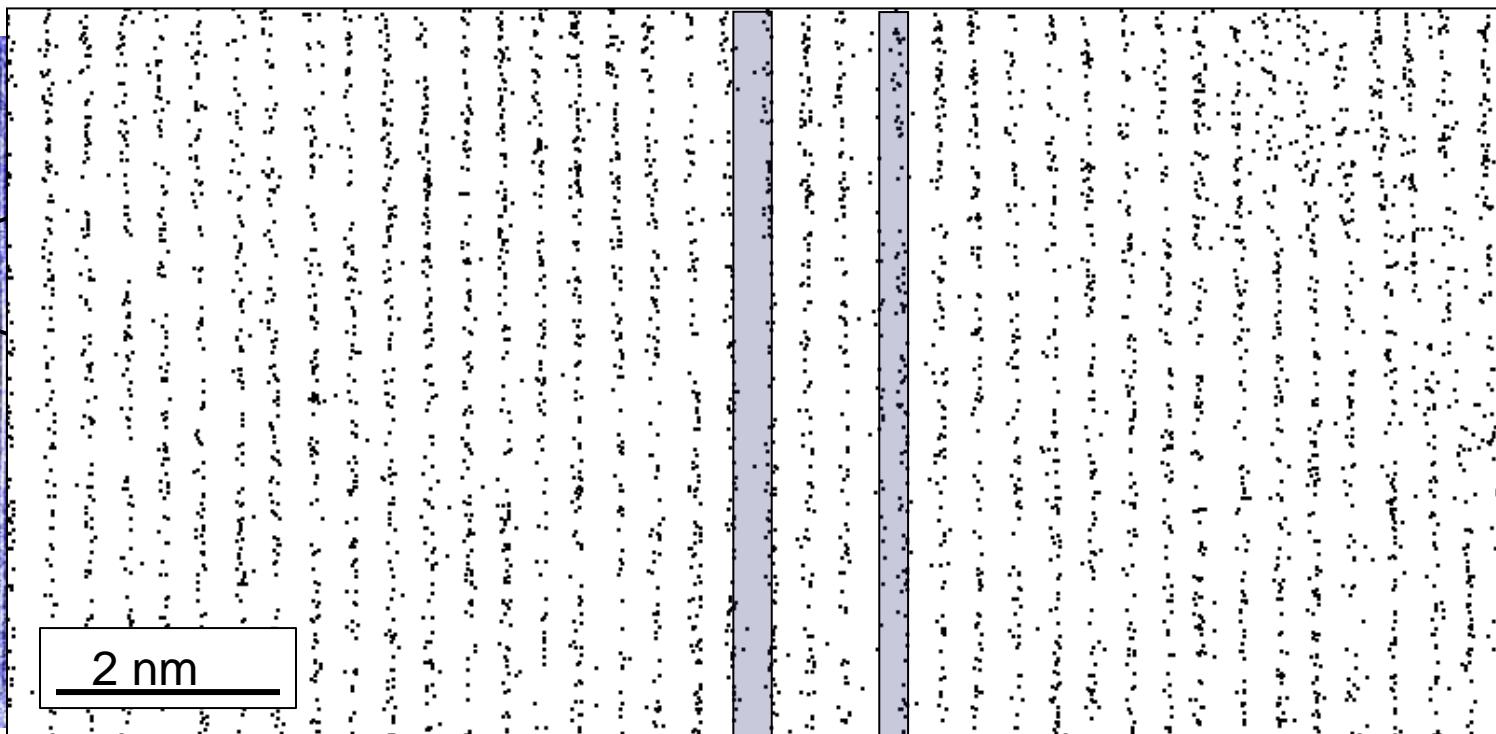


# Lattice plane reconstruction: APT crystallography



Fe<sub>3</sub>Al (only Al displayed)

0.33 nm 0.25 nm



Atom probe crystallography:  
Chemistry and structure in 3D

[1-12]  
[1-10]  
[111]

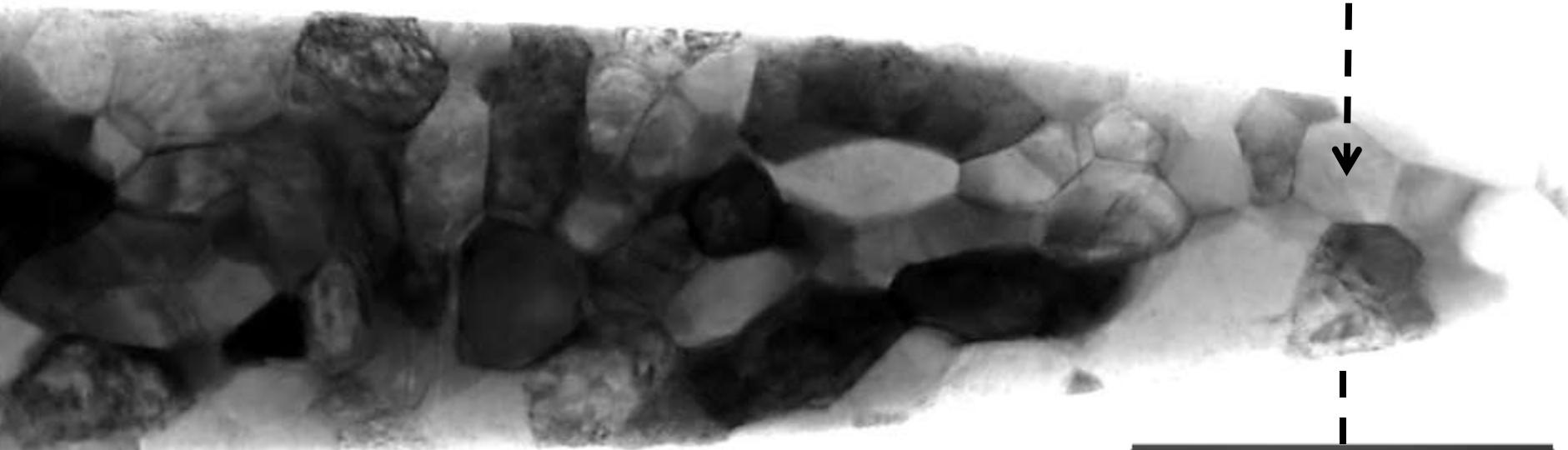
# Correlative TEM-APT probe for 5D GB segregation analysis



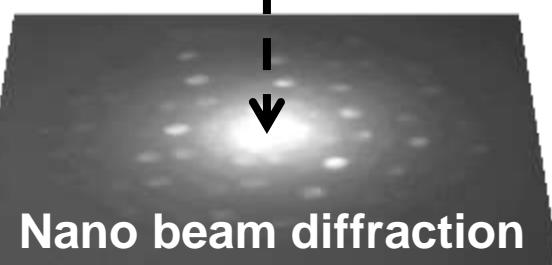
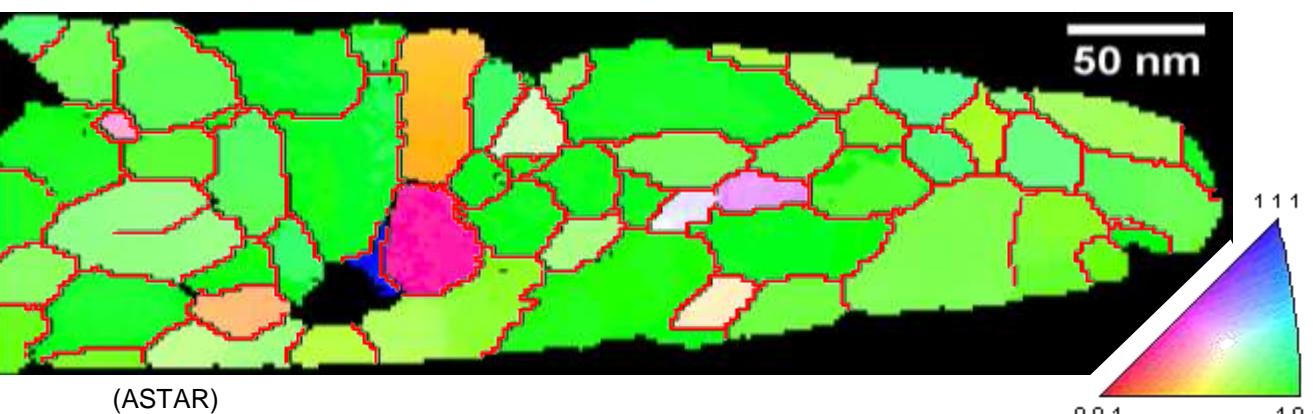
BF-STEM micrograph of cold-drawn Fe-C

100 nm

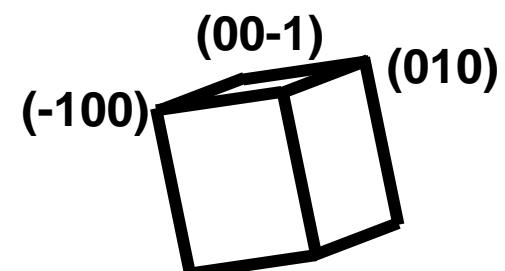
e<sup>-</sup> beam



Scanning nano beam diffraction



Nano beam diffraction

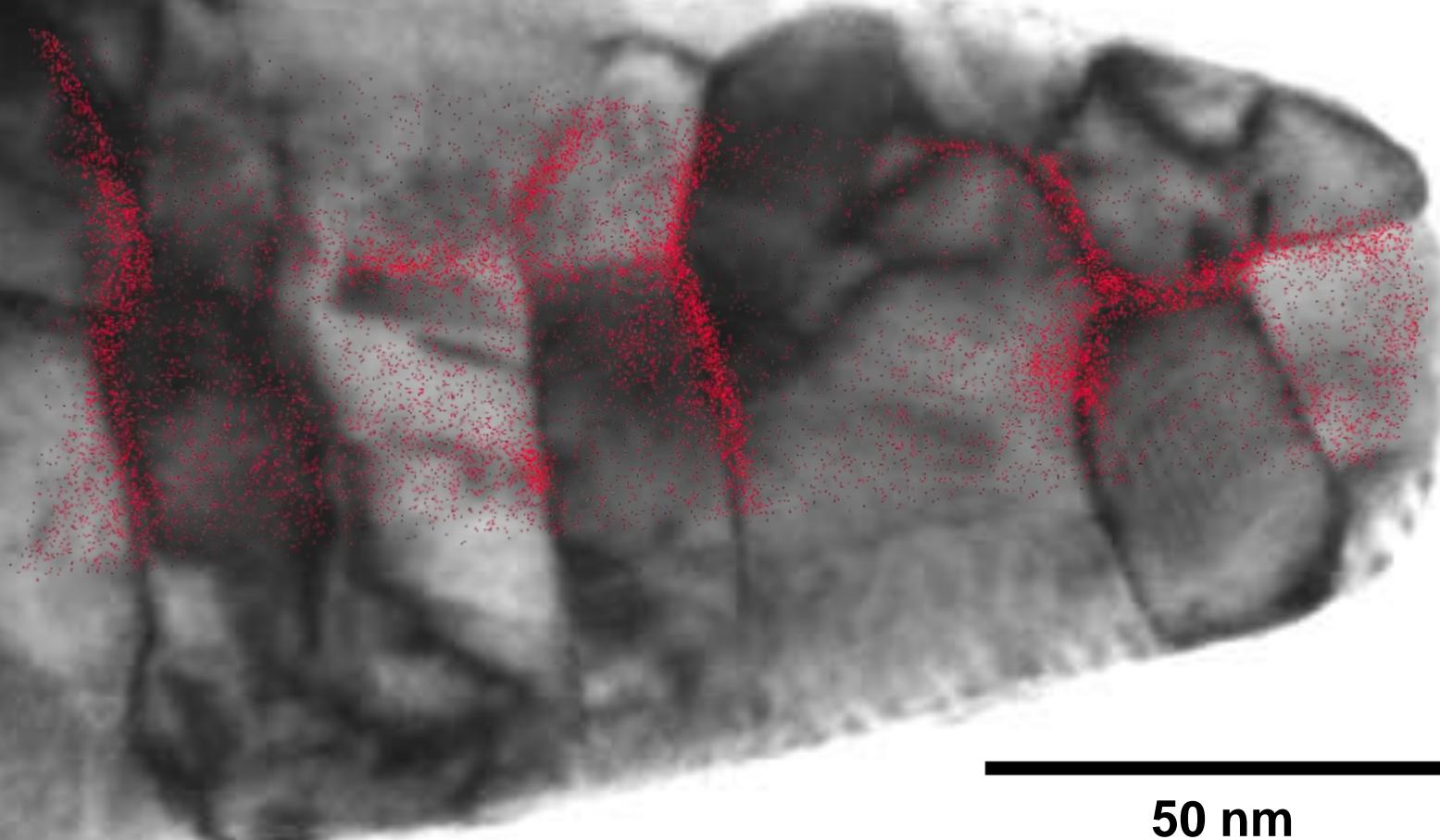


# Correlative TEM-APT probe for 5D GB segregation analysis



● Carbon atoms

5 crystal. parameters  
N chemical species



Kuzmina et al. Science 349, 1080 (2015)

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

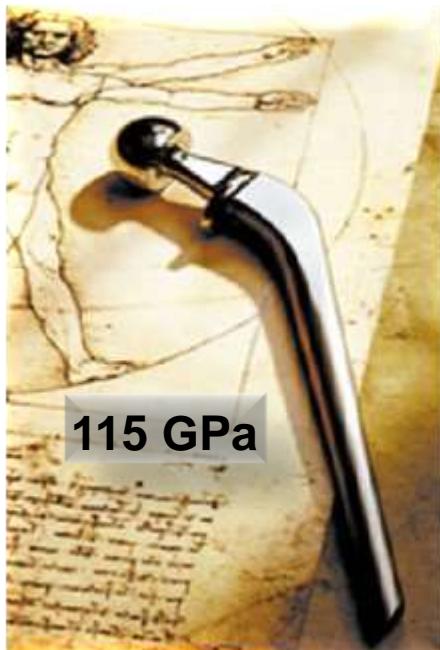
**Health:** Titanium

**Mobility:** Steel





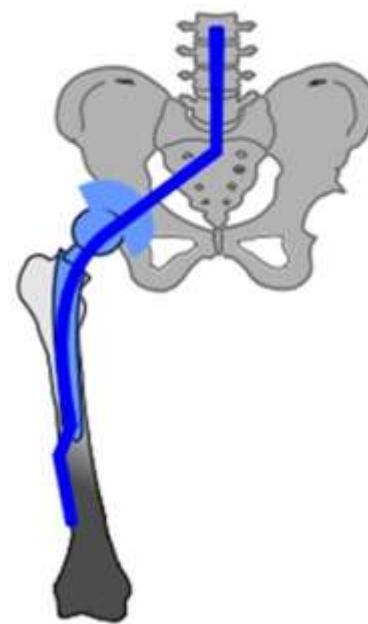
20-25 GPa



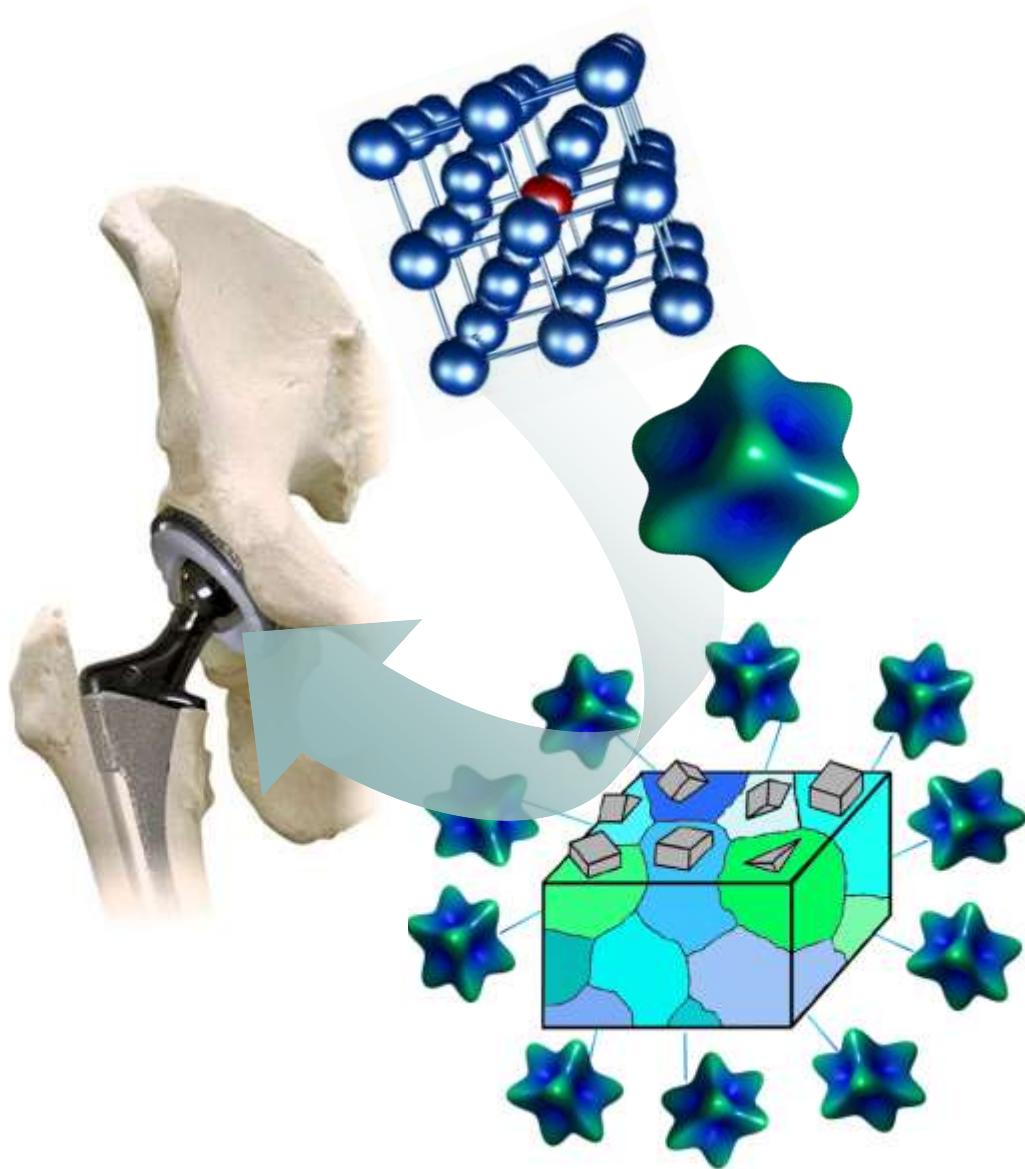
Medscape®

<http://www.medscape.com>

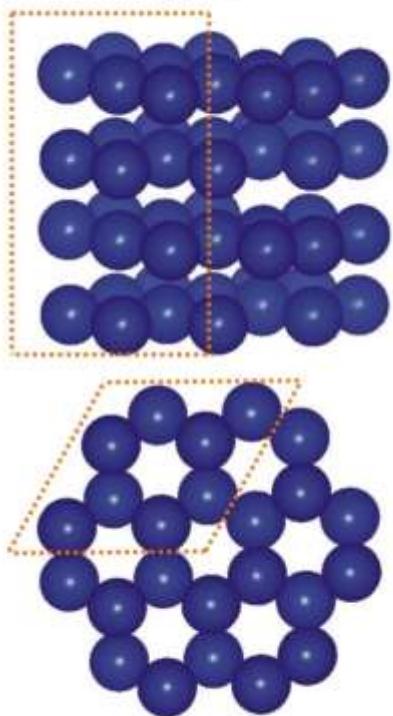
**Spannungs-Abschattung (Stress shielding)**  
**Elastische Fehlpassung:**  
**Knochenuflösung, Abrasion, Entzündung**



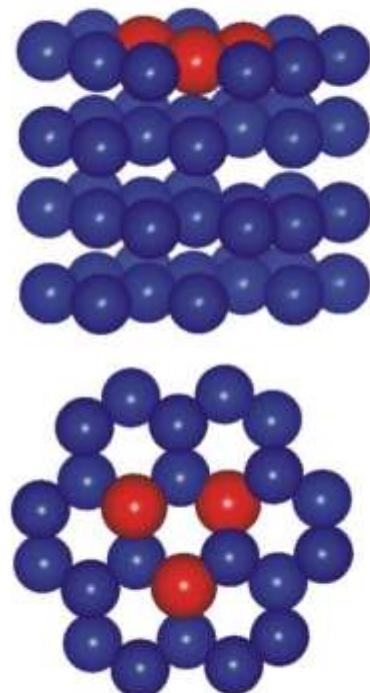
# ab-initio Simulation of elastic stiffness



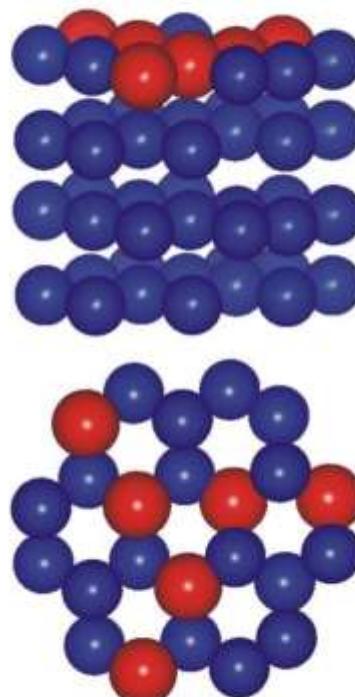
Ti hcp phase



15/1 Ti:X ratio

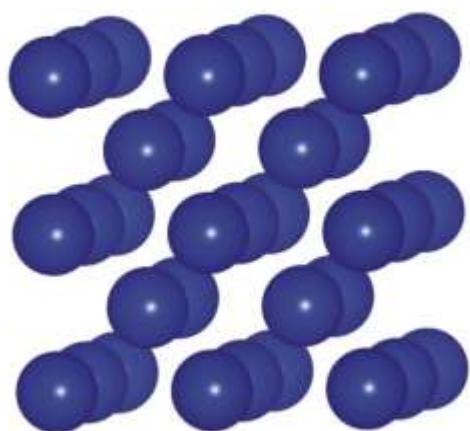


14/2 Ti:X ratio



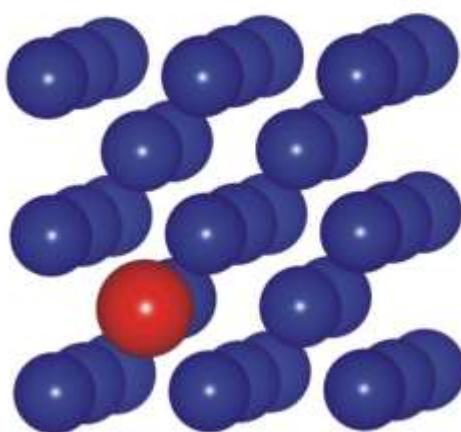
# Construct binary alloys in the cubic phase

Ti bcc phase



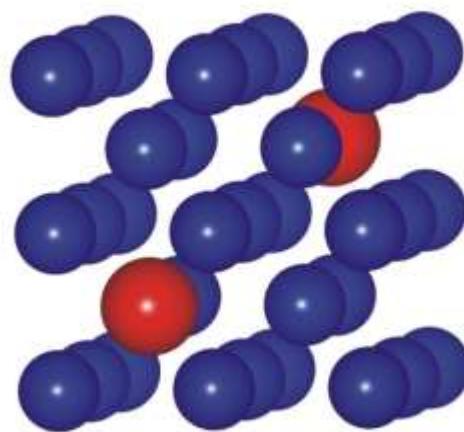
Ti atoms

15/1 Ti:X ratio

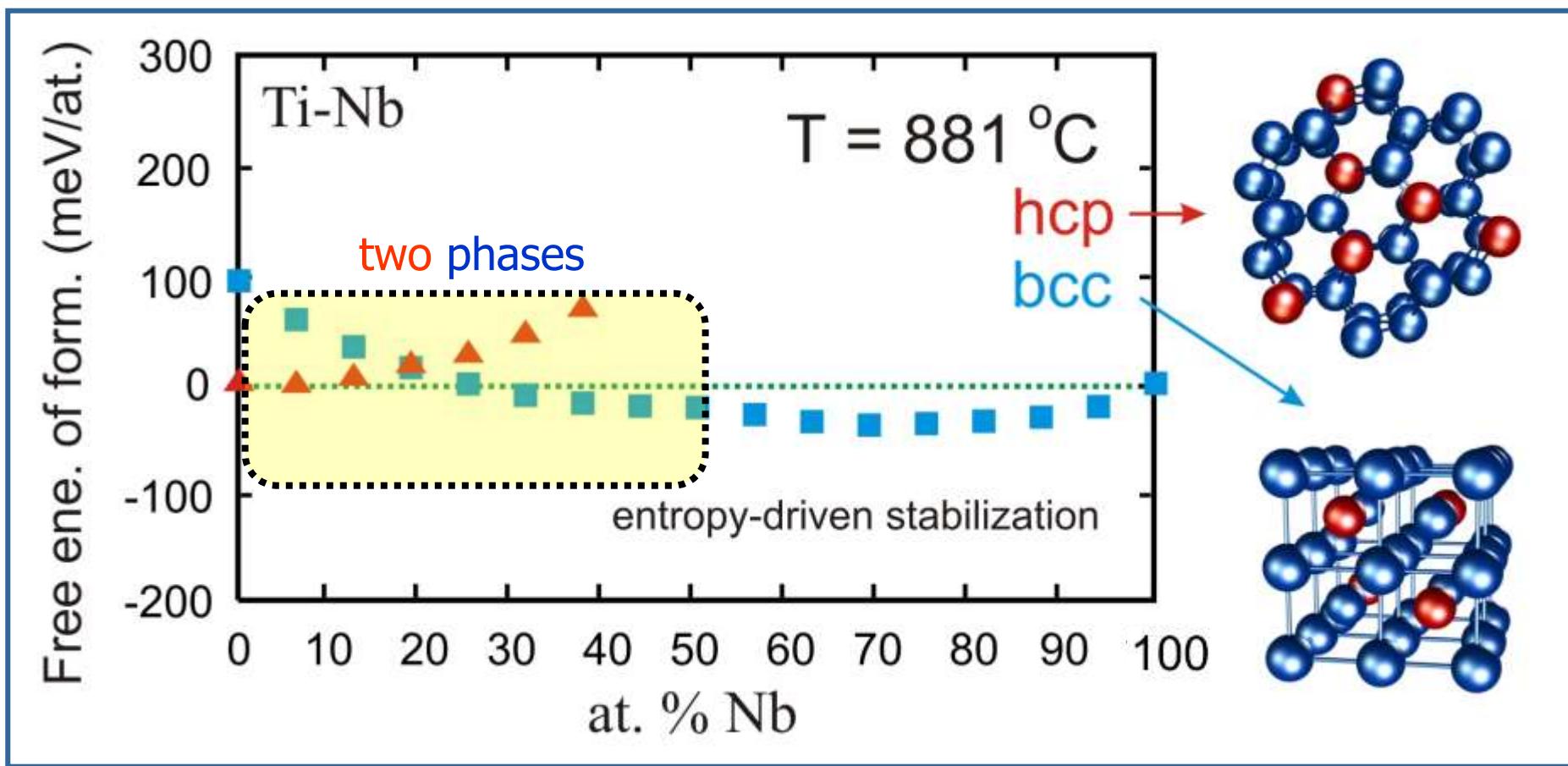


substituent X

14/2 Ti:X ratio



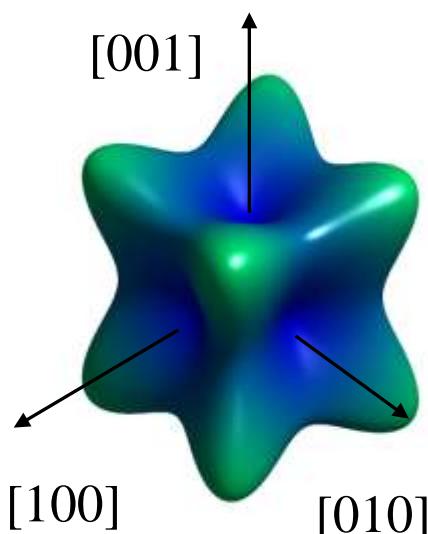
$$\text{Free energy } F(x,c,T) = U - T \cdot S$$



## Young's modulus surface plots

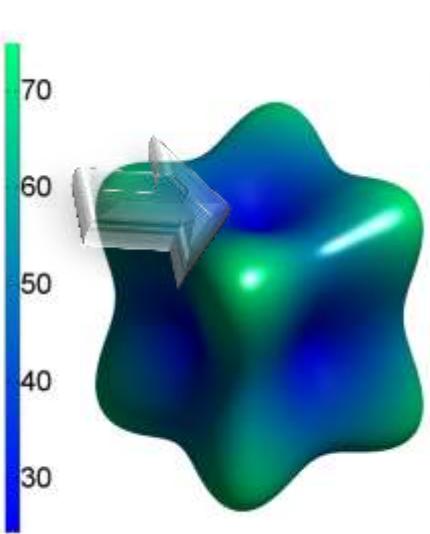
$$A_z = 2 C_{44} / (C_{11} - C_{12})$$

Ti-18.75at.%Nb



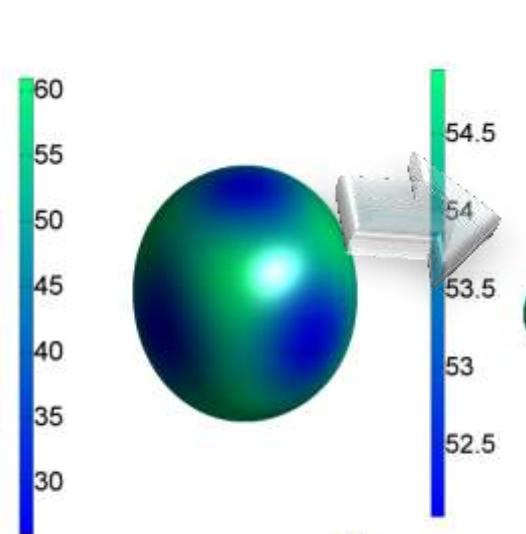
$$A_z = 3.210$$

Ti-25at.%Nb



$$A_z = 2.418$$

Ti-31.25at.%Nb



$$A_z = 1.053$$

Pure Nb



# Ab initio-based development of new alloys

