Microstructure Mechanics of Crystalline Materials

Introduction

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class times

Friday, 10 am – 14 pm at IMM / RWTH

(last class at MPI Düsseldorf)

lecture download page:
http://www.dierk-raabe.com/lectures/
http://www.mpie.de

19. April 2013
26. April 2013
3. May 2013
10. May 2013
31. May 2013
…..

Contents

Further reading

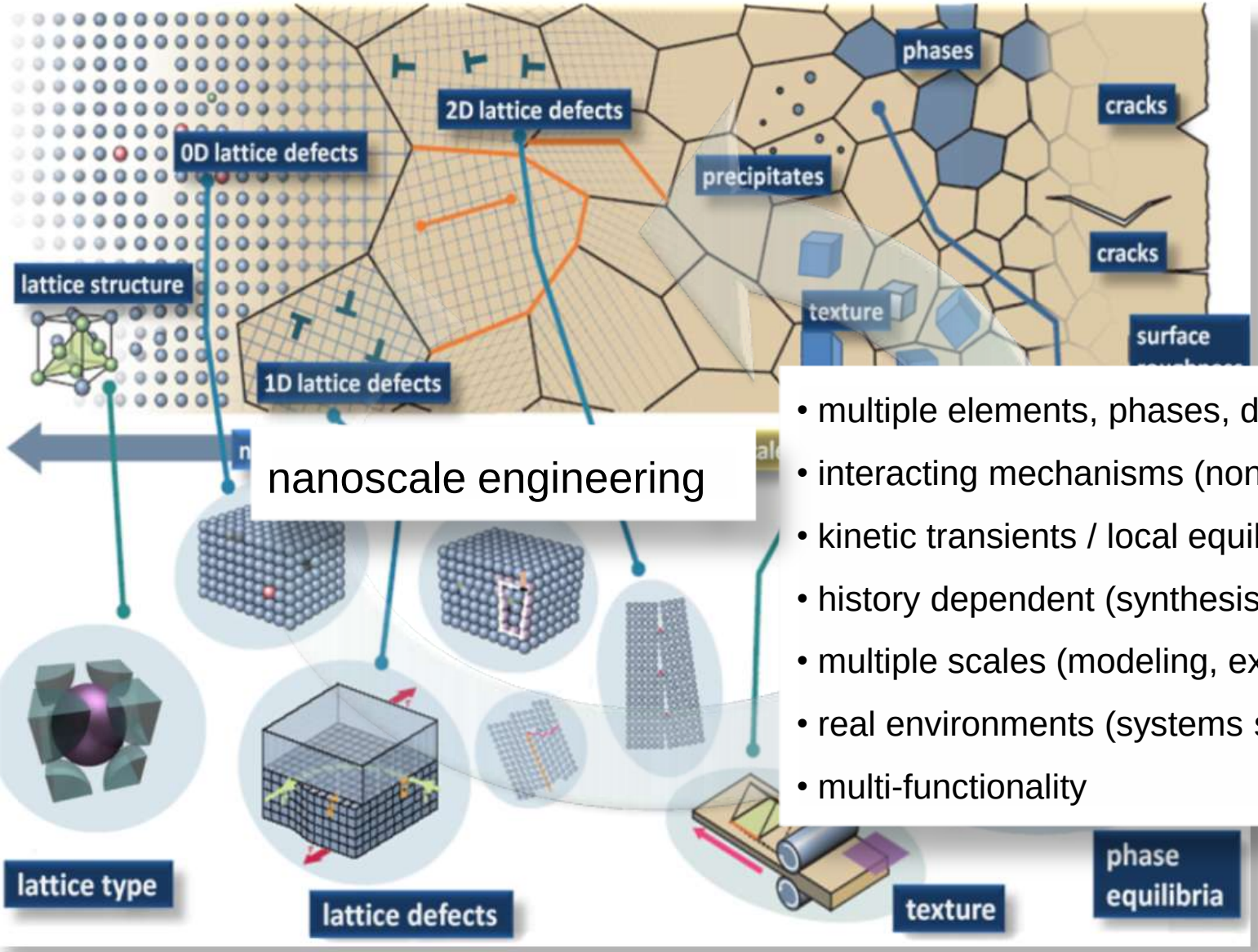
- Gottstein: Physical Metallurgy
- Reed-Hill: Physical Metallurgy Principles
- Hull and Bacon: Introduction to Dislocations, Butterworth-Heinemann
- Hirth and Lothe: Theory of Dislocations

- 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

Overview

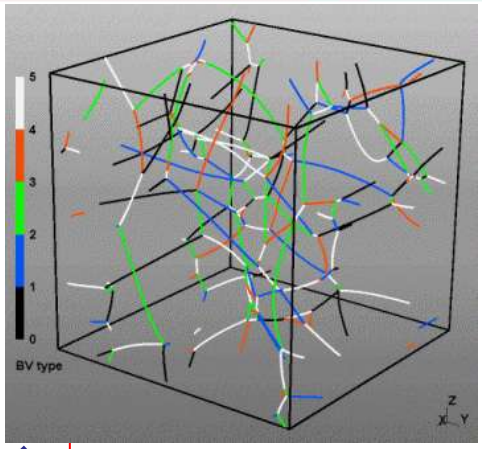
- Introduction to the scales
- Introduction to the engineering background
- Quantum mechanics primer
- Some examples

Scientific mission: complex materials in real environments



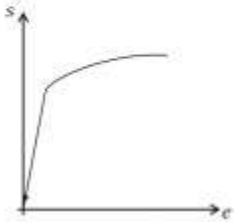
- multiple elements, phases, defects
- interacting mechanisms (non-linearity)
- kinetic transients / local equilibrium
- history dependent (synthesis, processing)
- multiple scales (modeling, experiment)
- real environments (systems science)
- multi-functionality

Inverse strength-ductility: phenomenological analysis



$\mathrm{d}\sigma/\mathrm{d}\varepsilon$

σ

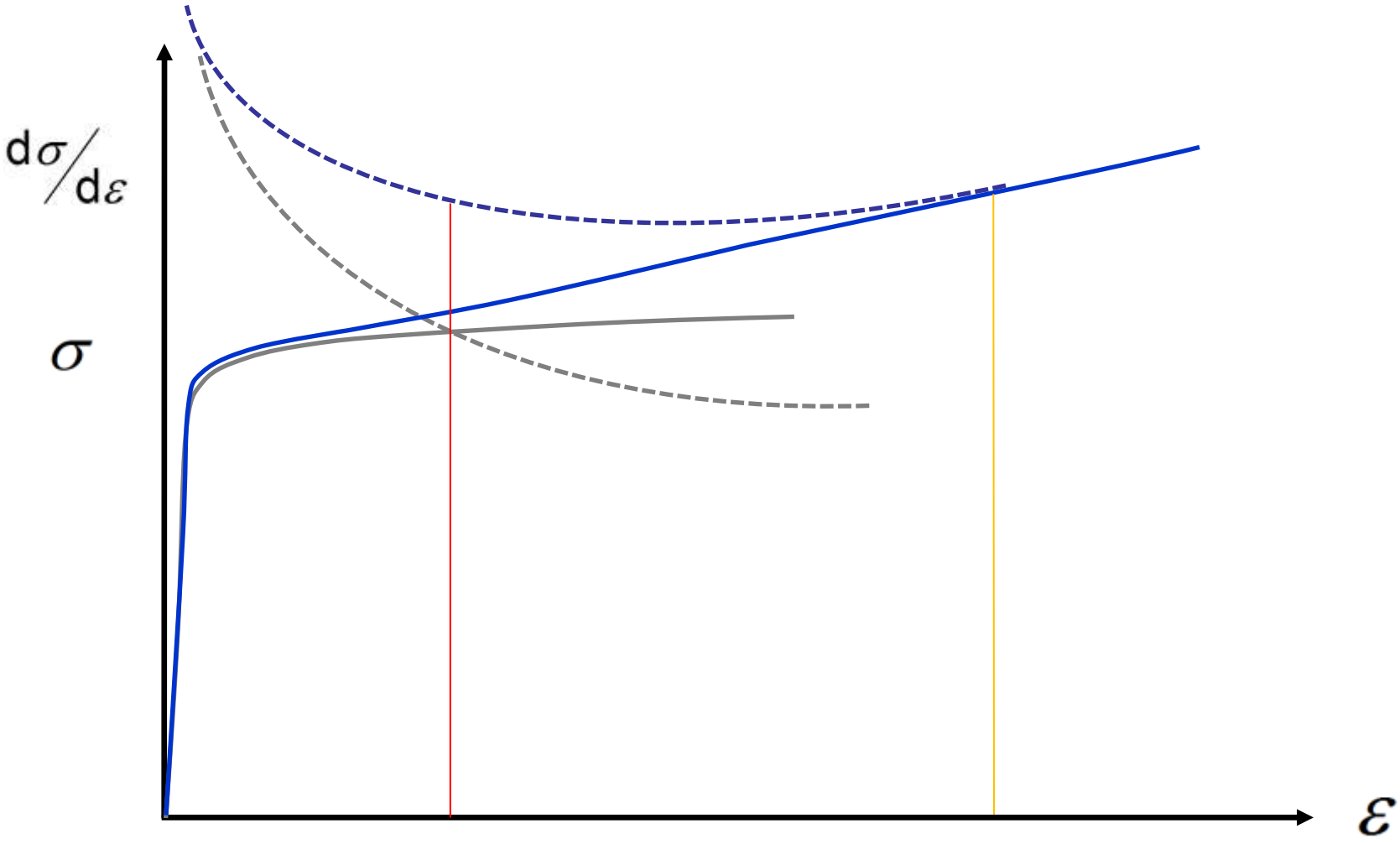


ε true strain

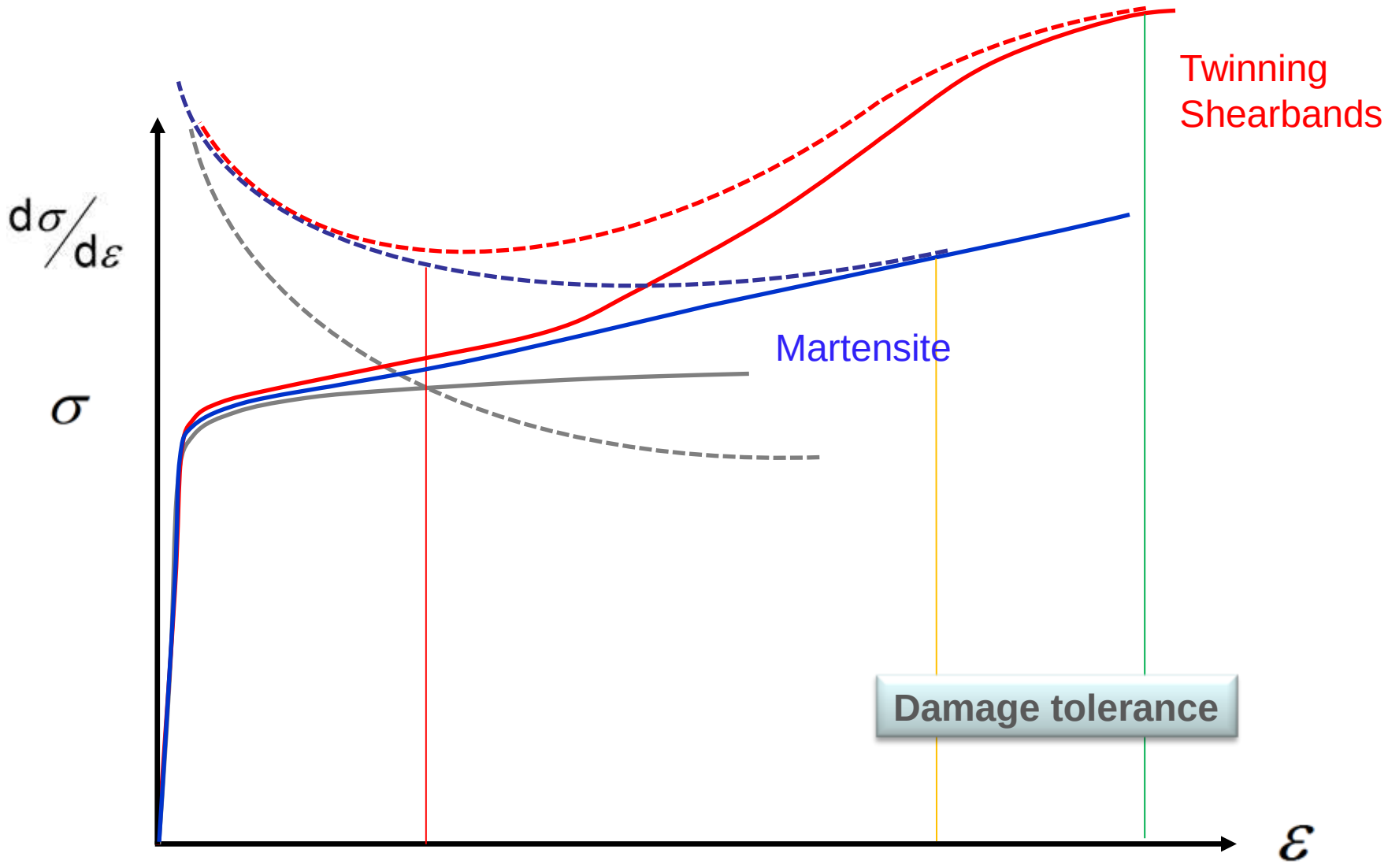
σ stress

ε

Inverse strength-ductility: phenomenological analysis

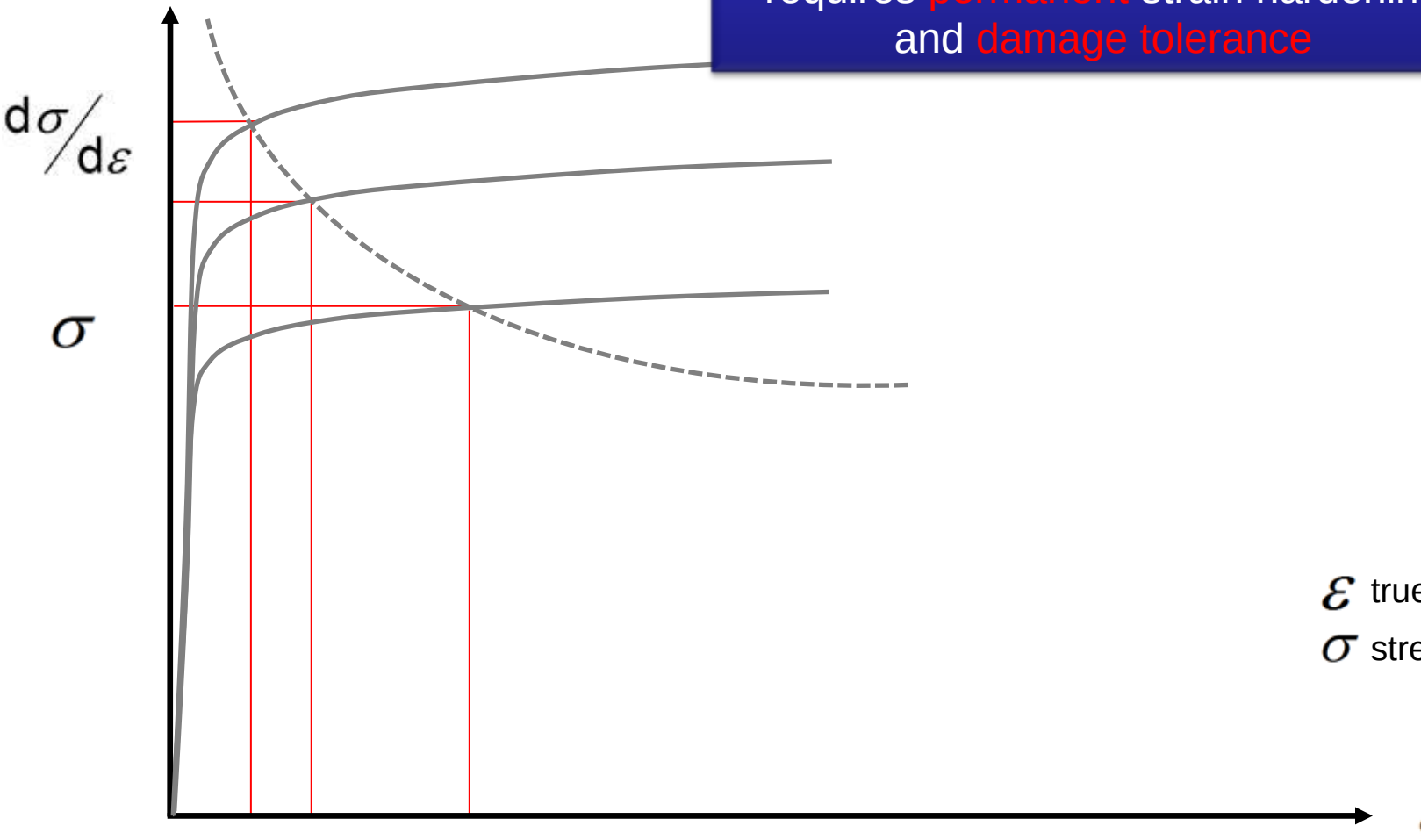


Inverse strength-ductility: phenomenological analysis



Inverse strength-ductility: phenomenological analysis

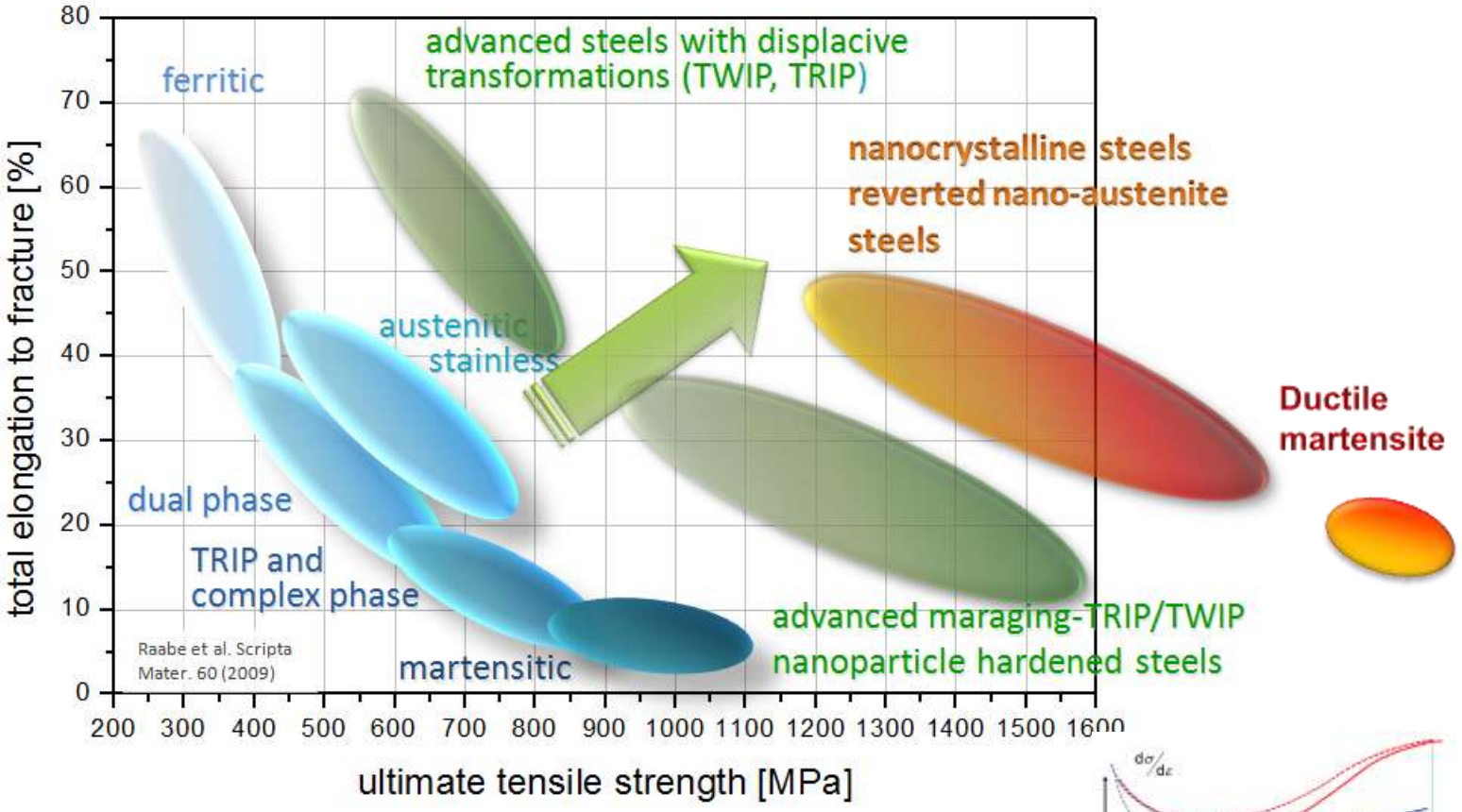
Design of ductile high strength alloys requires permanent strain hardening and damage tolerance

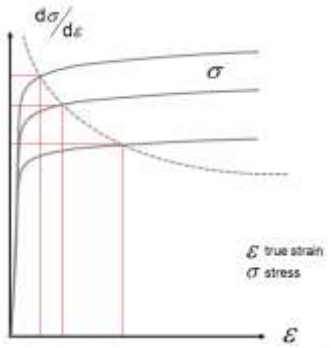


ε true strain

σ stress

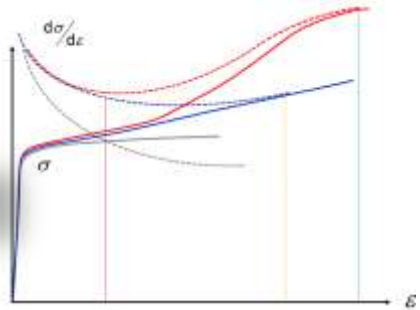
Local phase transformations enable high strength of bulk metals



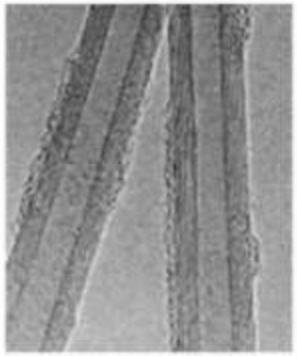


Inverse strength-ductility relation

Design strain hardening only where needed



Understanding the nanoscopic length scales and their effects



carbon nanotube
as size reference
(same scale bar)

wire drawing axis

10 nm

C isosurface (7 at.%)

C C2 C3 C4

Fe

remaining
cementite after wire
heavy drawing

carbon-
enriched ferrite

Ductile
martensite

Nano-
pearlite

> 6 GPa

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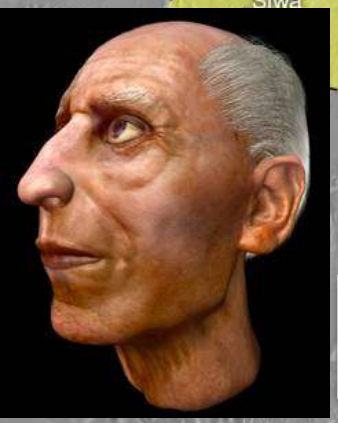
Dawn of the iron age in the mediterranean

37000 soldiers,
Hittite and other kingdoms

Hittite empire: iron age

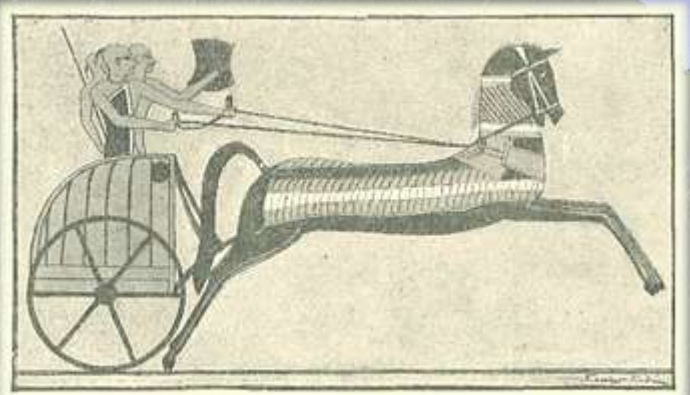
1274 BC:
Iron weapons
Large chariots



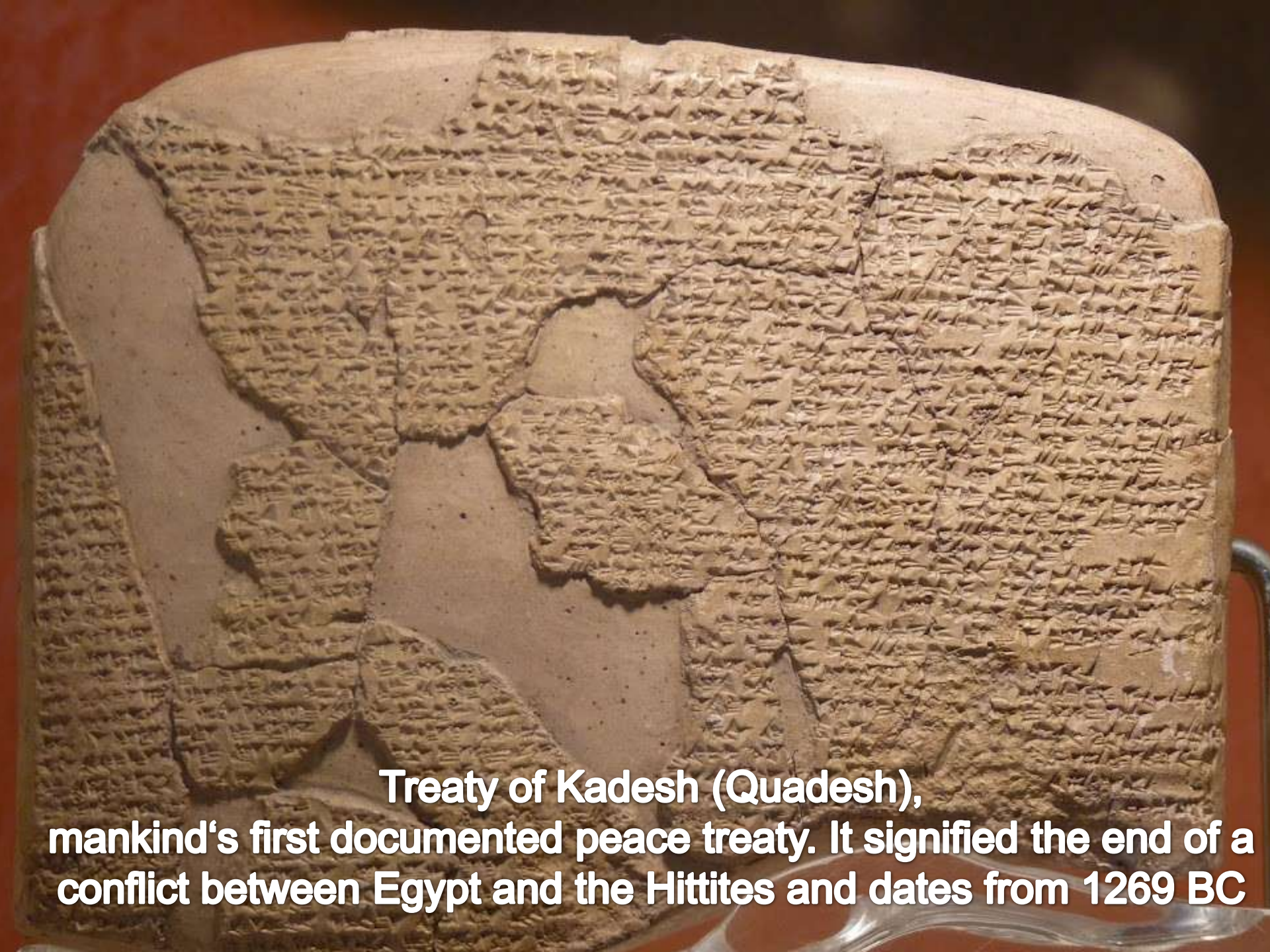
Ramses II.

Egypt empire: bronze age

20000 soldiers, 4 divisions
largest egypt army ever



A HITTITE CHARIOT WITH ITS THREE OCCUPANTS.[1]



Treaty of Kadesh (Quadesh),
mankind‘s first documented peace treaty. It signified the end of a conflict between Egypt and the Hittites and dates from 1269 BC

Answering societies' grand challenges with complex alloys

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

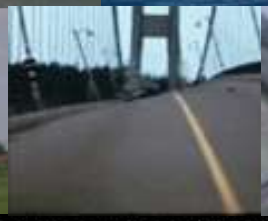
Complex Materials occupy key roles
(energy, transportation, health, safety, infrastructure)

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

Our mission: Understanding and designing complex materials and mechanisms for real environments from first principles



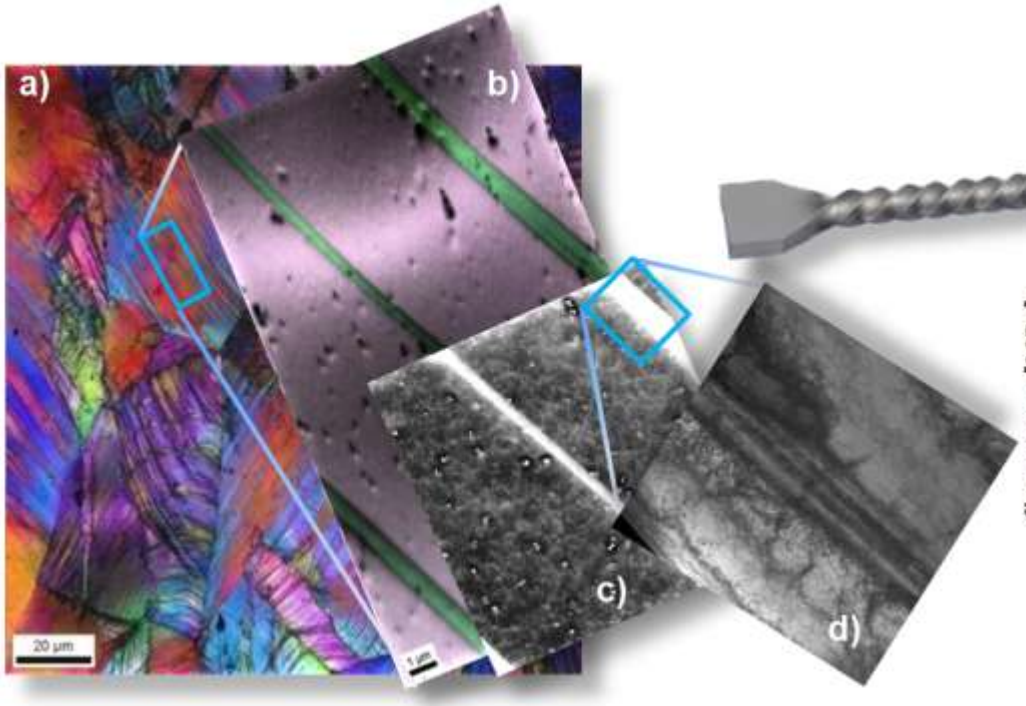


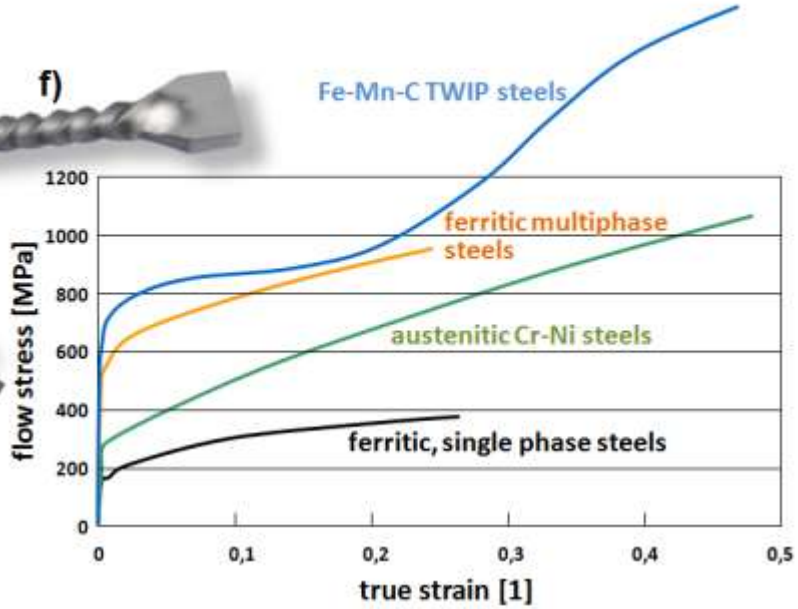


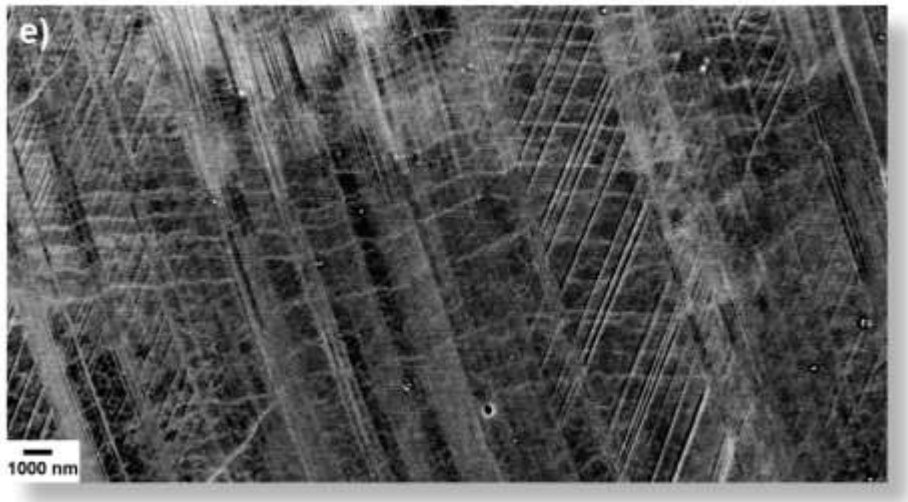
New materials for key technologies: mobility on land and water

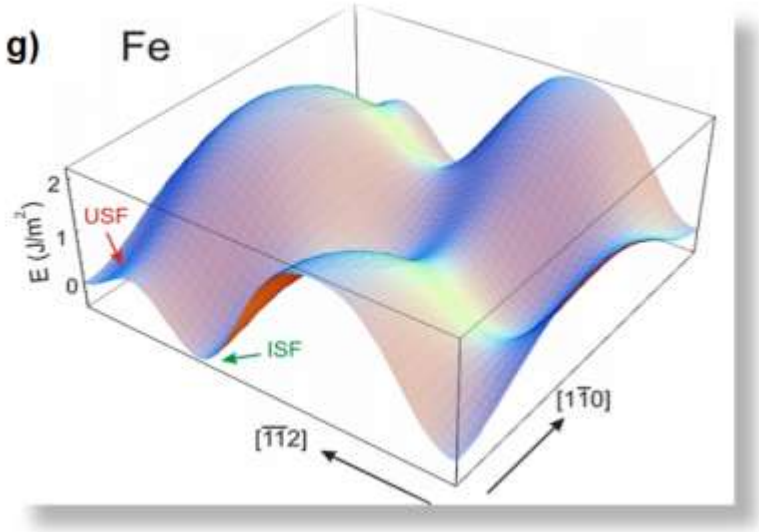
Steels
Magnesium
Aluminium
Titanium

Ab initio-based development of new alloys



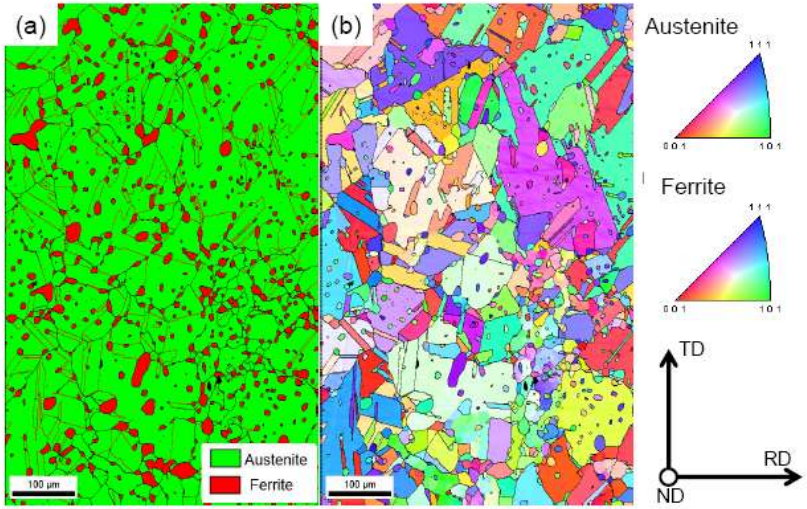


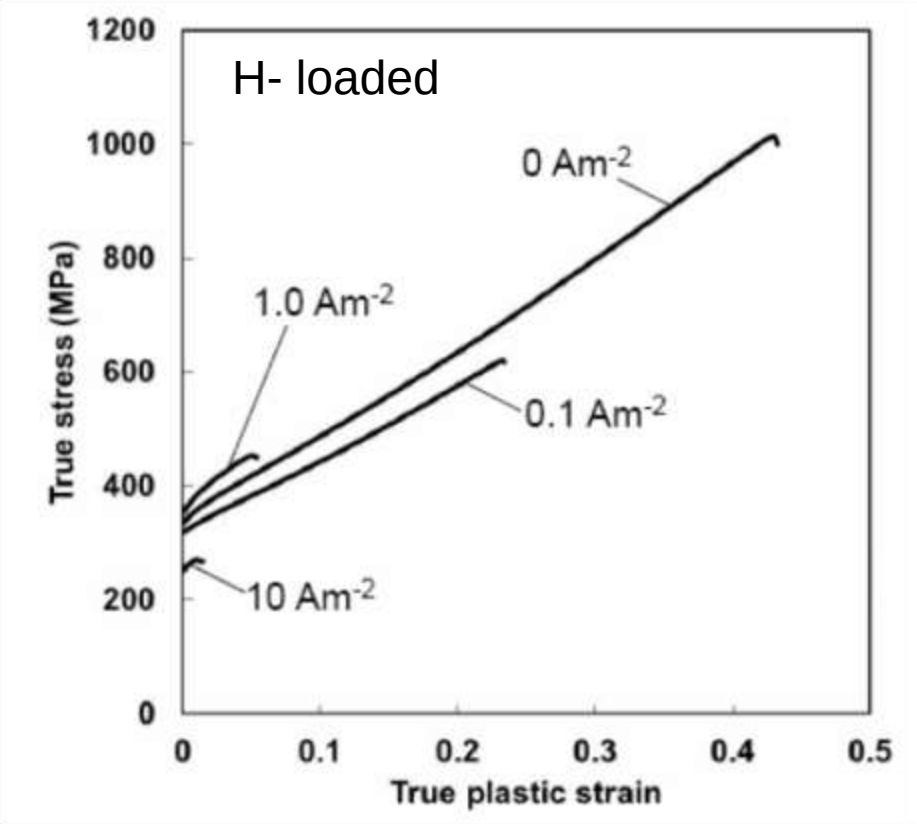




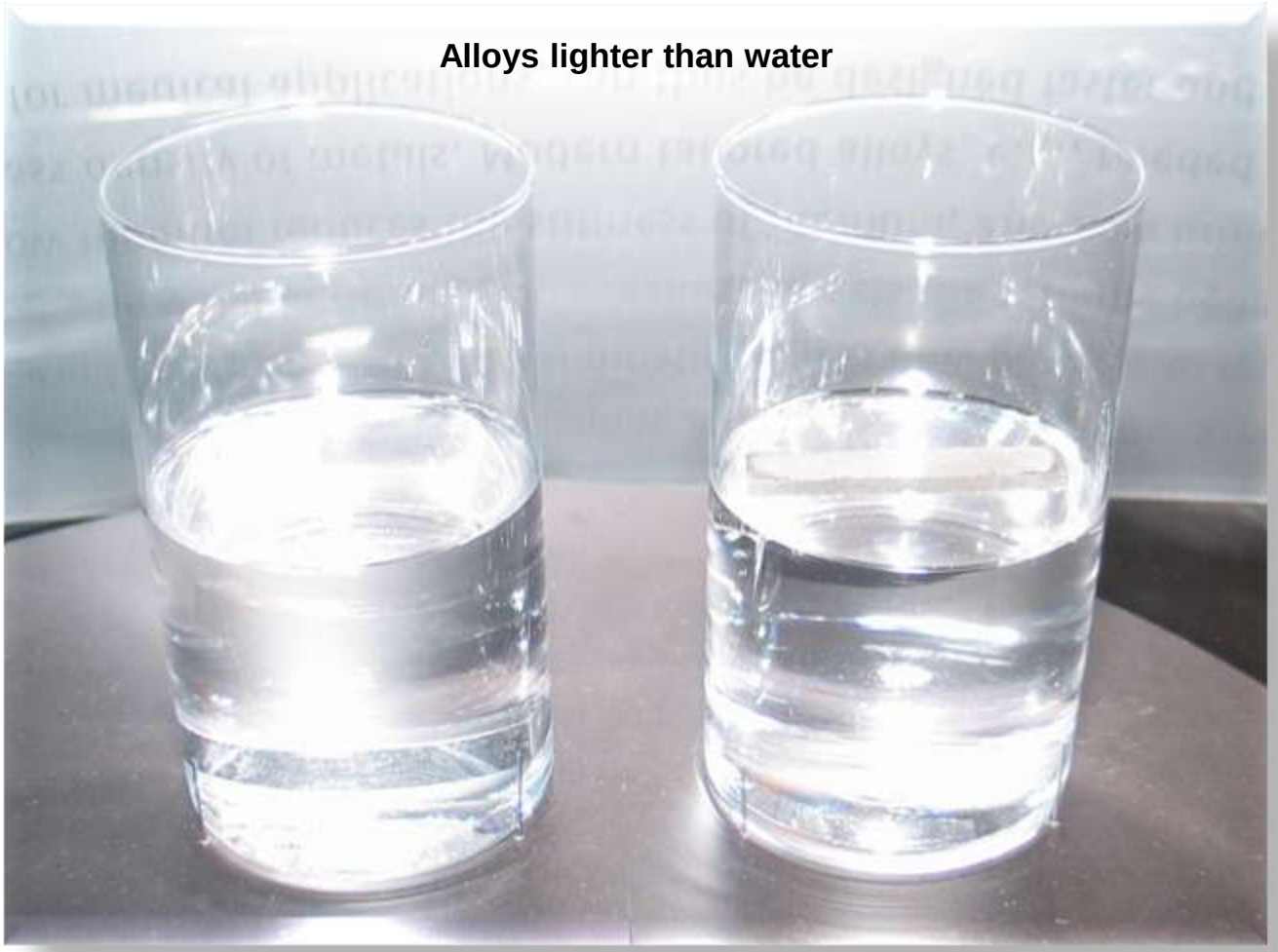
Rapid alloy prototyping: applied to TRIPLEX Fe-Mn-Al-C steels

Fe-24Mn–0.5C–8.6Al (wt%)

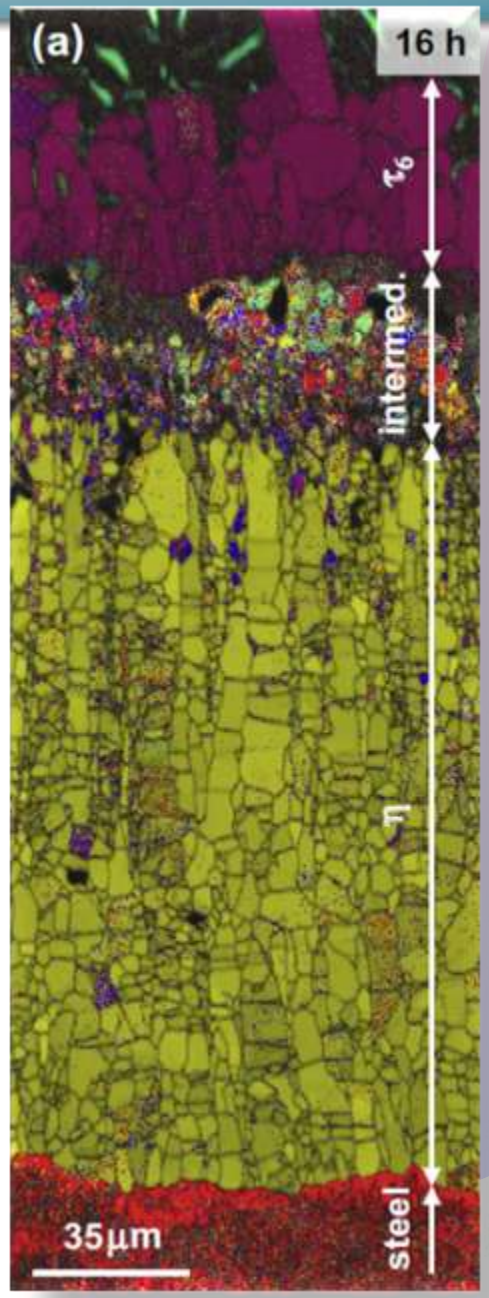




MPIE research focus: areas of high expertise



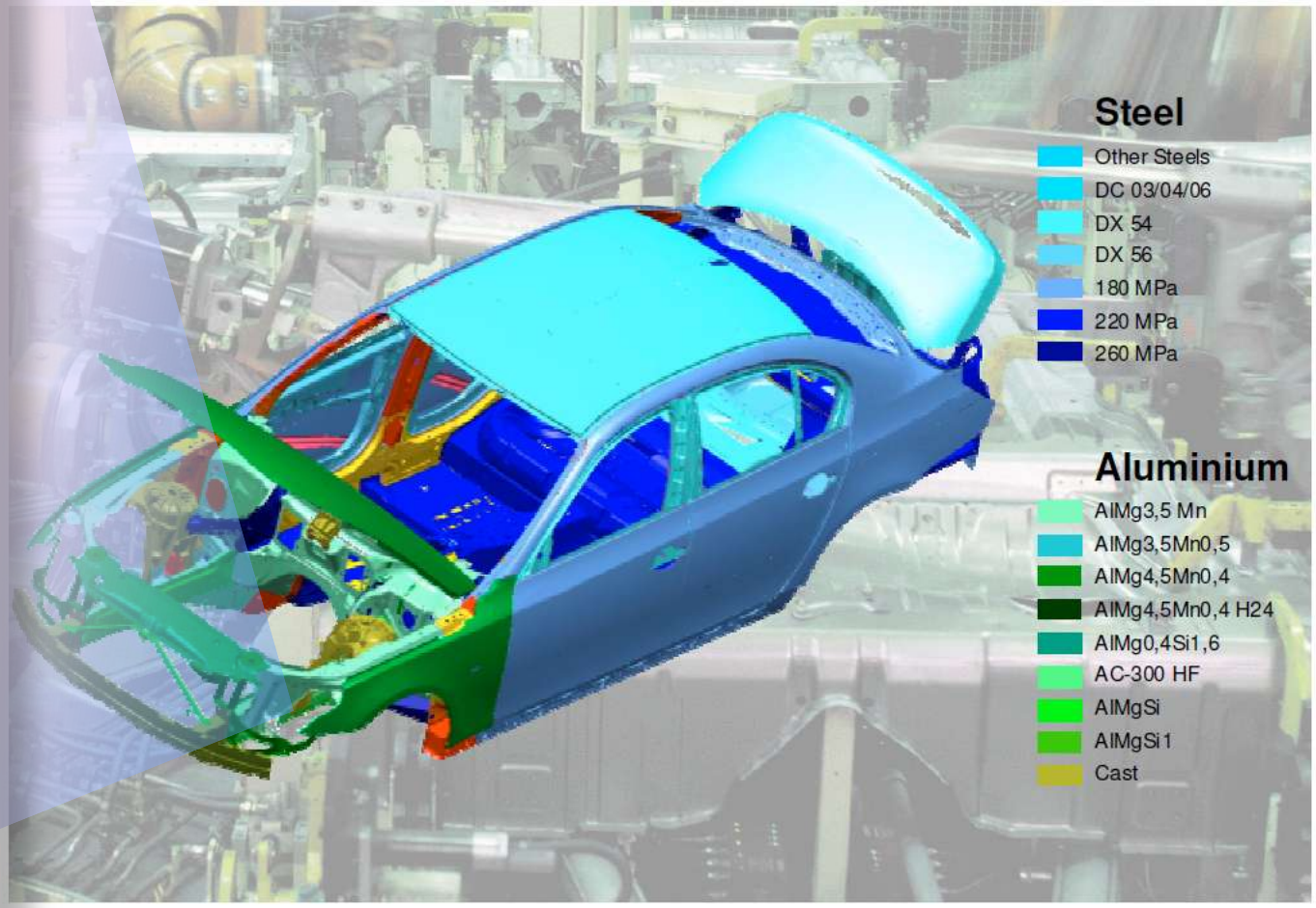
New materials automotive (courtesy BMW)



Car Body Structure.

Aluminium Front End / Steel passenger Cab.

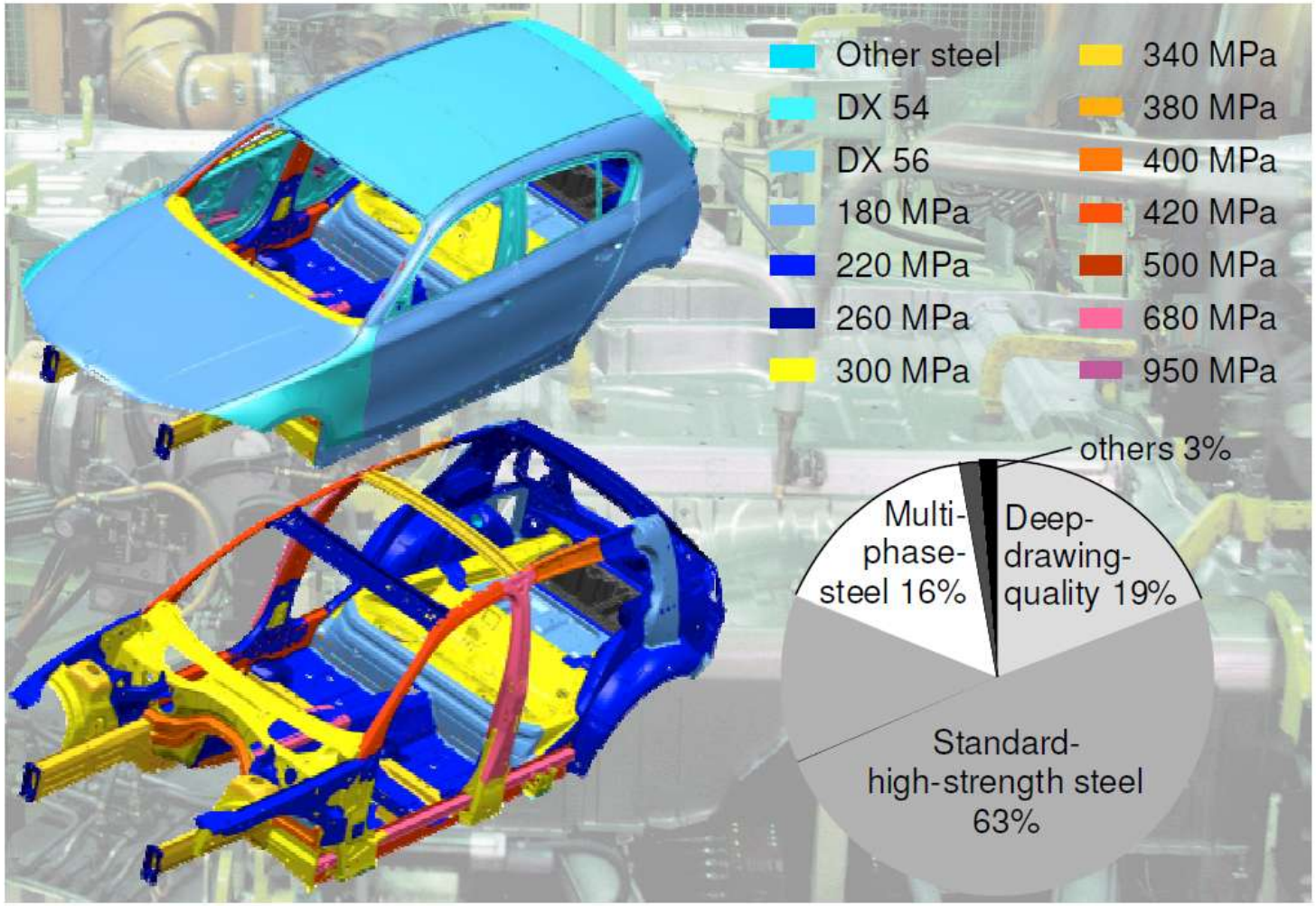
BMW 5 Series.



Car Body Structure.

High Strength Steel.

BMW 1 Series.

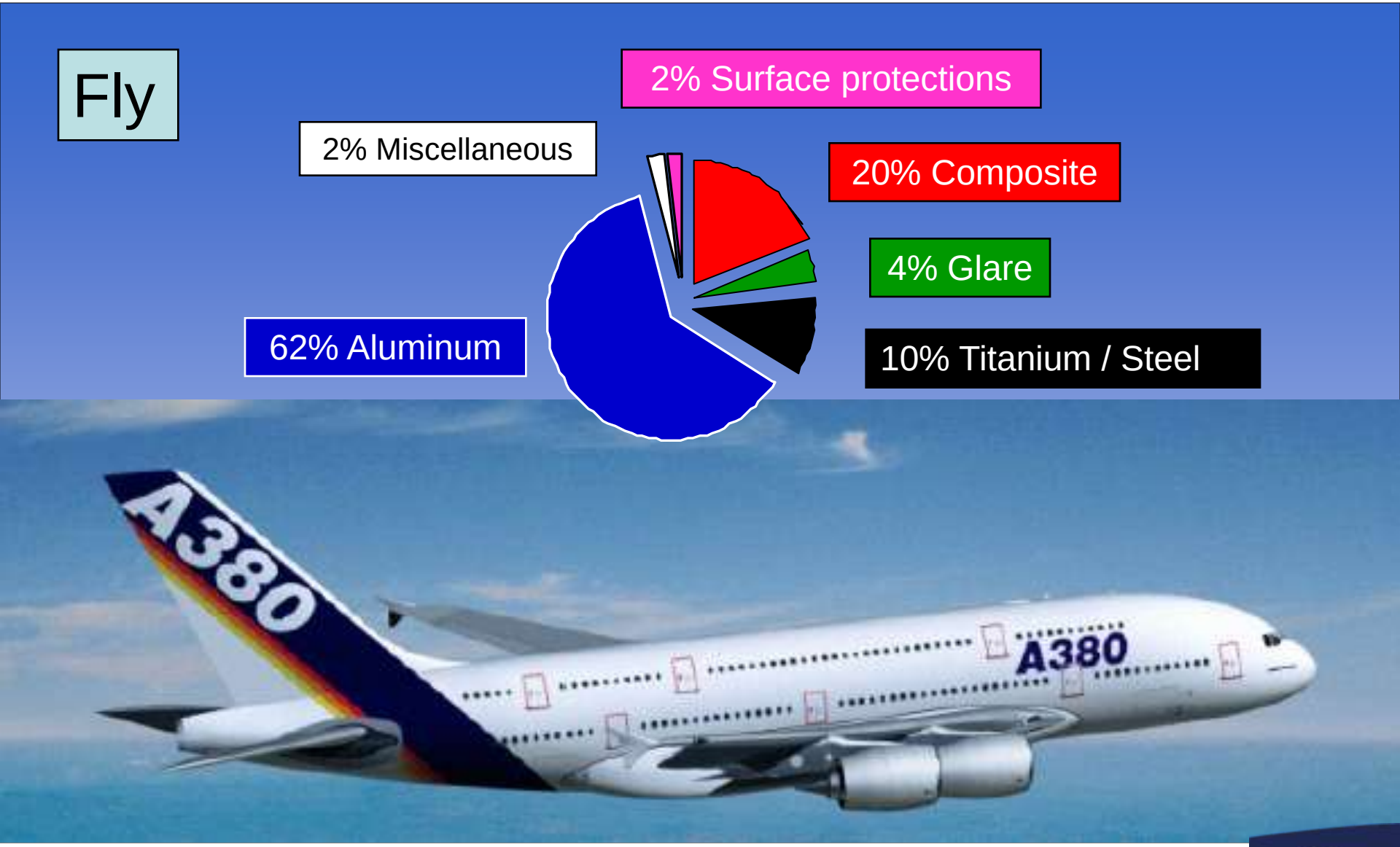


New materials for key technologies: Aero-space

Titanium
Aluminium
Magnesium
Nickel
Steels
Intermetallics

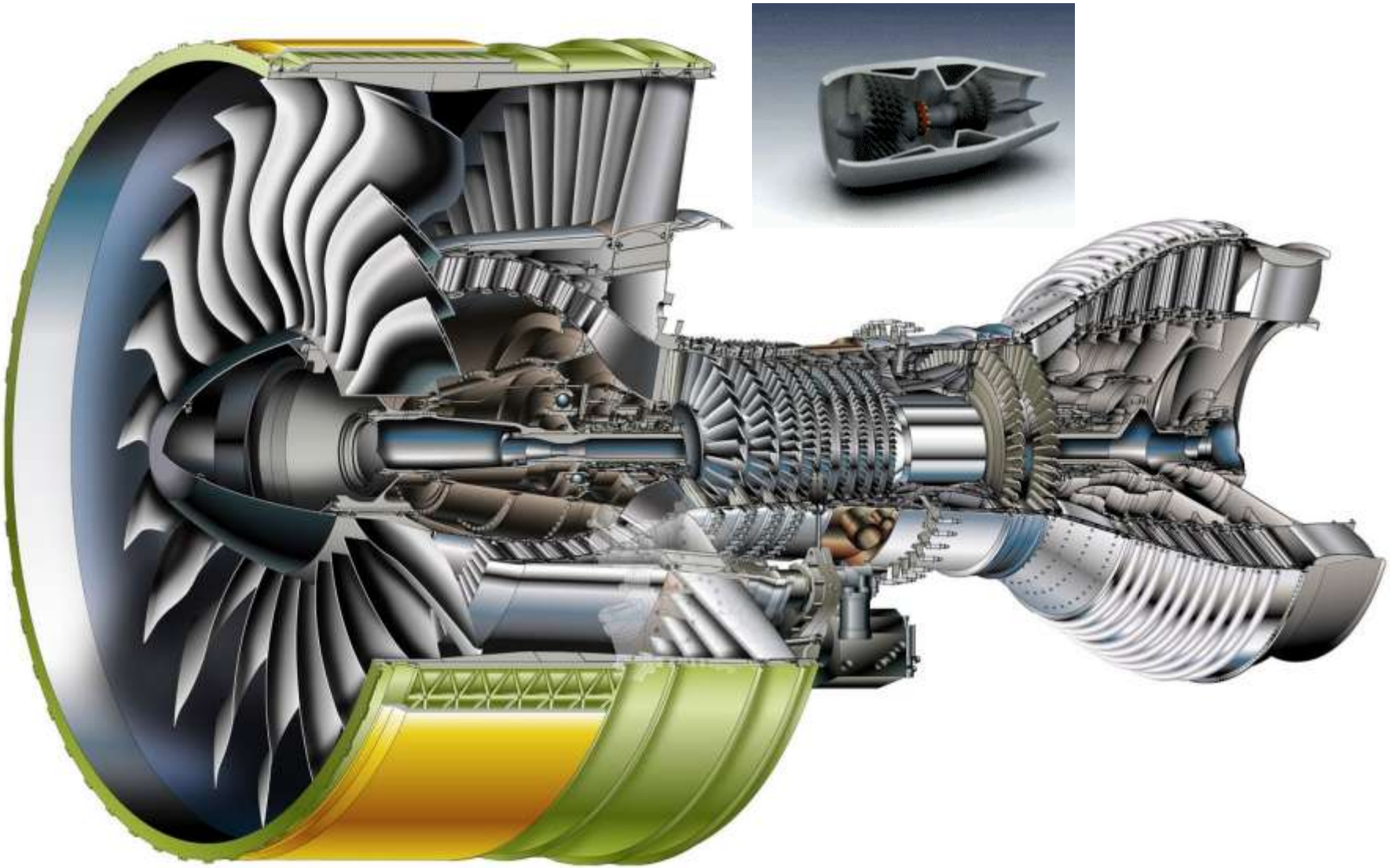
Technology Status A380 – Material Distribution (courtesy Airbus)

Fly

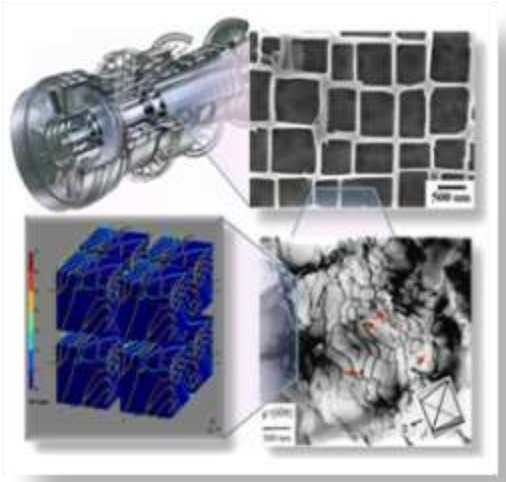


AIRBUS

New materials for key technologies: Aero-space



New materials for key technologies: Aero-space

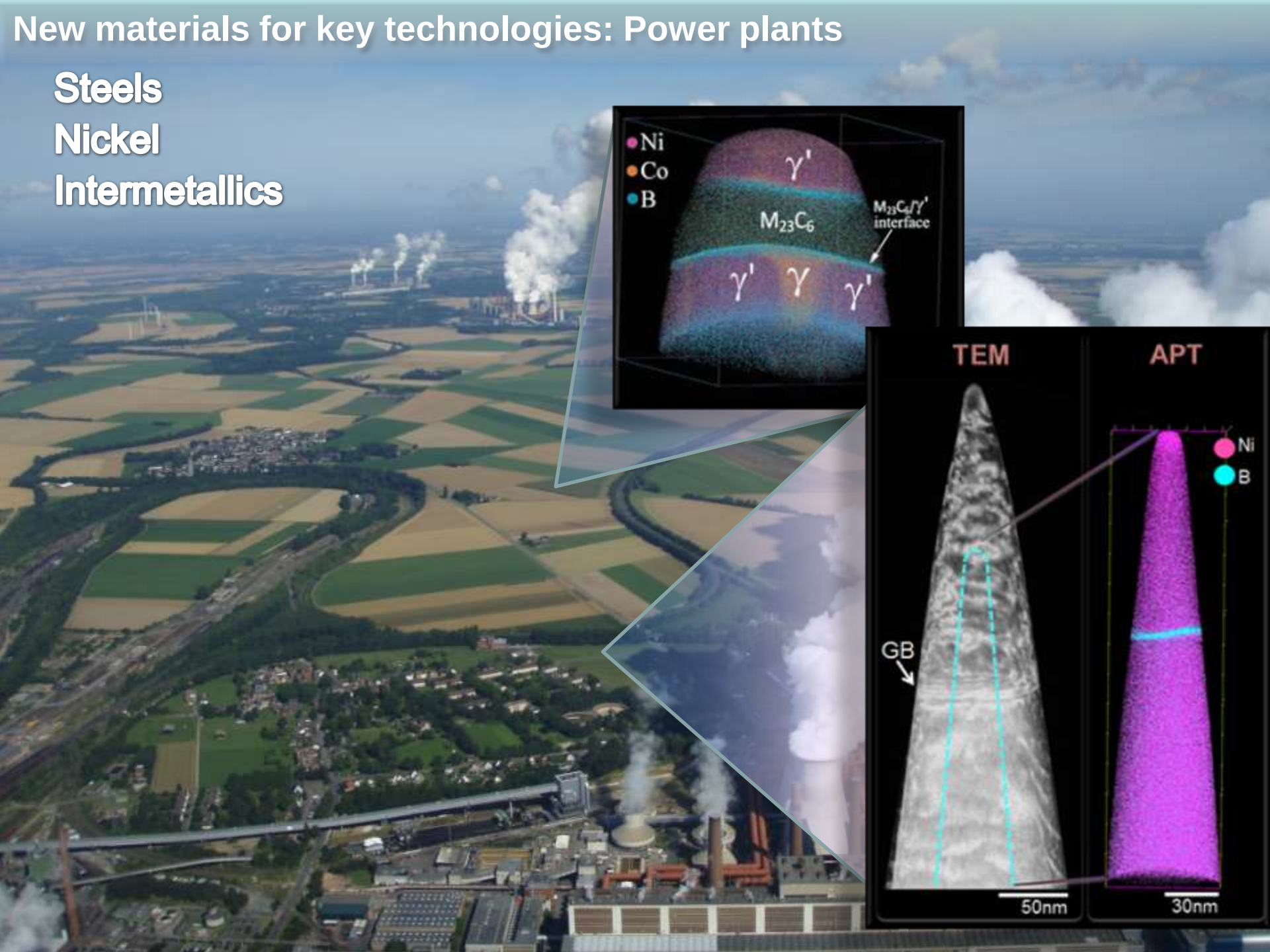


New materials for key technologies: Green energy

Steels
Copper

New materials for key technologies: Power plants

- Steels
- Nickel
- Intermetallics



New materials for key technologies: infrastructure

Steels

New materials for key technologies: health

TITANIUM
MAGNESIUM
COPPER
STEELS



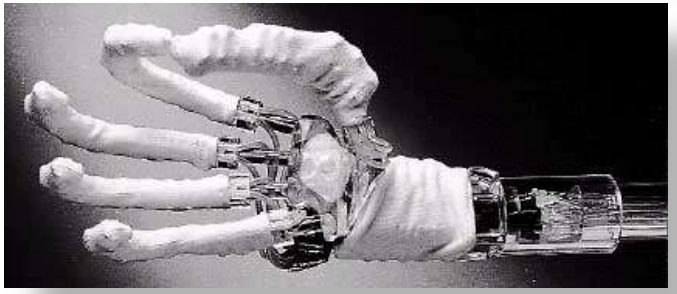






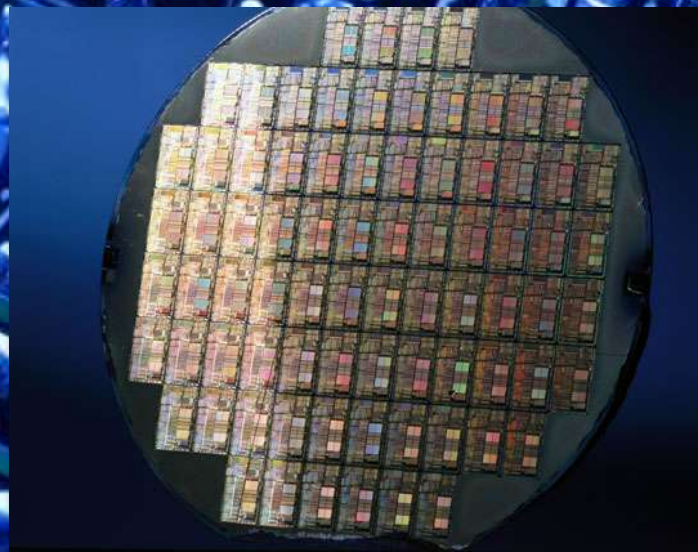






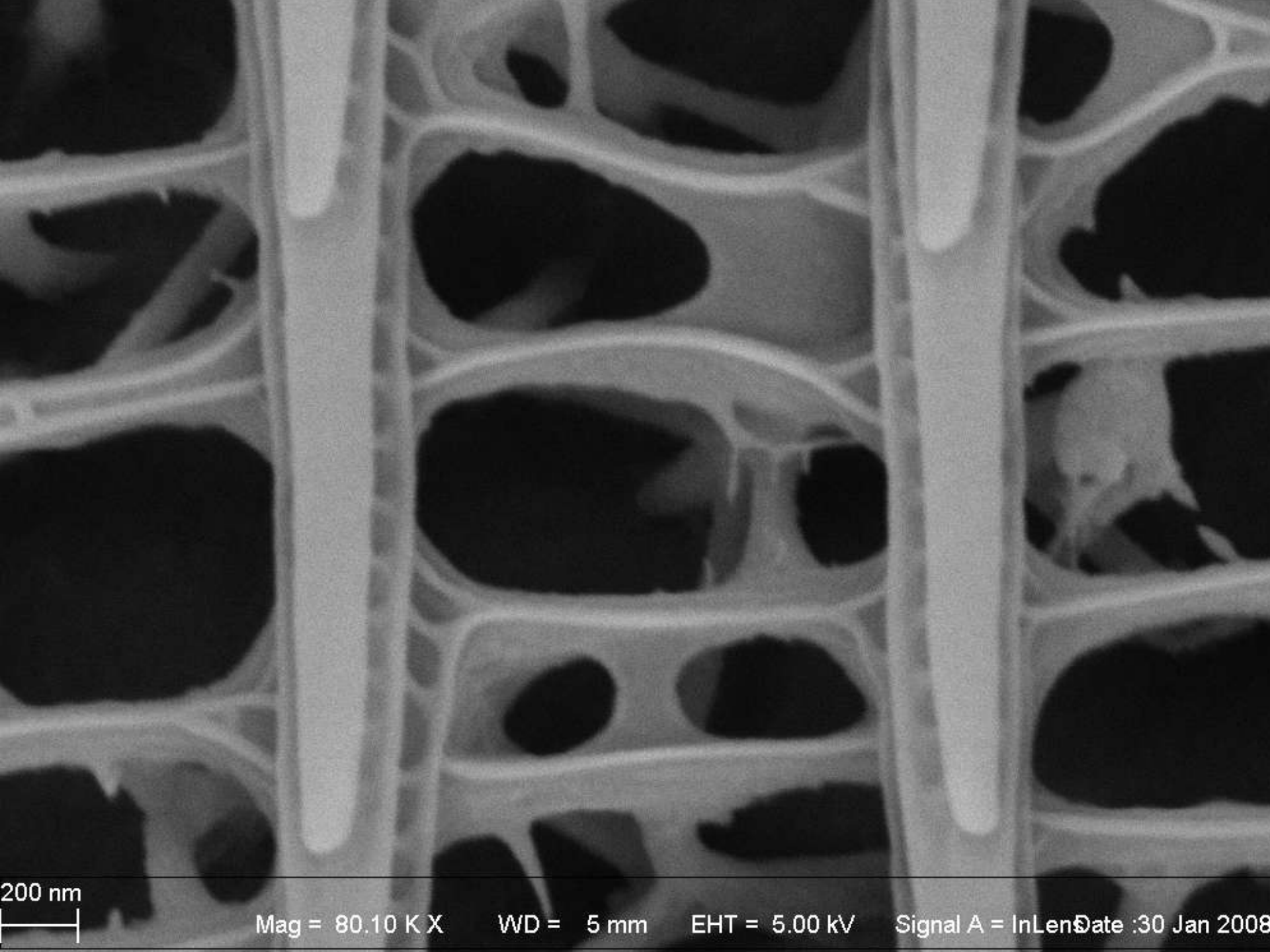
New materials for key technologies: functionals

- Gold
- Copper
- Solders
- III-V semiconductors



New materials for key technologies: communication

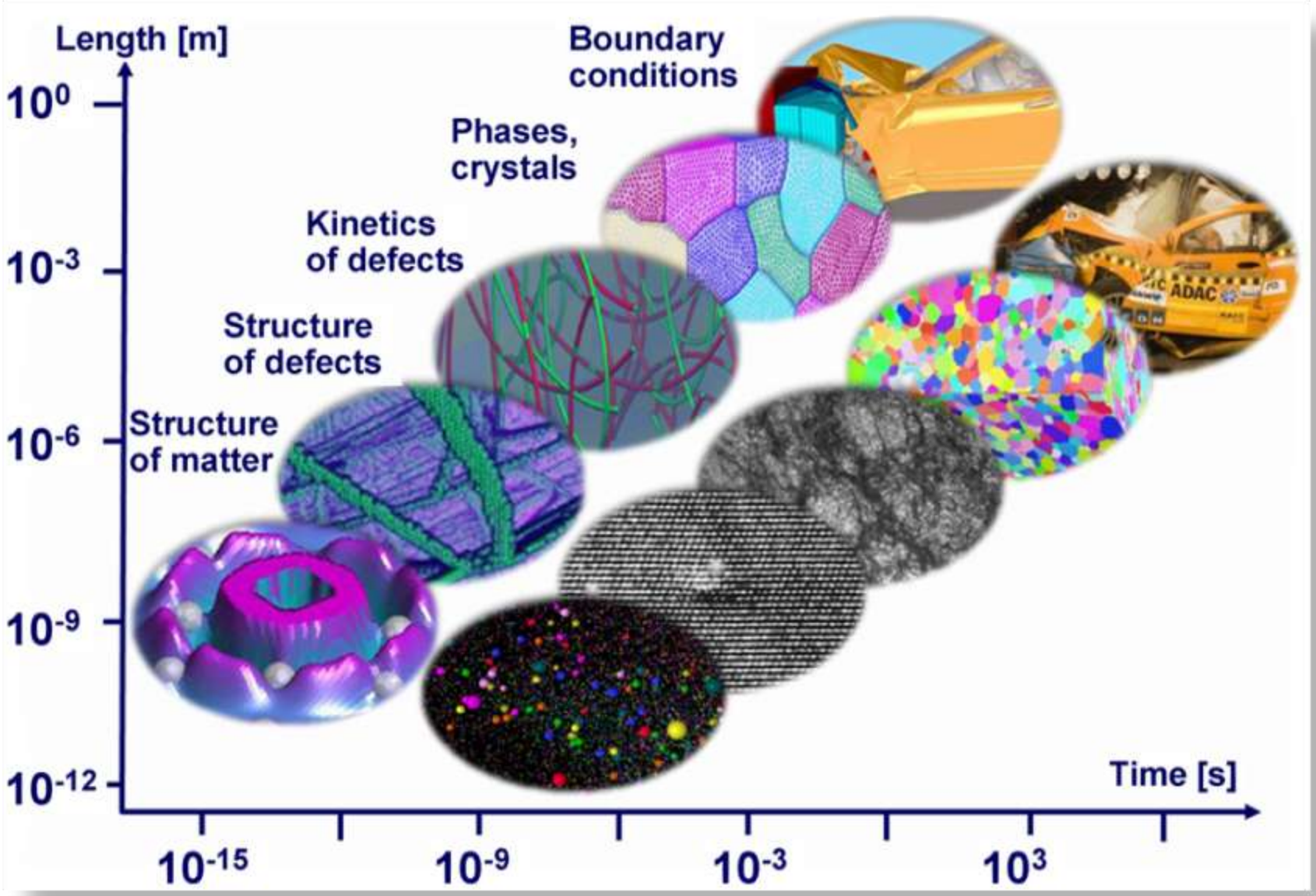
self healing materials, electronic polymers, regenerative Biomaterials, LED, energy storage, thermoelektrica…..


200 nm
Mag = 80.10 K X
WD = 5 mm
EHT = 5.00 kV
Signal A = InLens
Date :30 Jan 2008

Overview

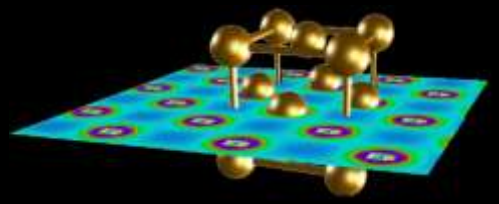
- Introduction to the scales
- Introduction to the engineering background
- Quantum mechanics primer
- Some examples

Multiscale Modeling and Experimentation



Ab initio Methods for materials science

- 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



Counts, Friák, Raabe, Neugebauer: Acta Mater. 57 (2009) 69

time-independent Schrödinger equation

h/(2π)

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

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

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

Raabe: Adv. Mater. 14 (2002)

time-independent Schrödinger equation for many particles

i Elektrons: Mass m_e ; Charge $q_e = -e$; Coordinates r_{ei}

j Cores: Mass m_n ; Charge $q_n = ze$; Coordinates r_{nj}

$$\left(-\frac{\hbar}{2m_e}\sum_i \nabla_i^2 - \frac{\hbar}{2m_n}\sum_j \nabla_j^2 + \sum_{\substack{i1,i2 \\ i1\neq i2}} \frac{e^2}{4\pi\varepsilon_0 \left| r_{e_{i1}} - r_{e_{i2}} \right|} + \sum_{\substack{j1,j2 \\ j1\neq j2}} \frac{z_{j1} z_{j2} e^2}{4\pi\varepsilon_0 \left| r_{n_{j1}} - r_{n_{j2}} \right|} + \sum_{i,j} \frac{z_j e^2}{4\pi\varepsilon_0 \left| r_{e_i} - r_{n_j} \right|} \right) \psi\left(r_{e_i}, r_{n_j}\right) = E\,\psi\left(r_{e_i}, r_{n_j}\right)$$

Raabe: Adv. Mater. 14 (2002)

Adiabatic Born-Oppenheimer approximation

Decoupling of cores and electrons

$$\psi(\mathrm{r_e}, \mathrm{r_n}) = \varphi(\mathrm{r_e})\phi(\mathrm{r_n})$$

Electrons

$$\left(-\frac{\hbar}{2m_e}\sum_i \nabla_i^2 + \sum_{\substack{i1,i2 \\ i1 \neq i2}} \frac{e^2}{4\pi\varepsilon_0 \left| r_{e_{i1}} - r_{e_{i2}} \right|} + \sum_{i,j} \frac{z_j e^2}{4\pi\varepsilon_0 \left| r_{e_i} - r_{n_j} \right|} \right) \varphi(r_{e_i}) = E\varphi(r_{e_i})$$

Atom cores

$$\left(-\frac{\hbar}{2m_n}\sum_j \nabla_j^2 + \sum_{\substack{j1,j2 \\ j1 \neq j2}} \frac{z_{j1} z_{j2} e^2}{4\pi\varepsilon_0 \left| r_{n_{j1}} - r_{n_{j2}} \right|} + \sum_{i,j} \frac{z_j e^2}{4\pi\varepsilon_0 \left| r_{e_i} - r_{n_j} \right|} \right) \phi(r_{n_j}) = E\phi(r_{n_j})$$

Raabe: Adv. Mater. 14 (2002)

Hohenberg-Kohn-Sham Theorem: density function theory

Ground state energy is a unique function of the particle density

$$E_0 = E(n(r))$$

The Functional E(n(r)) has a minimum regarding variation in particle density at equilibrium density $n_0(r)$

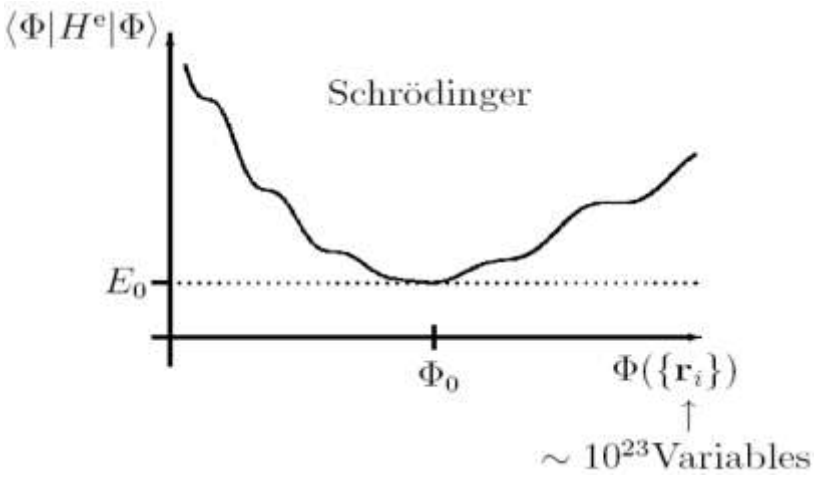
$$E = E(n_0(r)) = \min\{E(n(r))\}$$

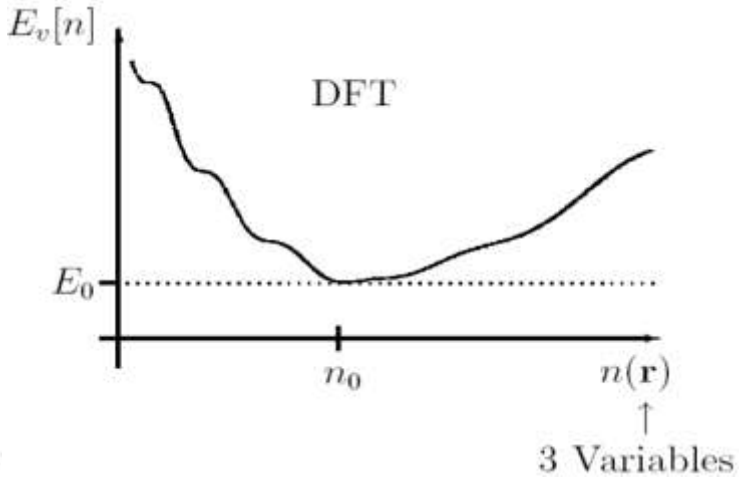
$$\left.\frac{\partial E(n(r))}{\partial n(r)}\right|_{n(r)=n_0(r)} = 0$$

Hohenberg Kohn, Phys. Rev. 136 (1964) B864

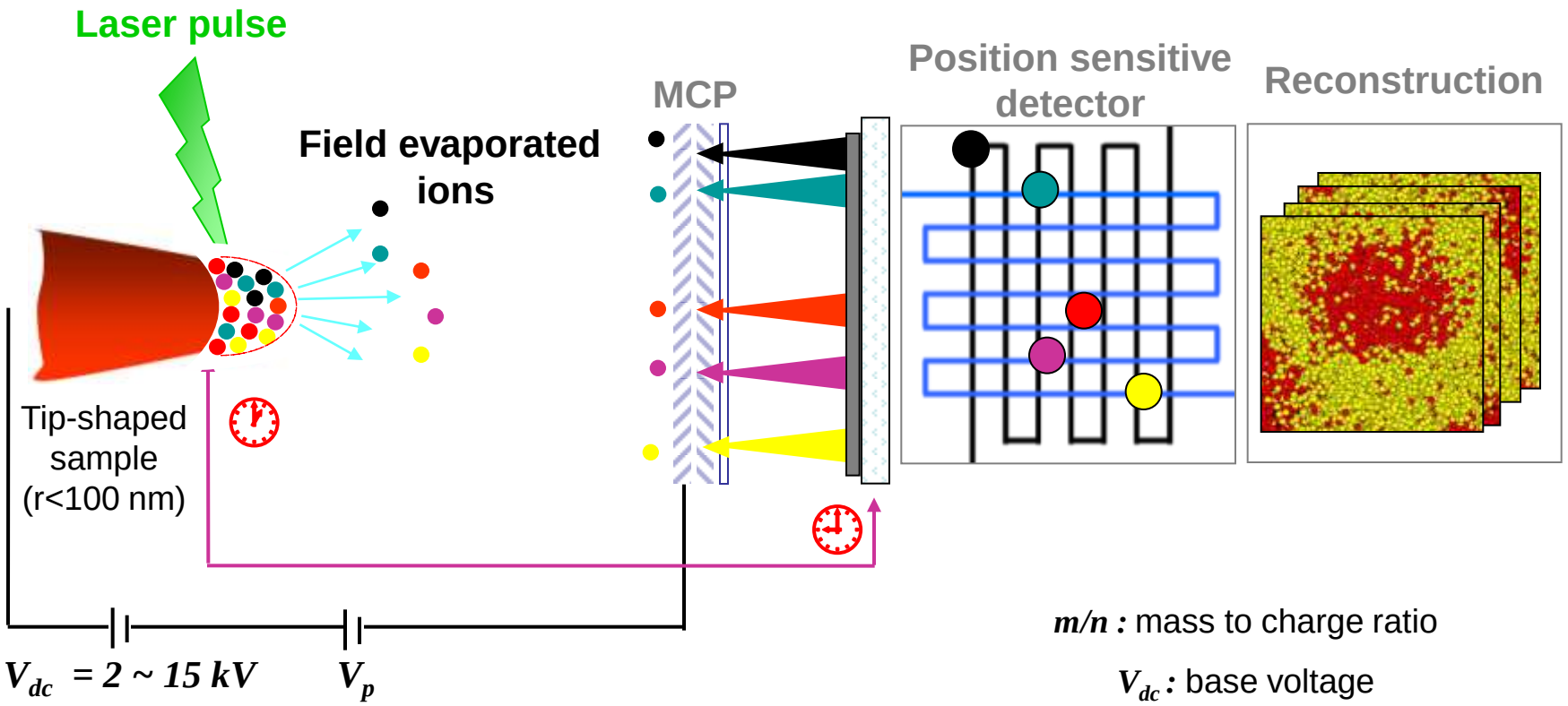
Ab initio: theoretical methods

- Density functional theory (DFT), generalized gradient approximation (GGA); also LDA
- Vienna ab-initio simulation package (VASP) code or SPHINX; different pseudo-potentials, Brillouin zone sampling, supercell sizes, and cut-off energies, different exchange-correlation functions, M.-fit
- Entropy: non-0K, dynamical matrix, configuational analytical





Atom Probe Tomography (APT)



$$\frac{m}{n} = 2e(\alpha V_{dc} + \beta V_P)\left(\frac{t}{L}\right)^2$$

m/n : mass to charge ratio

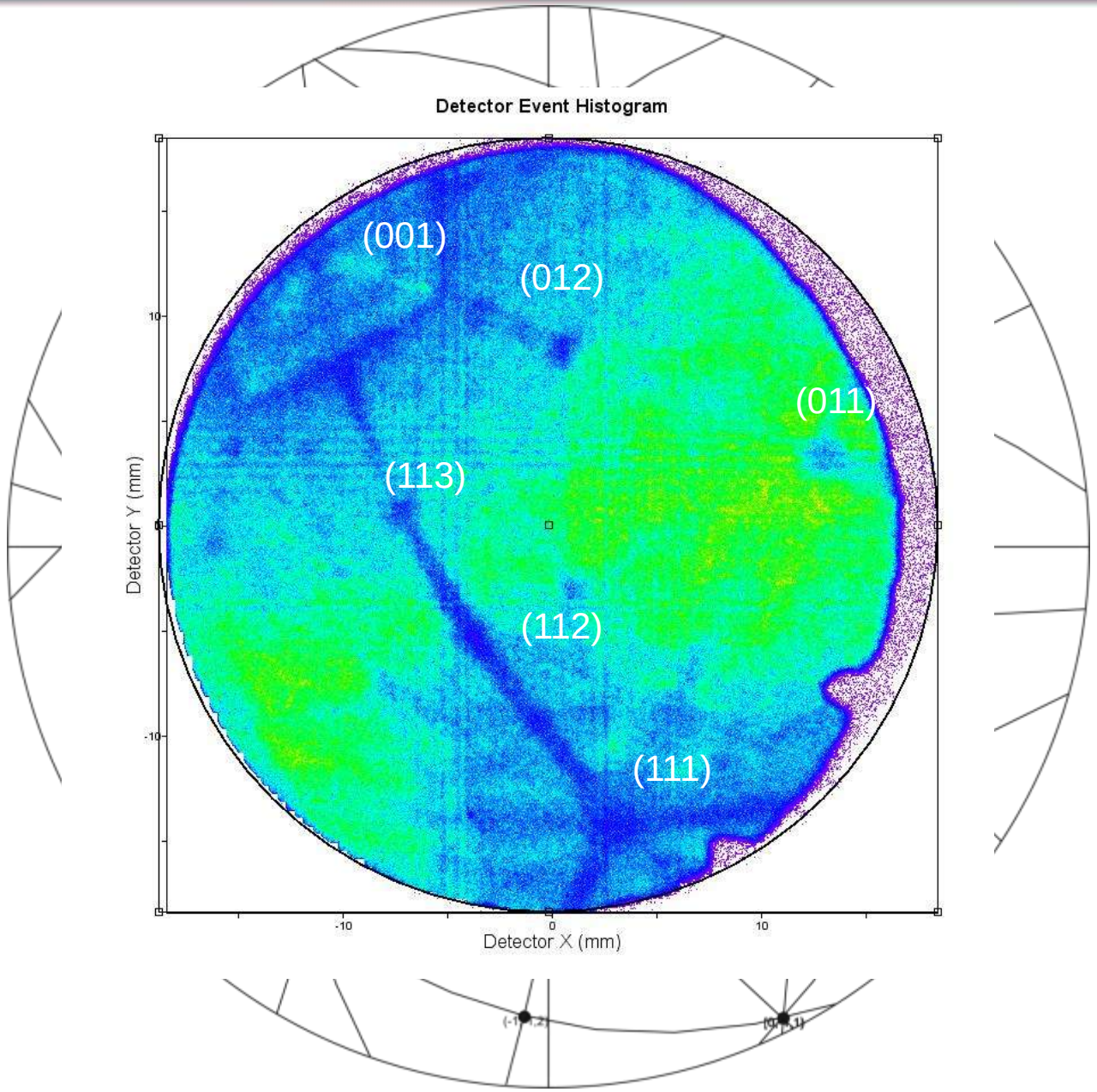
V_{dc} **:** base voltage

V_P **:** pulse voltage

***t*:** time of flight

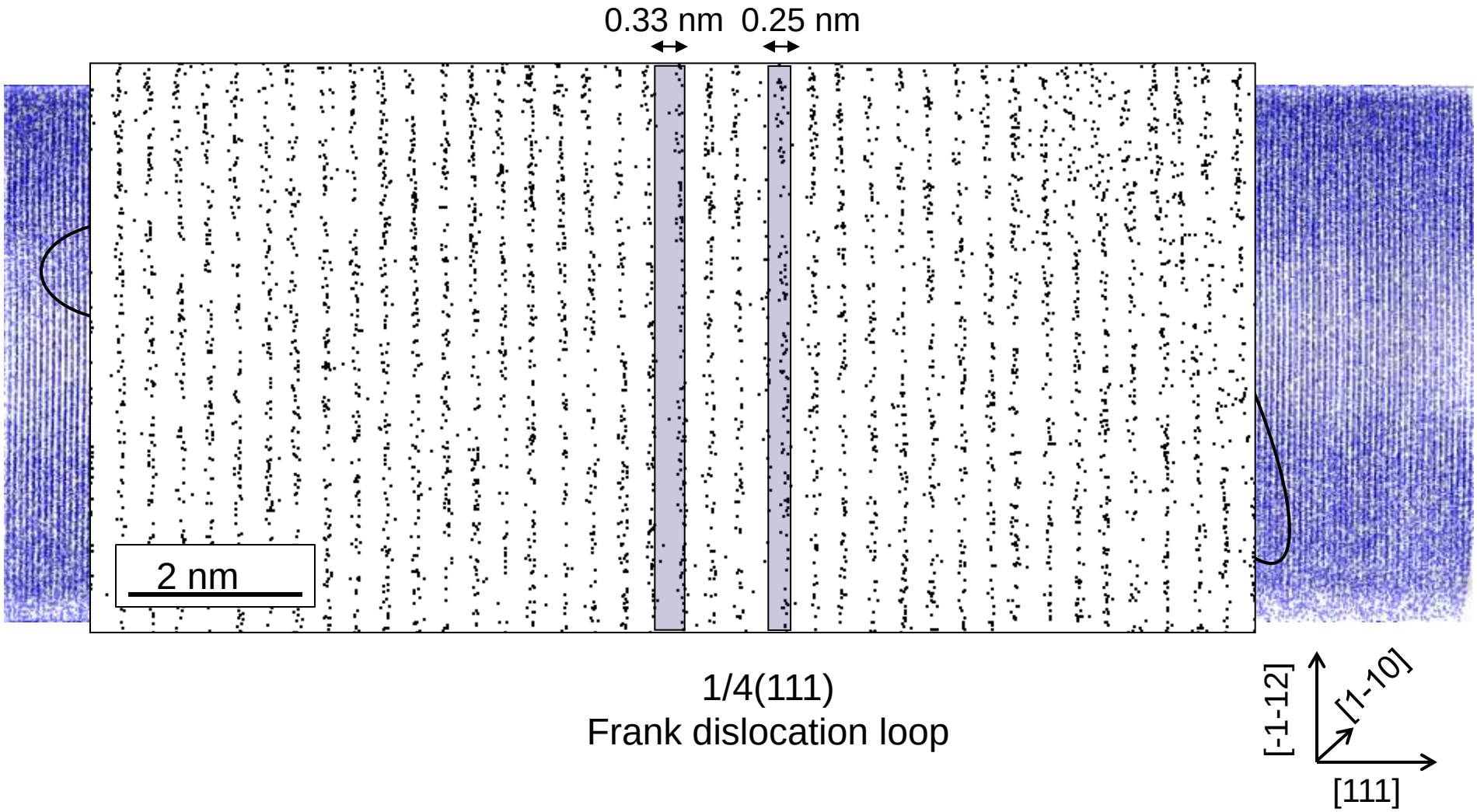
***L*:** distance specimen - detector

Field desorption image



Lattice plane reconstruction

Fe_3Al ordered phase (only Al displayed)



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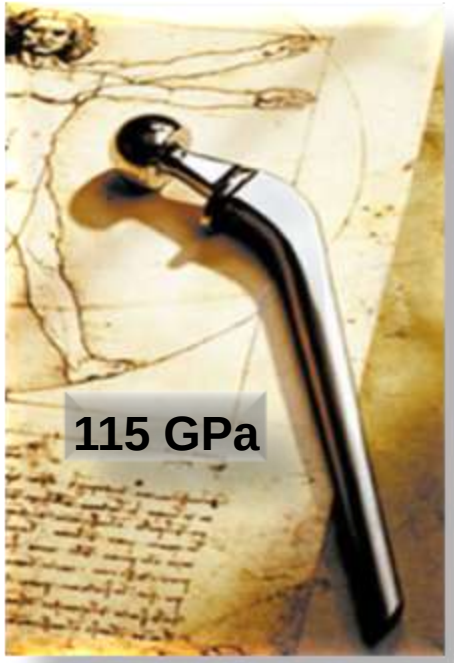
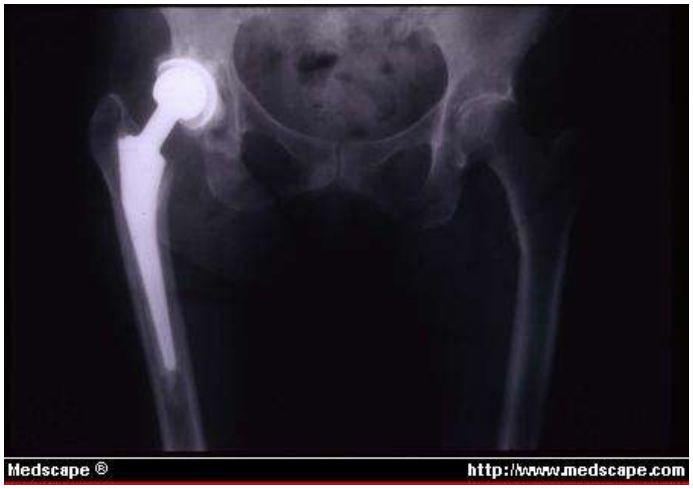
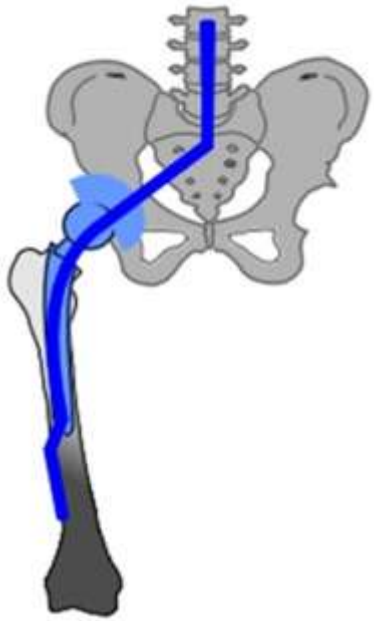
  - Health: Titanium
  - Mobility: Steel

Neue Biowerkstoffe: Titanimplantate mit kubischer Gitterstruktur

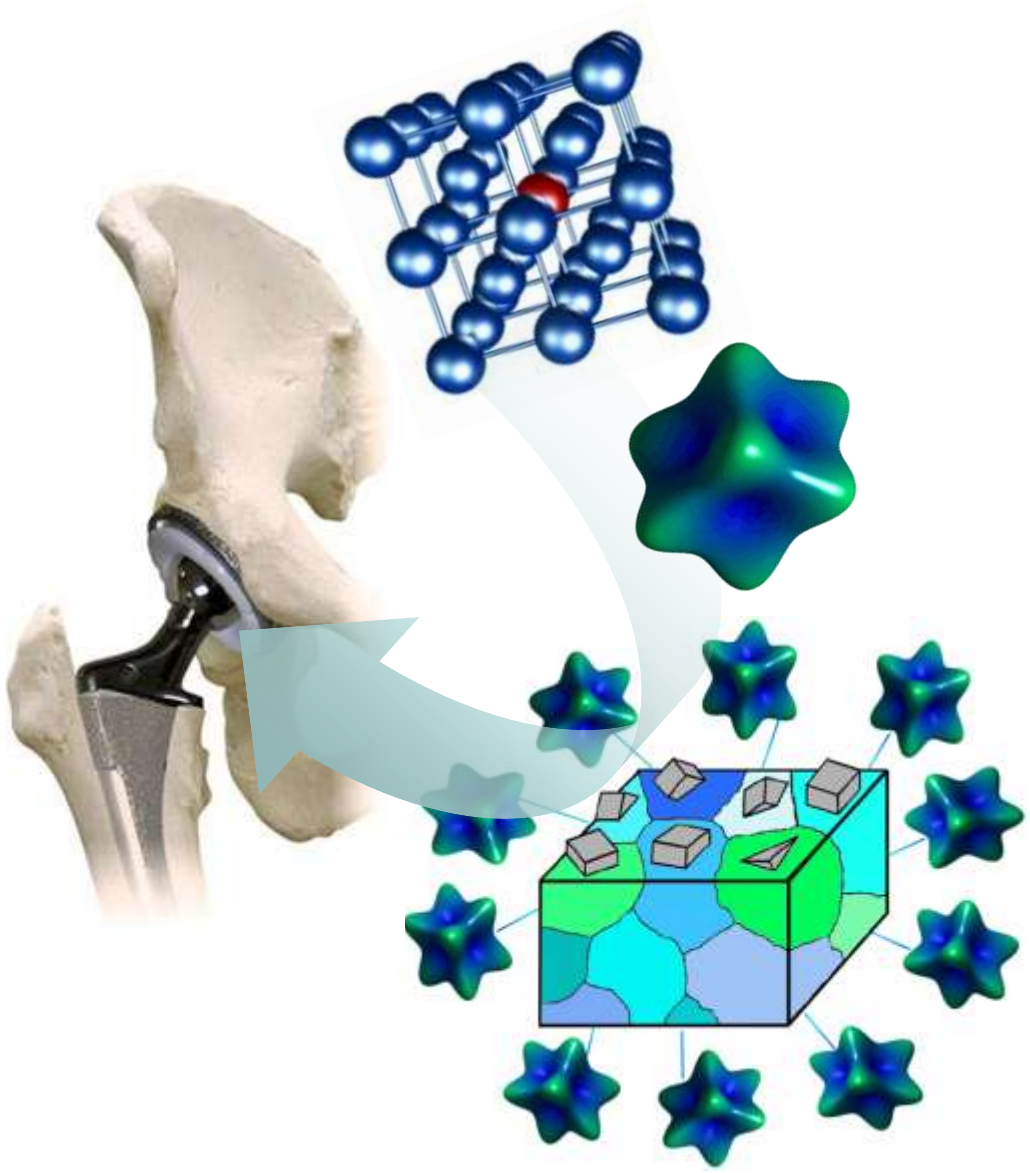




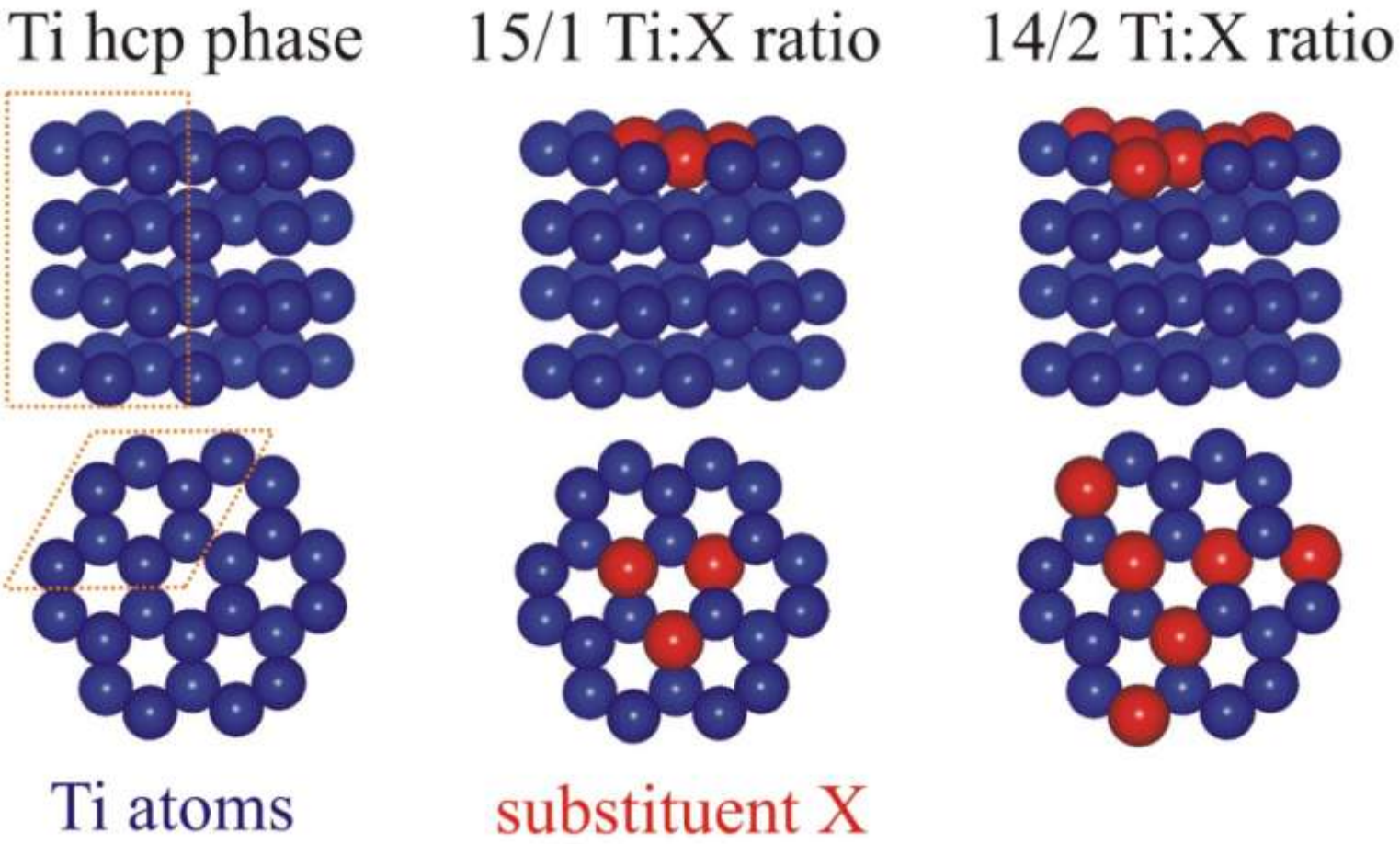


Spannungs-Abschattung (Stress shielding)
Elastische Fehlpassung:
Knochenauflösung, Abrasion, Entzündung

Von ab-initio zur Vielkristall-Steifigkeit

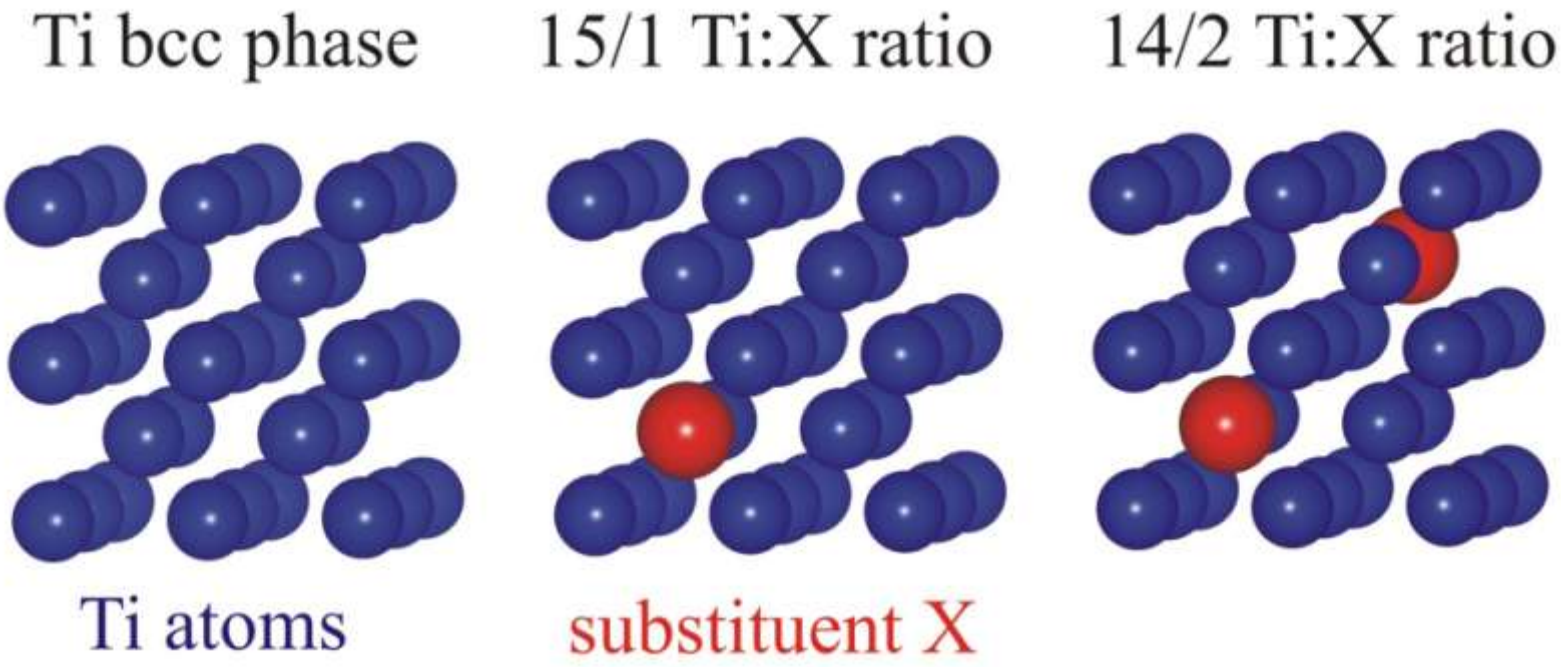


Construct binary alloys in the hexagonal phase



Raabe, Sander, Friák, Ma, Neugebauer: Acta Mater. 55 (2007) 4475

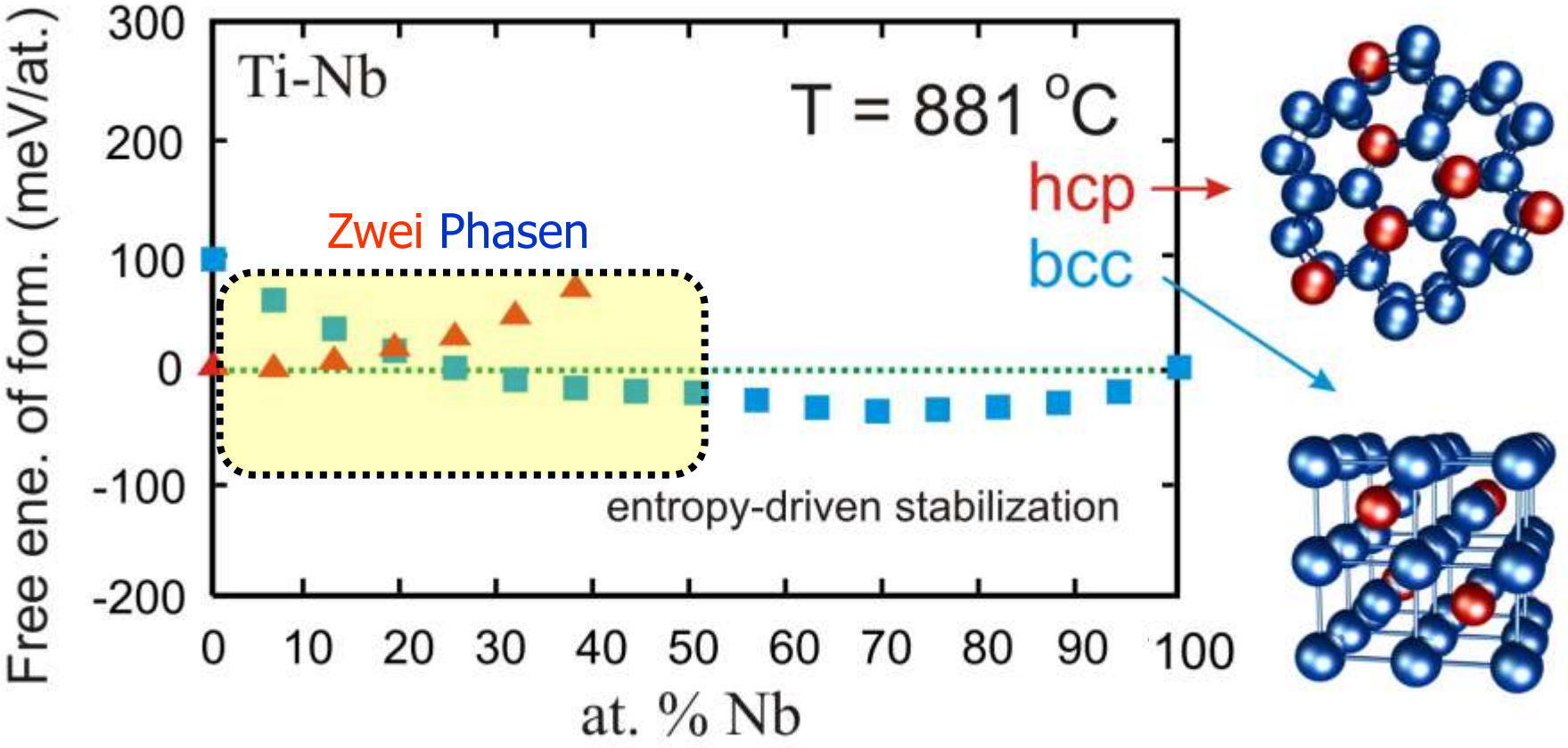
Construct binary alloys in the cubic phase



Raabe, Sander, Friák, Ma, Neugebauer: Acta Mater. 55 (2007) 4475

Neue Biowerkstoffe: Titanimplantate mit kubischer Gitterstruktur

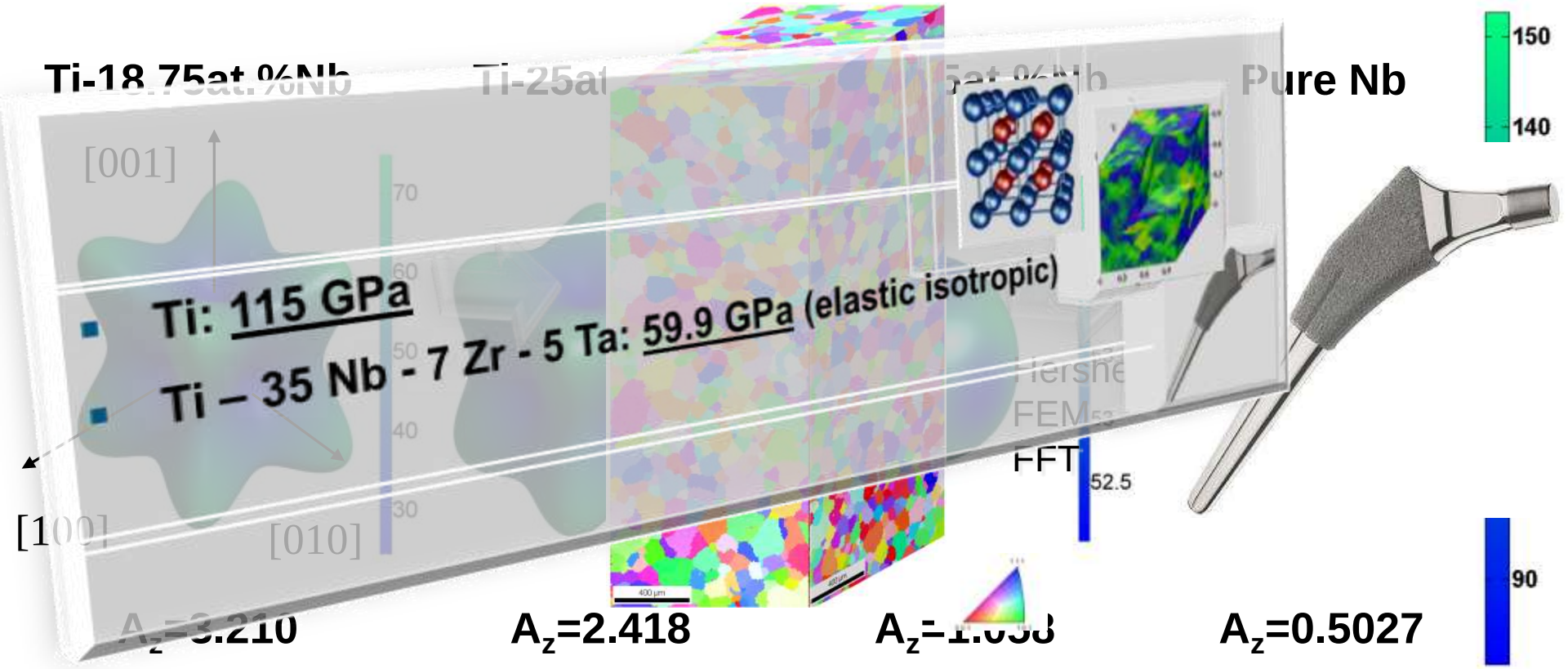
Freie Energie F(x,c,T) = U – T · S
U: Dichtefunktional-Theorie (DFT)
S: Konfigurationsentropie
Elastischer Tensor
Vielkristall-Steifigkeit (Homogenisierung)



Ab initio alloy design: Elastic properties: Ti-Nb system

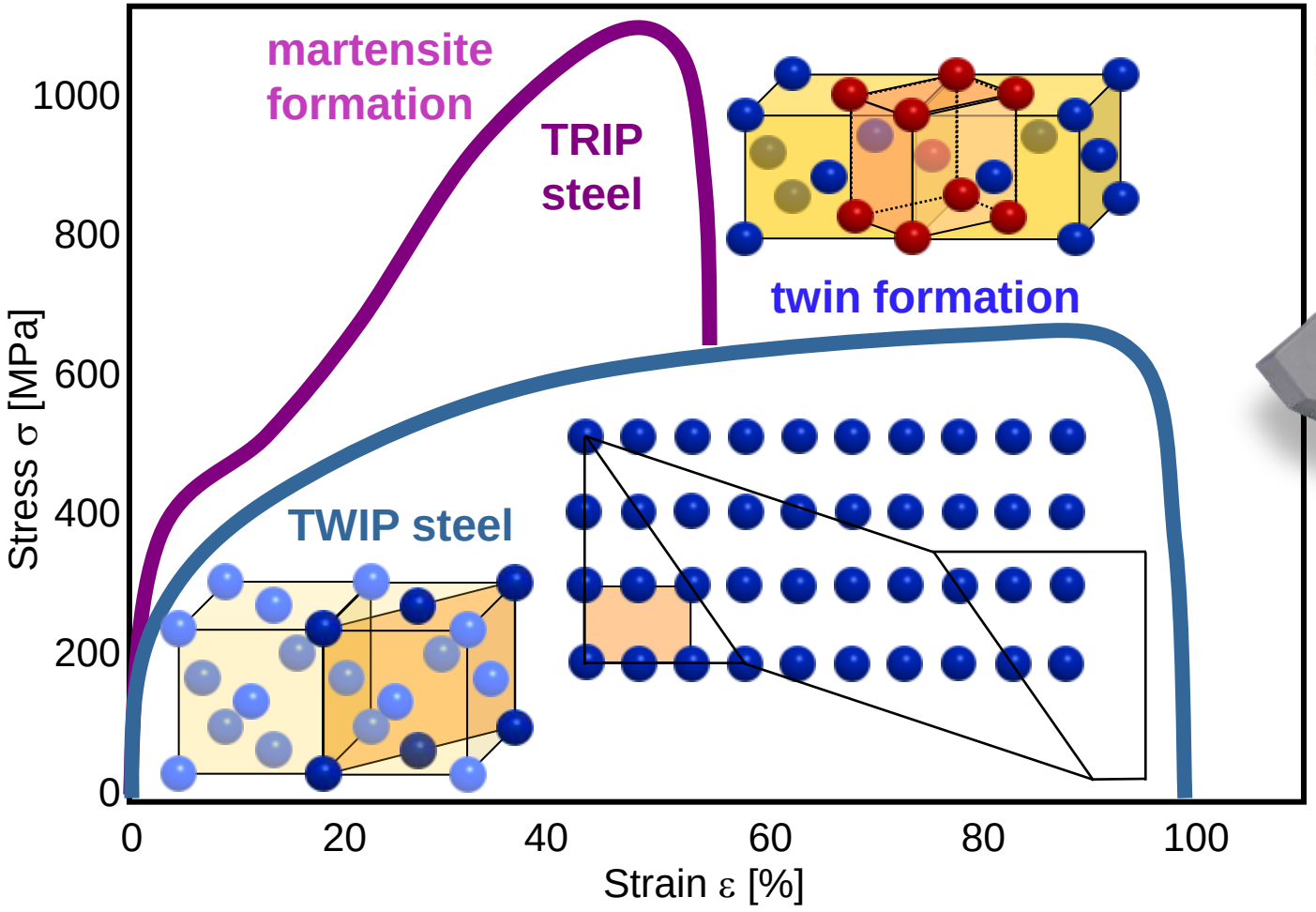
Young's modulus surface plots

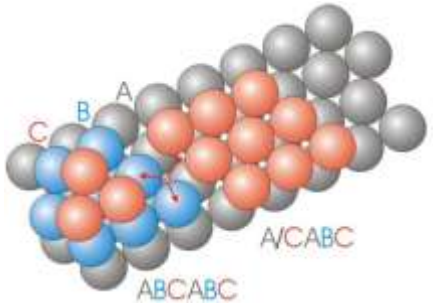
$A_z = 2\,C_{44}/(C_{11} - C_{12})$

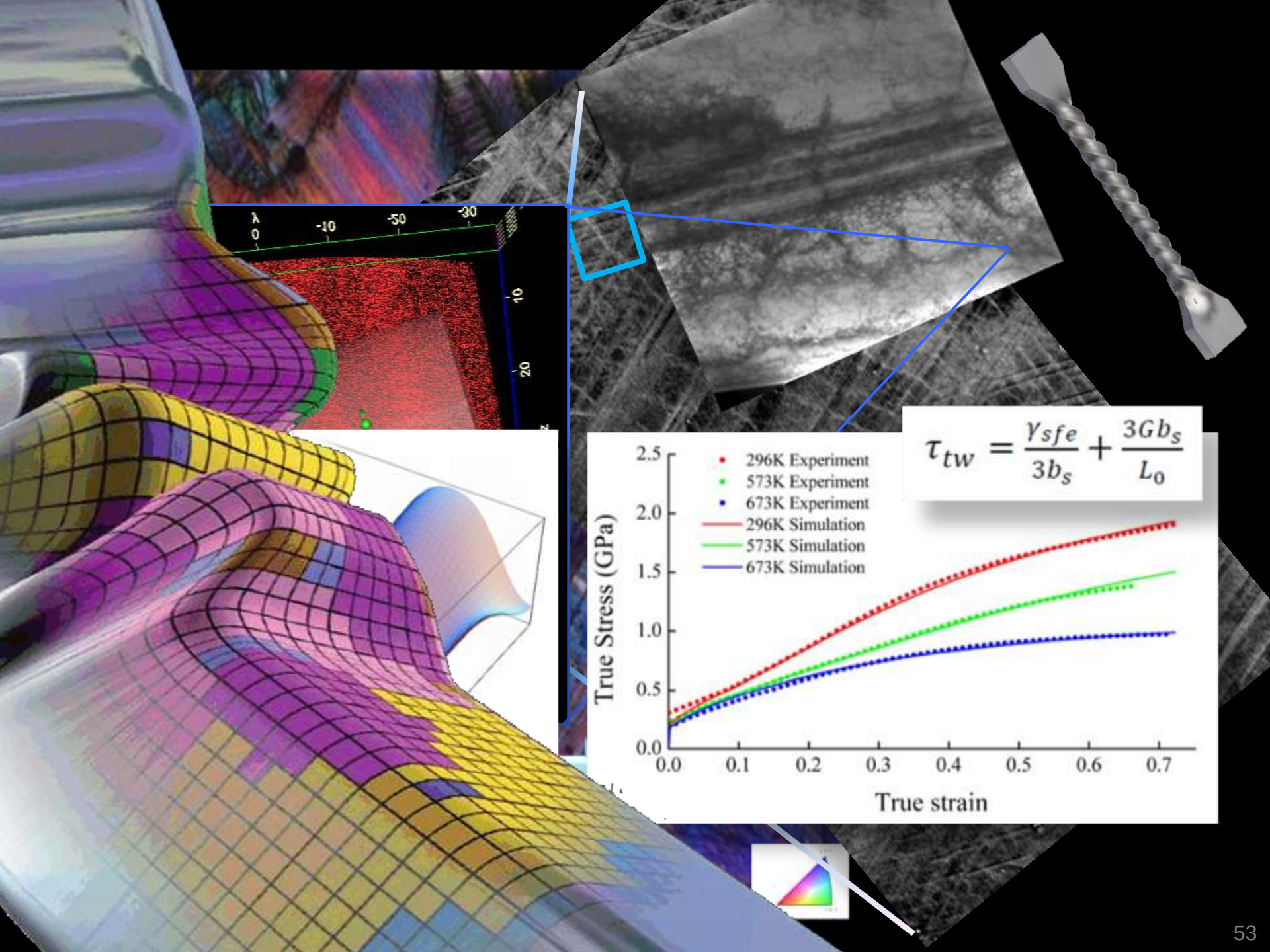


Ma, Friák, Neugebauer, Raabe, Roters: phys. stat. sol. B 245 (2008) 2642

Ab-initio methods for the design of high strength steels






0
-10
-30
-50
10
20
$\tau_{tw} = \frac{\gamma_{sfe}}{3b_s} + \frac{3Gb_s}{L_0}$
296K Experiment
573K Experiment
673K Experiment
296K Simulation
573K Simulation
673K Simulation
True Stress (GPa)
True strain
2.5
2.0
1.5
1.0
0.5
0.0
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7

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Acta Materialia 61 (2013) 1773–1784

Acta MATERIALIA

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Thermodynamics of carbon solubility in ferrite and vacancy formation in cementite in strained pearlite

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Received 27 August 2012; received in revised form 30 November 2012; accepted 1 December 2012
Available online 8 January 2013

Abstract

In order to investigate the thermodynamic driving force for the experimentally observed accumulation of C in ferritic layers of severely plastically deformed pearlitic wires, the stabilities of C interstitials in ferrite and of C vacancies in cementite are investigated as a function of uniaxial stain, using density-functional theory. In the presence of an applied strain along [1 1 0] or [1 1 1], the C interstitial in ferrite is significantly stabilized, while the C vacancy in cementite is moderately destabilized by the corresponding strain states in cementite [1 0 0] and ([0 1 0]). The enhanced stabilization of the C interstitial gives rise to an increase in the C concentration within the ferritic layers by up to two orders of magnitude. Our results thus suggest that in addition to the generally assumed non-equilibrium, dislocation-based mechanism, there is also a strain-induced thermodynamic driving force for the experimentally observed accumulation of C in ferrite.

Keywords: Density-functional theory; Ferrite; Cementite; Carbon interstitial; Vacancy formation energy

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Available online at www.sciencedirect.com
ScienceDirect
Acta Materialia 55 (2007) 4475–4487

Acta MATERIALIA
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Theory-guided bottom-up design of β-titanium alloys as biomaterials based on first principles calculations: Theory and experiments

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Received 17 March 2007; received in revised form 10 April 2007; accepted 12 April 2007
Available online 1 June 2007

Abstract

In this study we present a new strategy for the theory-guided bottom up design of β-Ti alloys for biomedical applications using a quantum mechanical approach in conjunction with experiments. Parameter-free density functional theory calculations are used to provide theoretical guidance in selecting and optimizing Ti-based alloys with respect to three constraints: (i) the use of non-toxic alloy elements; (ii) the stabilization of the body centered cubic β-phase at room temperature; (iii) the reduction of the elastic stiffness compared to existing Ti-based alloys. Following the theoretical predictions, the alloys of interest are cast and characterized with respect to their crystallographic structure, microstructure, texture, and elastic stiffness. Due to the complexity of the ab initio calculations, the simulations have been focused on a set of binary systems of Ti with two different high melting body-centered cubic metals, namely, Nb and Mo. Various levels of model approximations to describe mechanical and thermodynamic properties are tested and critically evaluated. The experiments are conducted both, on some of the binary alloys and on two more complex engineering alloy variants, namely, Ti–35 wt.% Nb–7 wt.% Zr–5 wt.% Ta and Ti–20 wt.% Mo–7 wt.% Zr–5 wt.% Ta.

Keywords: Ab initio; Metallurgy; Quantum mechanics; Materials design; Bcc

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Acta Materialia 57 (2009) 69–76

Acta MATERIALIA
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Using *ab initio* calculations in designing bcc Mg–Li alloys for ultra-lightweight applications

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Received 30 April 2008; received in revised form 22 August 2008; accepted 22 August 2008
Available online 1 October 2008

Abstract

Ab initio calculations are becoming increasingly useful to engineers interested in designing new alloys, because these calculations are able to accurately predict basic material properties only knowing the atomic composition of the material. In this paper, single crystal elastic constants of 11 bcc Mg–Li alloys are calculated using density functional theory (DFT) and compared with available experimental data. Based on DFT determined properties, engineering parameters such as the ratio of bulk modulus over shear modulus (B/G) and the ratio of Young's modulus over mass density (Y/ρ) are calculated. Analysis of B/G and Y/ρ shows that bcc Mg–Li alloys with 30–50 at.% Li offer the most potential as lightweight structural material. Compared with fcc Al–Li alloys, bcc Mg–Li alloys have a lower B/G ratio, but a comparable Y/ρ ratio. An Ashby map containing Y/ρ vs B/G shows that it is not possible to increase both Y/ρ and B/G by changing only the composition of a binary alloy.

Keywords: Magnesium alloys; Brittle-to-ductile transition; Density functional; *Ab initio* electron theory; Elastic behavior

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Acta Materialia 60 (2012) 3011–3021

Acta MATERIALIA

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The relation between ductility and stacking fault energies in Mg and Mg–Y alloys

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Received 28 September 2011; received in revised form 1 February 2012; accepted 4 February 2012
Available online 7 March 2012

Abstract

The underlying mechanisms that are responsible for the improved room-temperature ductility in Mg–Y alloys compared to pure Mg are investigated by transmission electron microscopy and density functional theory. Both methods show a significant decrease in the intrinsic stacking fault I_1 energy (I_1 SFE) with the addition of Y. The influence of the SFE on the relative activation of different competing deformation mechanisms (basal, prismatic, pyramidal slip) is discussed. From this analysis we suggest a key mechanism which explains the transition from primary basal slip in hexagonal close-packed Mg to basal plus pyramidal slip in solid solution Mg–Y alloys. This mechanism is characterized by enhanced nucleation of $\langle c+a \rangle$ dislocations where the intrinsic stacking fault I_1 (ISF_1) acts as heterogeneous source for $\langle c+a \rangle$ dislocations. Possible electronic and geometric reasons for the modification of the SFE by substitutional Y atoms are identified and discussed.

Keywords: Magnesium alloys; Transmission electron microscopy (TEM); Density functional theory (DFT); Dislocation structure; Ductility

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Acta Materialia 60 (2012) 6025–6032

Acta MATERIALIA

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Elastic properties of face-centred cubic Fe–Mn–C studied by nanoindentation and ab initio calculations

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Received 22 March 2012; received in revised form 10 July 2012; accepted 11 July 2012
Available online 16 August 2012

Abstract

We have studied experimentally and theoretically the influence of C and Mn content on the Young's modulus of Fe–Mn–C alloys. Combinatorial thin film and bulk samples were characterized regarding their structure, texture and Young's modulus. The following chemical composition range was investigated: 1.5–3.0 at.% C, 28.0–37.5 at.% Mn and 60.6–69.8 at.% Fe. The experimental lattice parameters change marginally within 3.597–3.614 Å with the addition of C and are consistent with ab initio calculations. The Young's modulus data are in the range of 185 ± 12–251 ± 59 GPa for the bulk samples and the thin film, respectively. C has no significant effect on the Young's modulus of these alloys within the composition range studied here. The ab initio calculations are 15–22% larger than the average Young's modulus values of the as-deposited and polished thin film at 3 at.% C. The comparison of thin film and bulk samples results reveals similar elastic properties for equivalent compositions, indicating that the applied research strategy consisting of the combinatorial thin film approach in conjunction with ab initio calculations is useful to study the composition dependence of the structure and elastic properties of Fe–Mn–C alloys. The very good agreement between the presented calculations and the experimentally determined lattice parameters and Young's modulus values implies that the here-adopted simulation strategy yields a reliable description of carbon in Fe–Mn alloys, important for future alloy design.

Keywords: Iron alloys; Sputtering; Elastic behaviour; Ab initio electron theory; Nanoindentation