Nanostructuring of 1 Million tons: designing steels using quantum mechanics and atom probe tomography

D. Raabe, D. Ponge, P. Choi, S. Zaefferer,
T. Hickel, M. Friak, J. Neugebauer

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

Foundation: 1917
Kaiser-Wilhelm-Institut für Eisenforschung

Since 1971: Basic corporate budget financed by Max-Planck-Society (50%) and VDEh (50%)

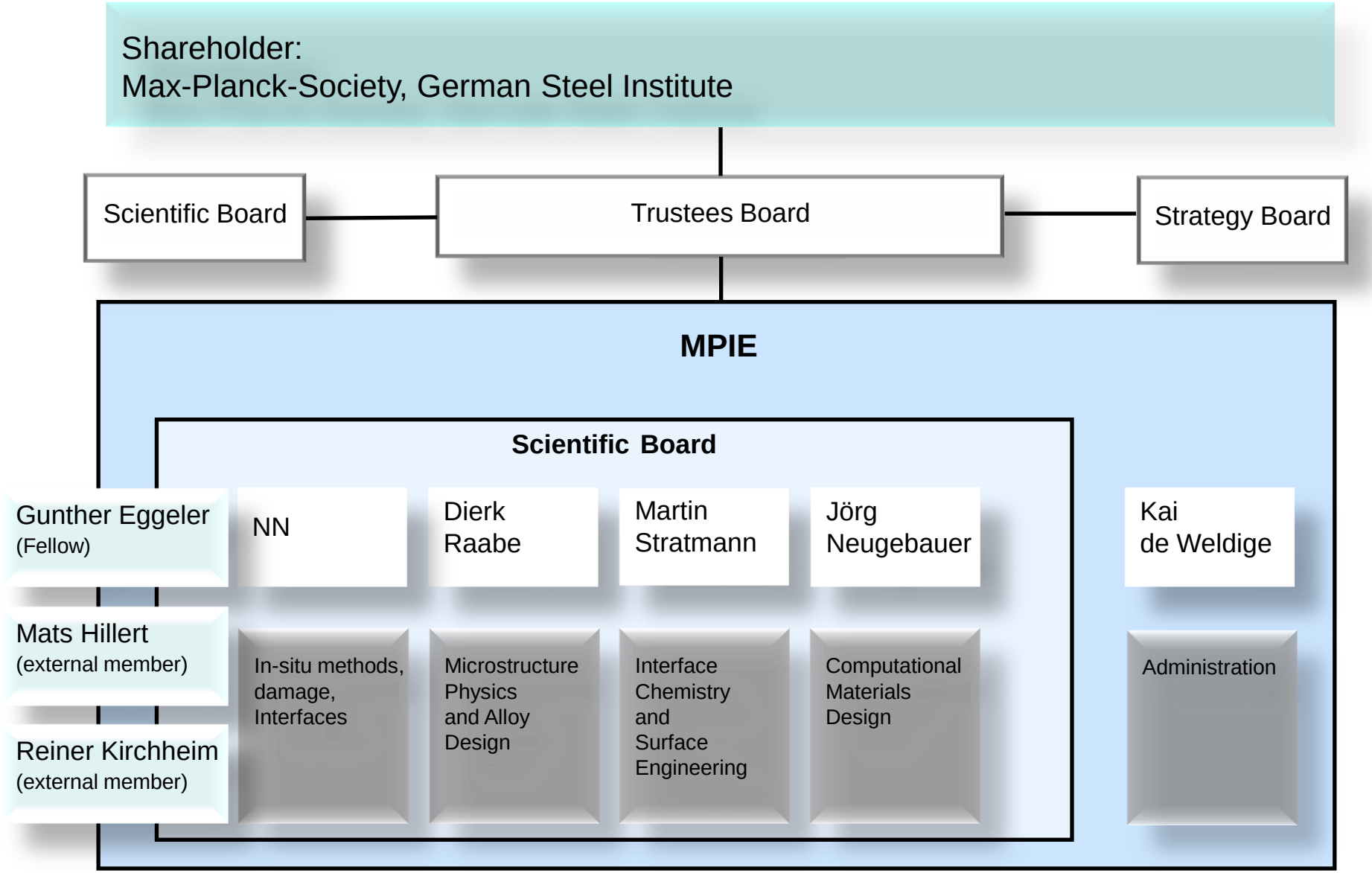
Total budget: 16,4 Mio. €
(40% MPG, 38% VDEh, 22% third party funds)

Personnel: 250

Max Planck

Basic science of
complex engineering alloys and processes

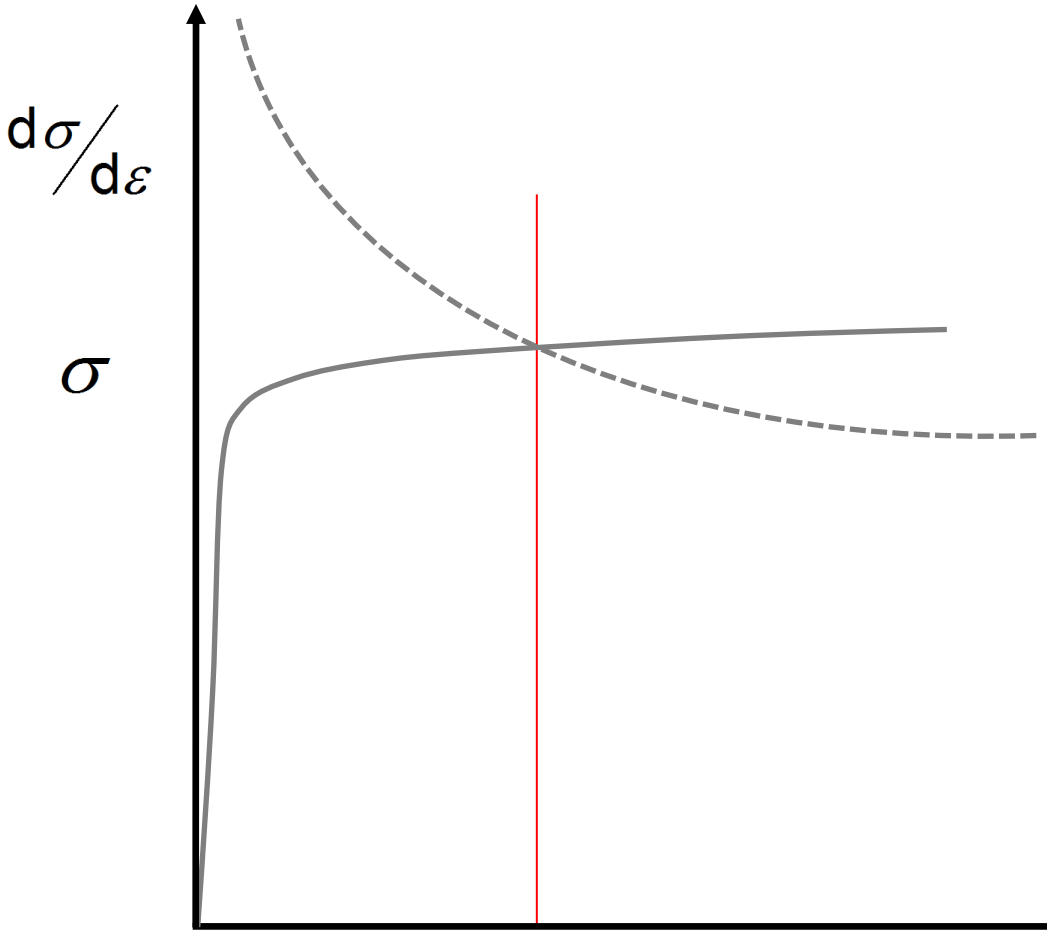
MPIE departments



Overview

- Atomistic design of complex alloys (ab initio, APT)
- Nanostructuring by selective phase transformation
- Conclusions and challenges

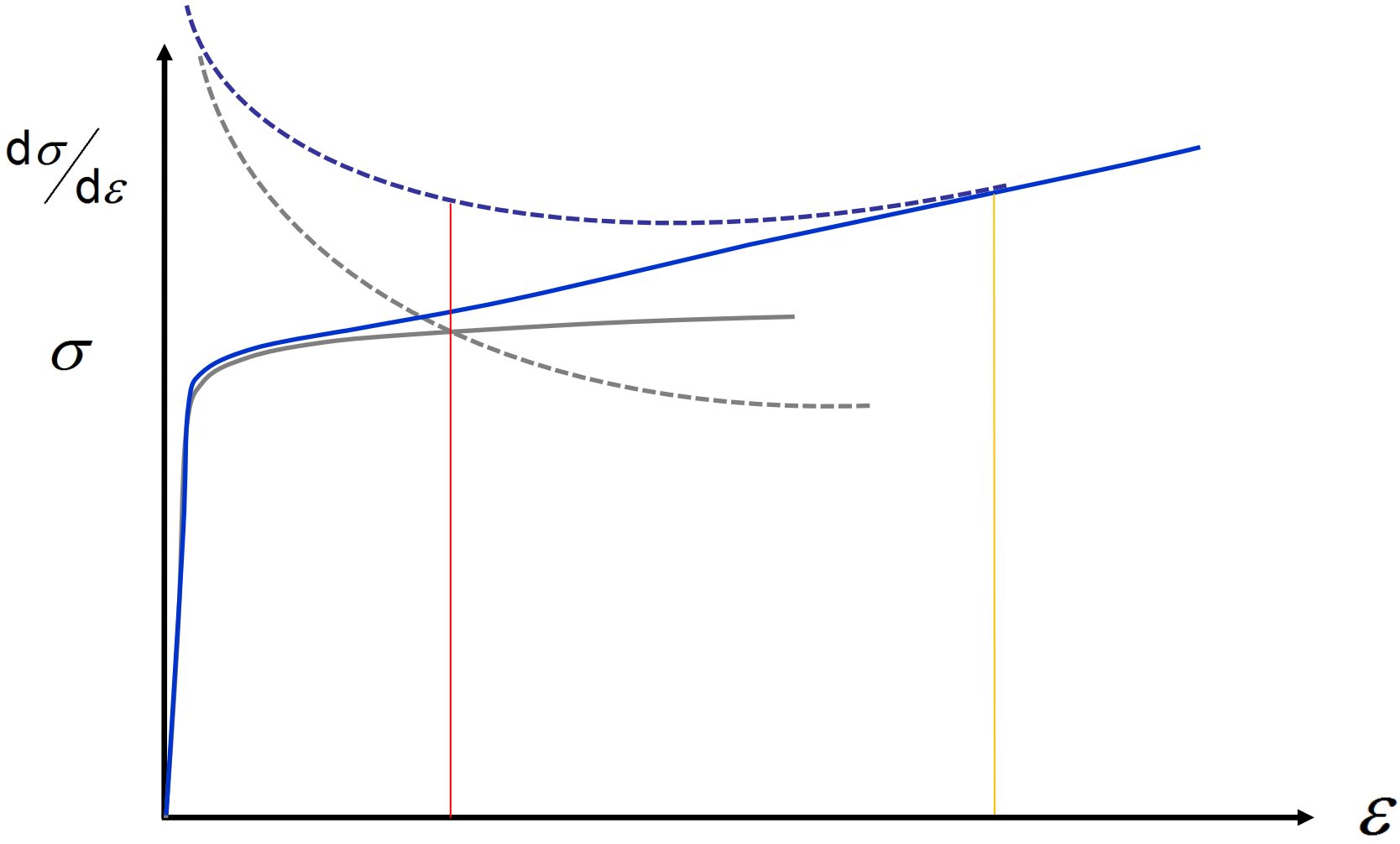
Inverse strength-ductility: phenomenological analysis



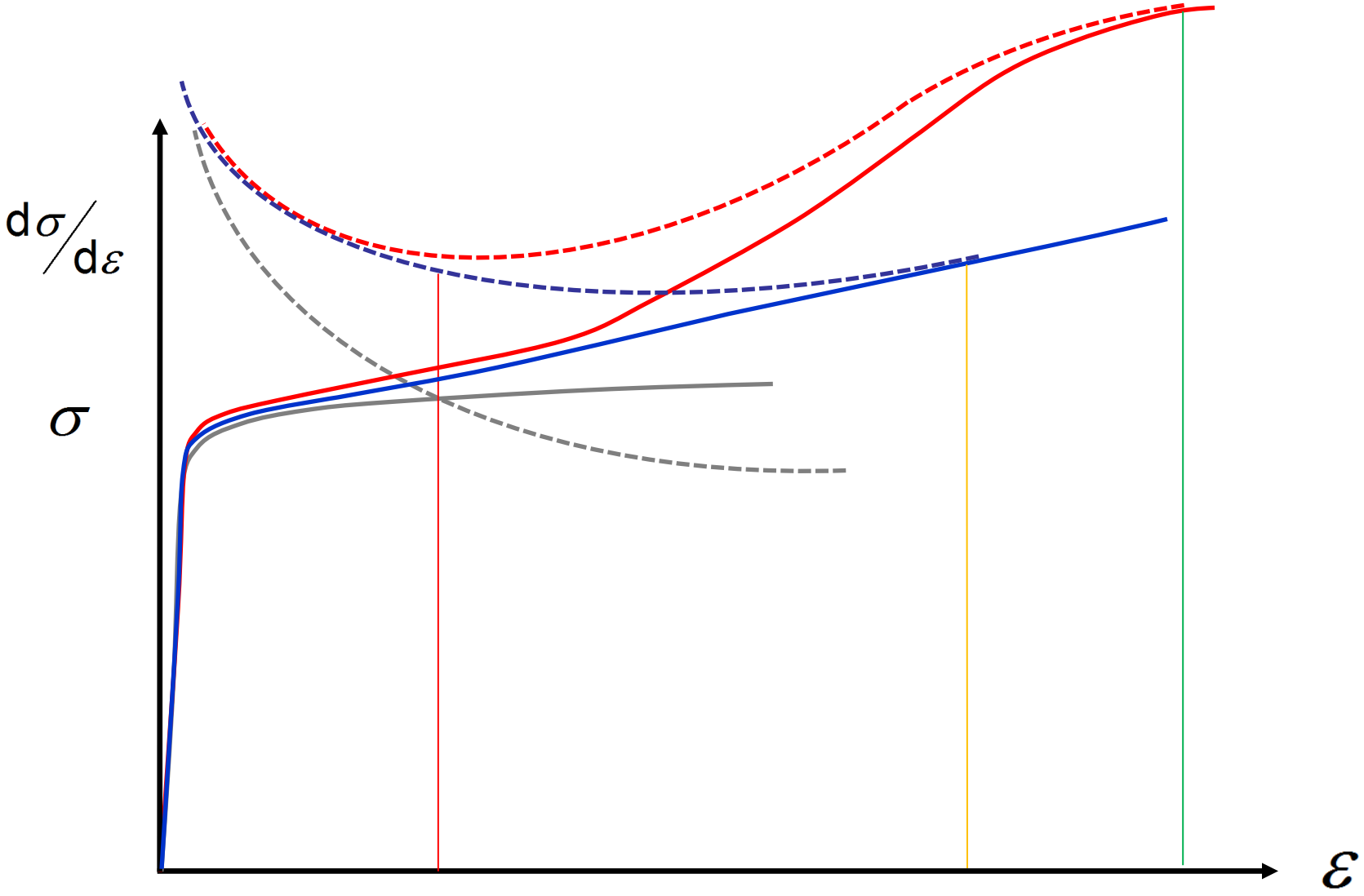
ε true strain

σ stress

Inverse strength-ductility: phenomenological analysis

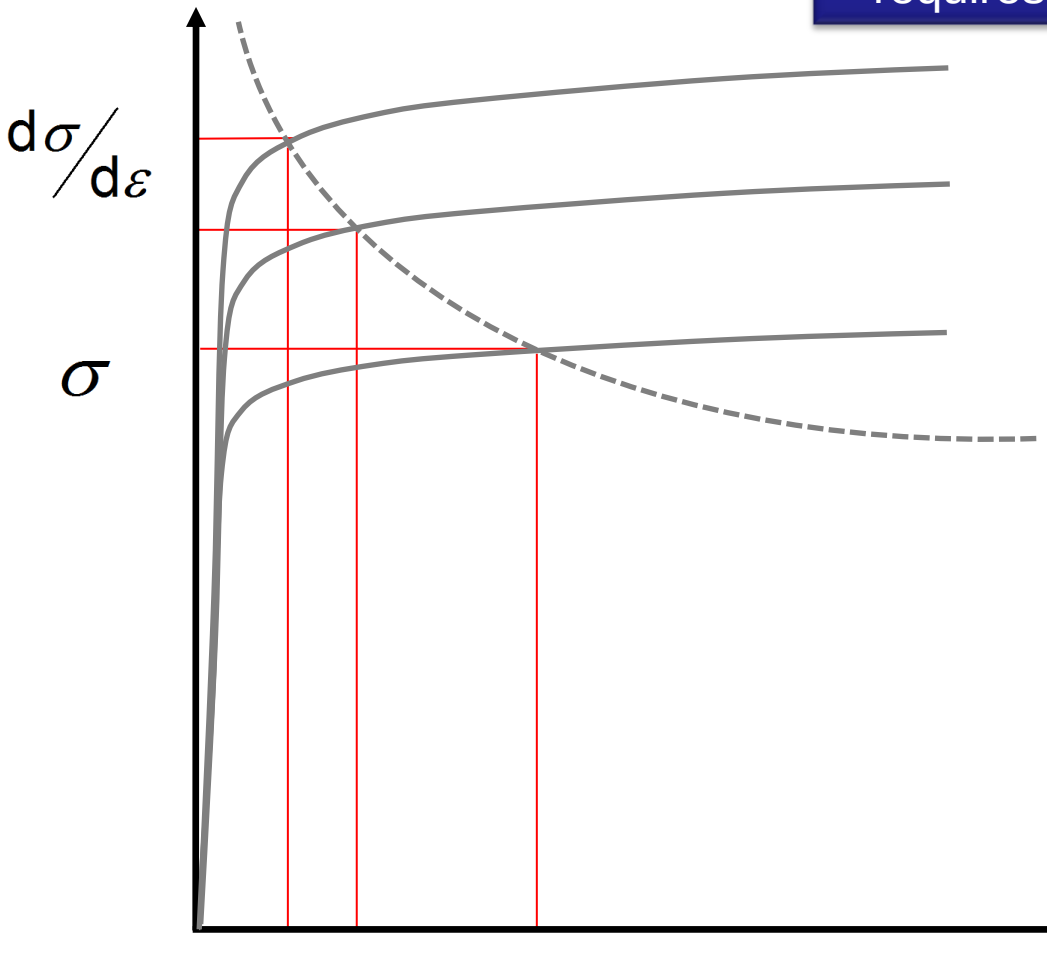


Inverse strength-ductility: phenomenological analysis



Inverse strength-ductility: phenomenological analysis

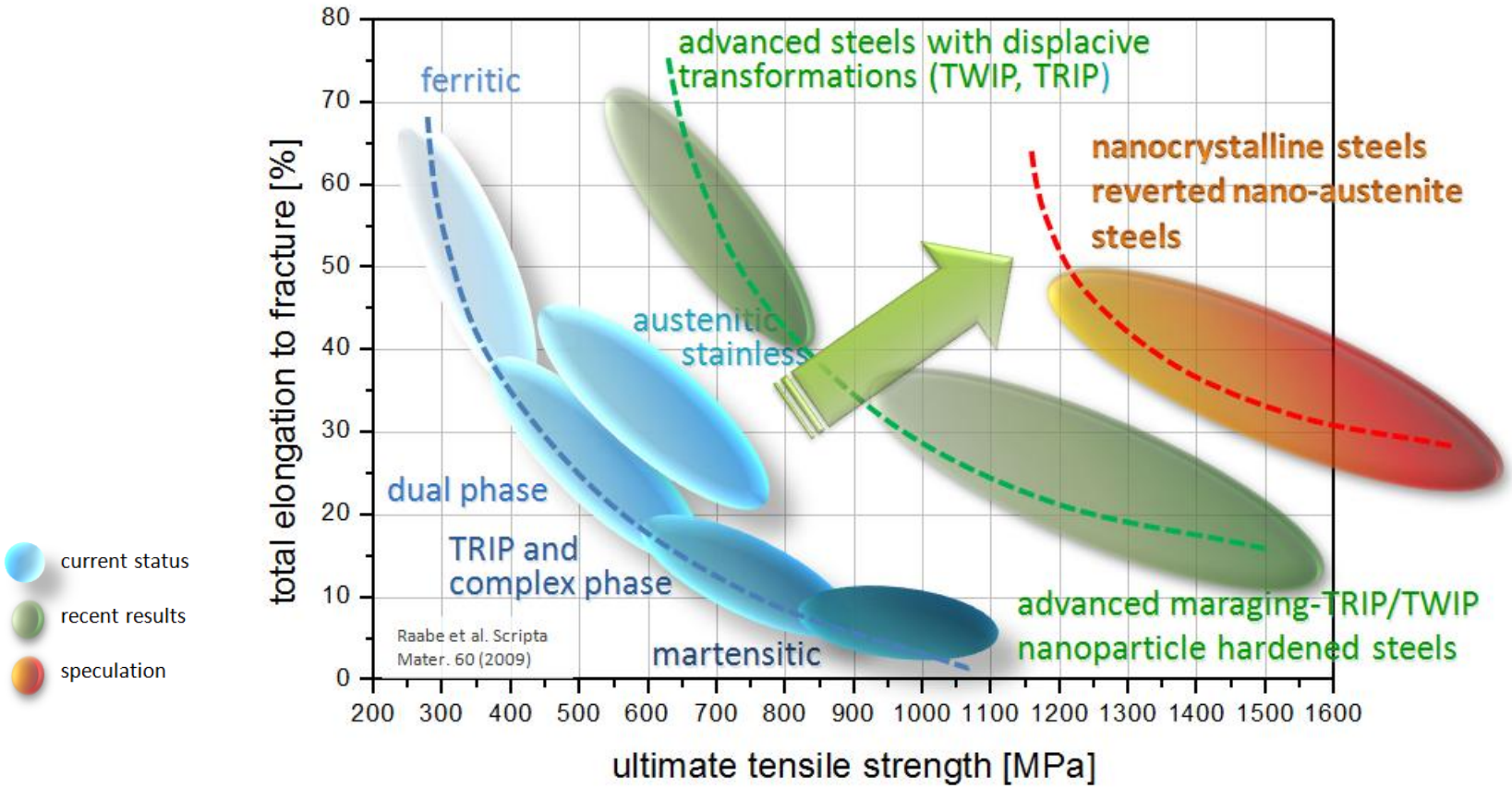
Design of ductile high strength alloys requires permanent strain hardening



ε true strain

σ stress

From atomistic understanding towards designing new materials



Inverse strength-ductility relation (strain hardening where needed, use smart mechanisms) ?

Limits of strength?

How to synthesize?

!

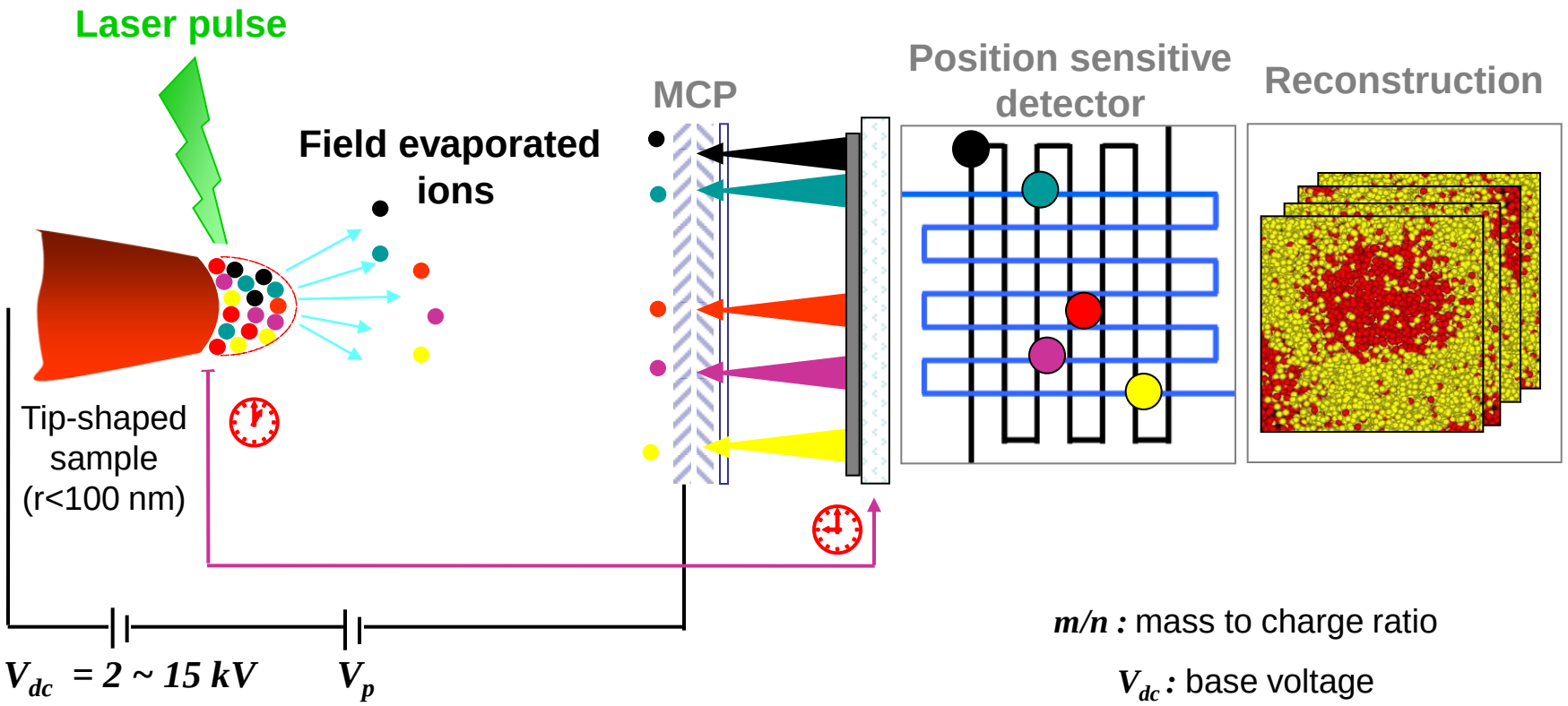
Ab initio modeling

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

Suited for designing steels?

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

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

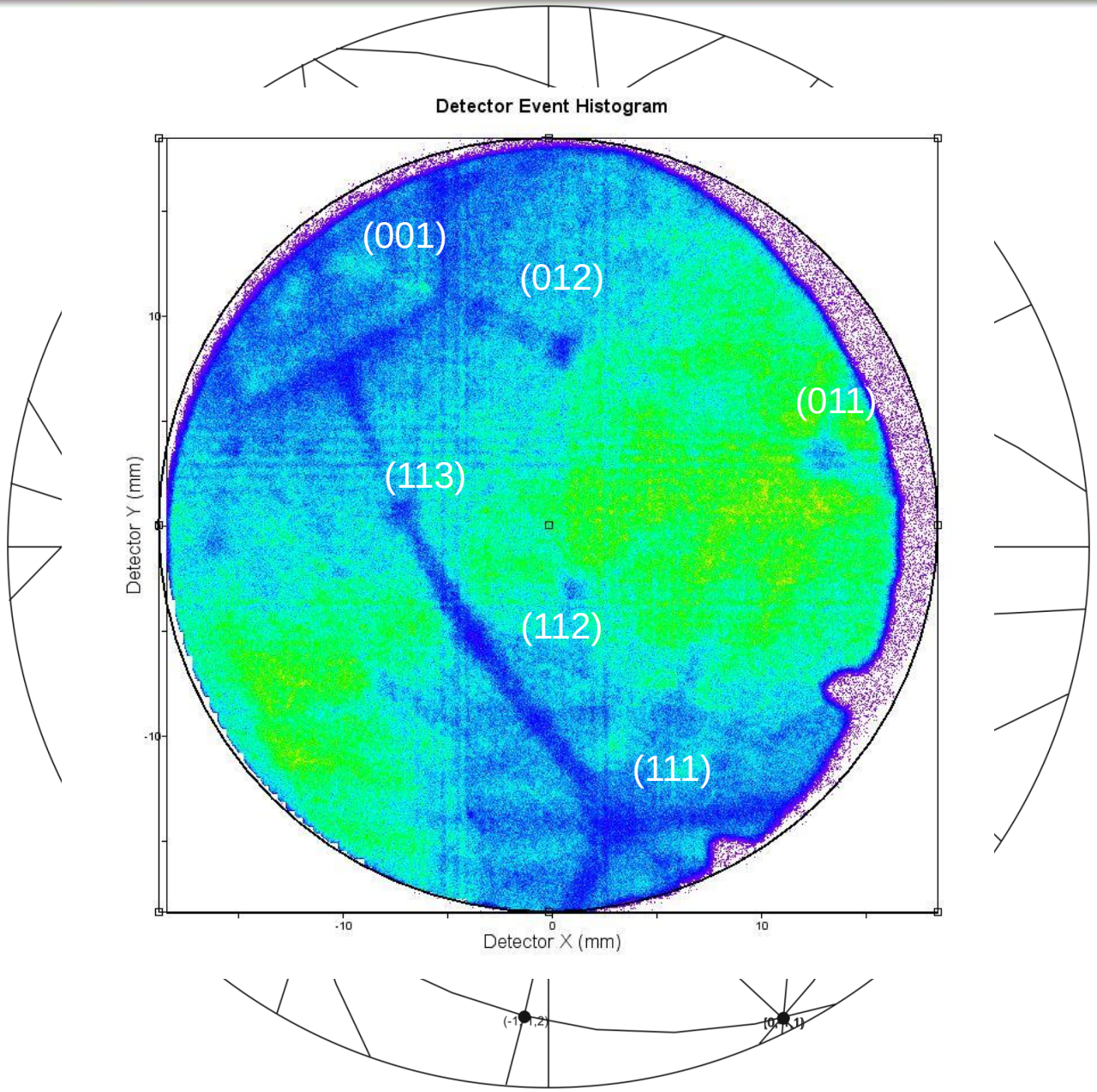
V_P **:** pulse voltage

t **:** time of flight

L **:** distance specimen - detector

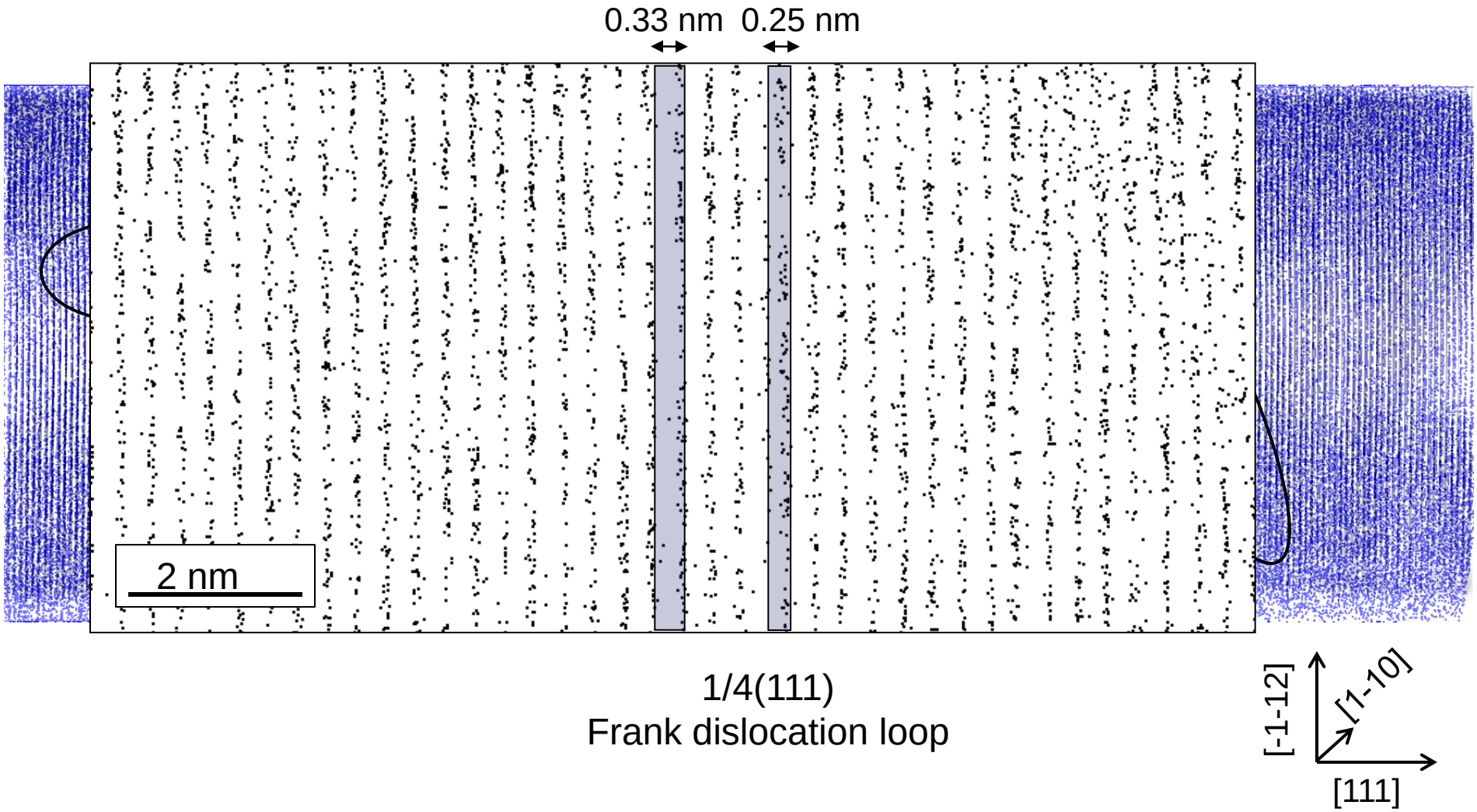
Dmitrieva et al. Acta Mater. 59 (2011) 364

Field desoprtion image

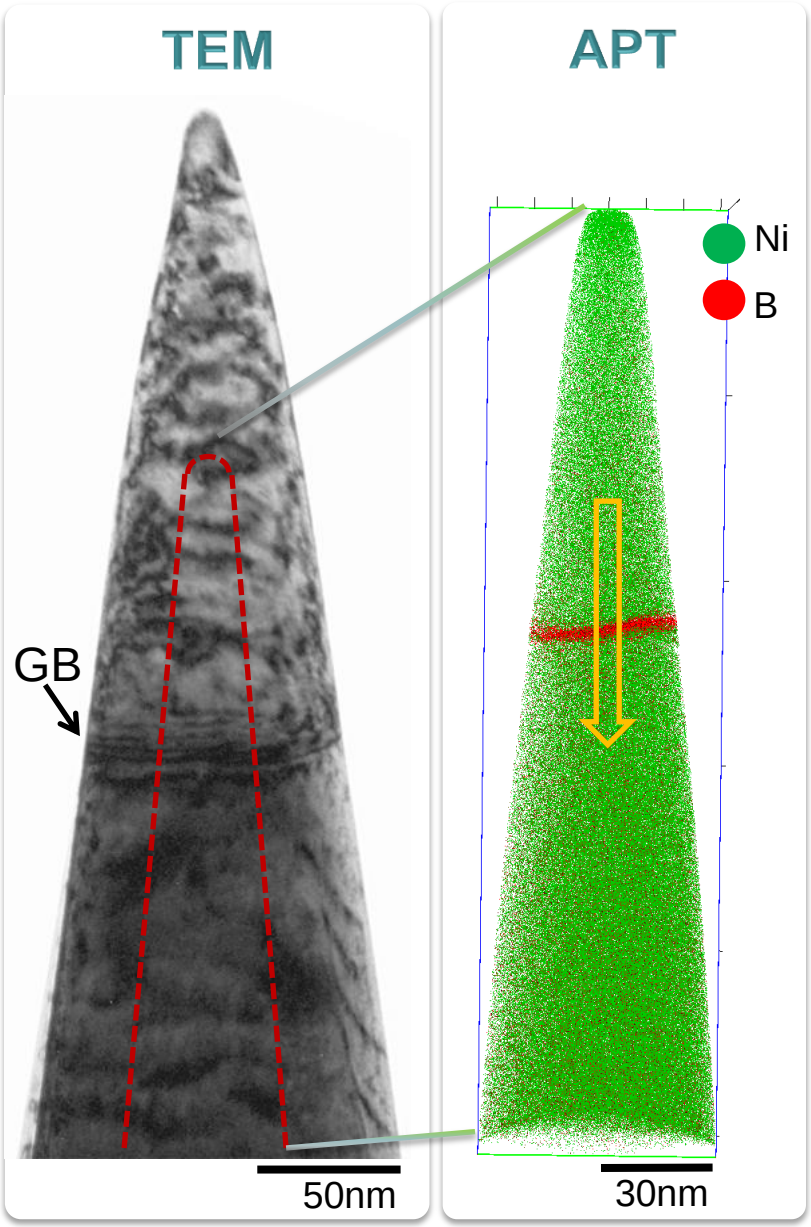


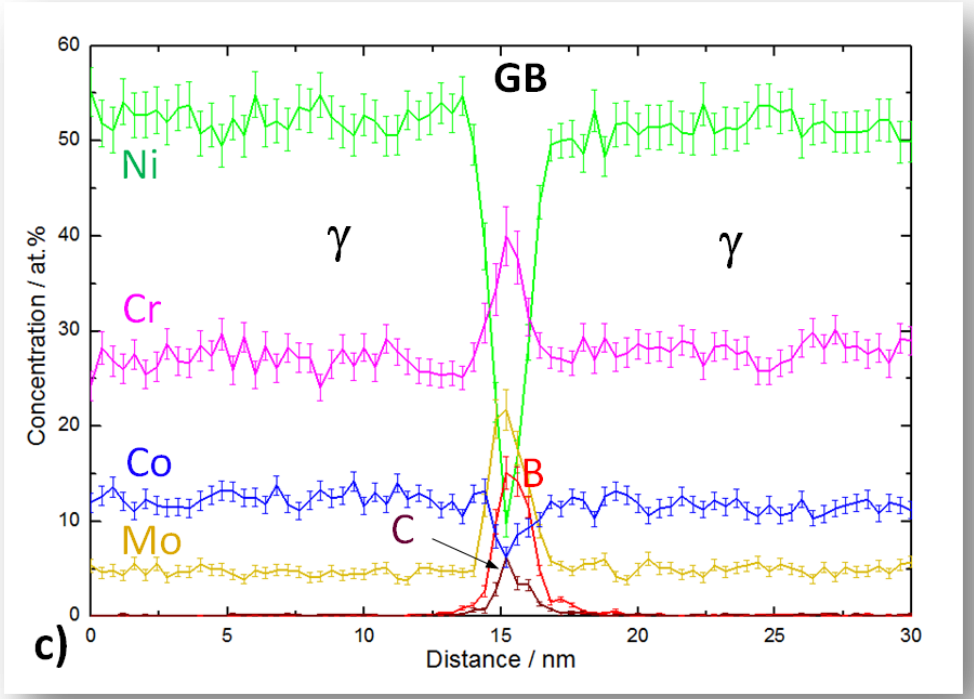
Lattice plane reconstruction

Fe_3Al ordered phase (only Al displayed)

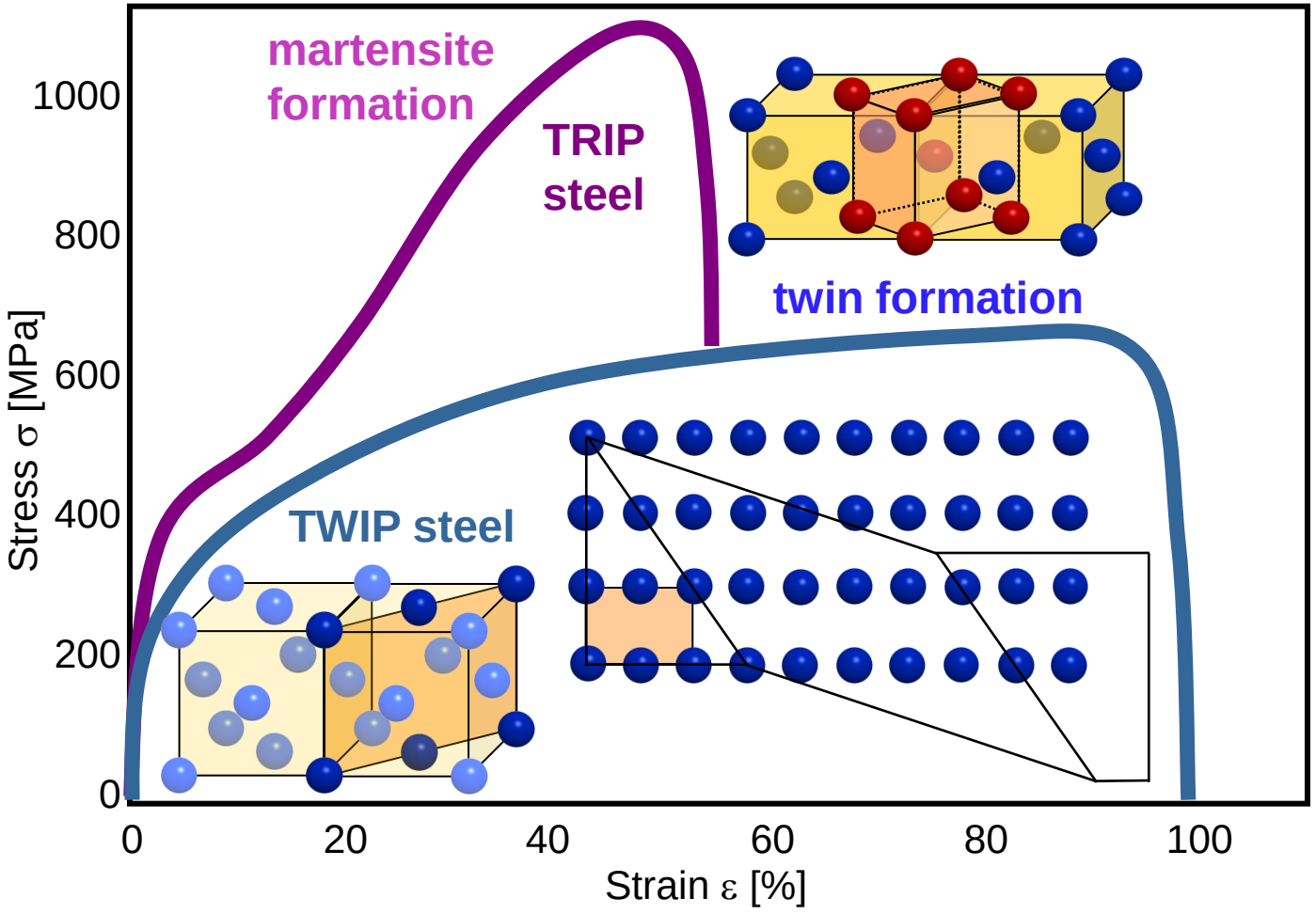


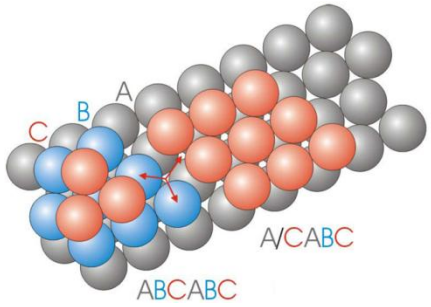
Joint TEM and APT analysis

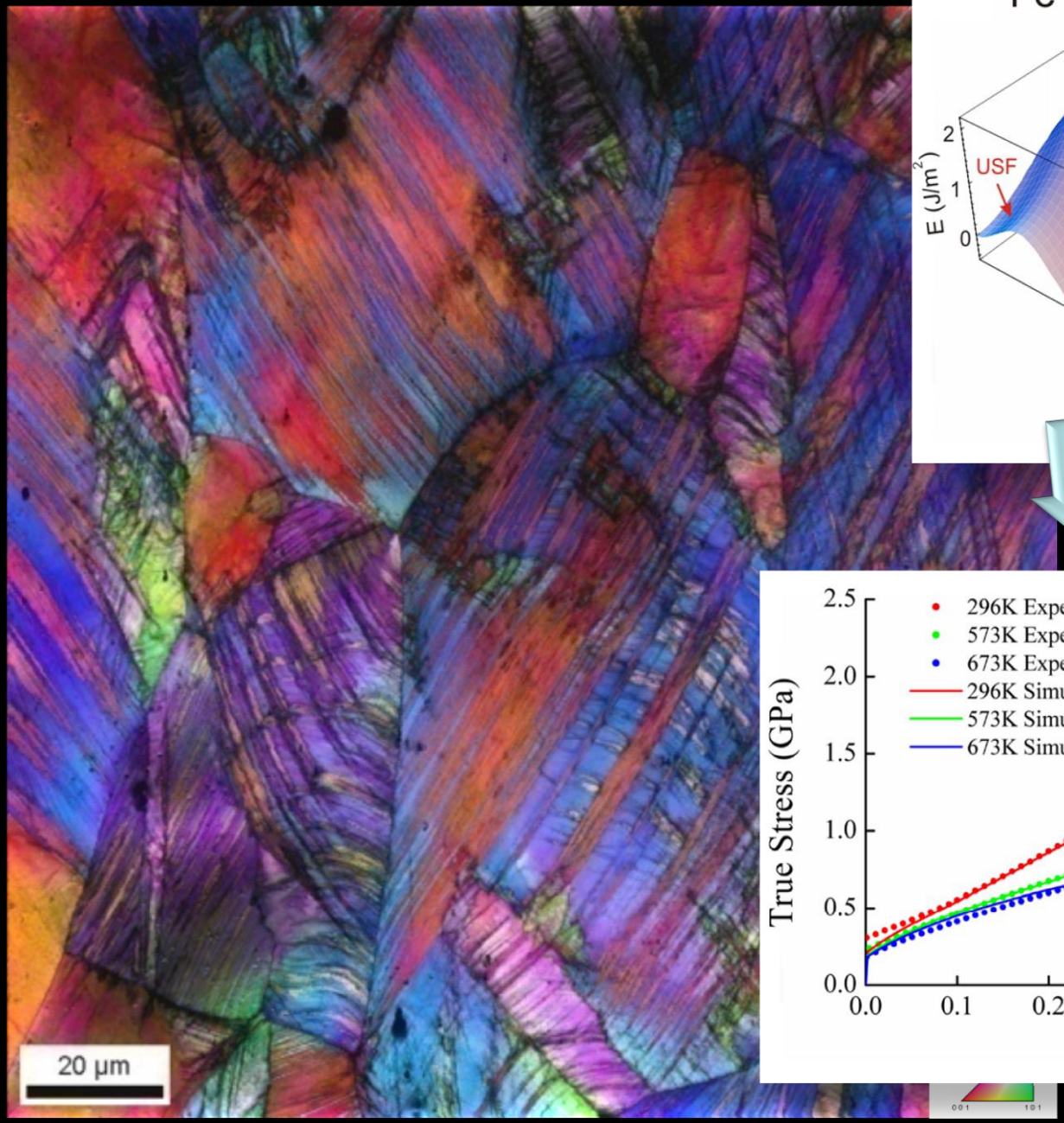


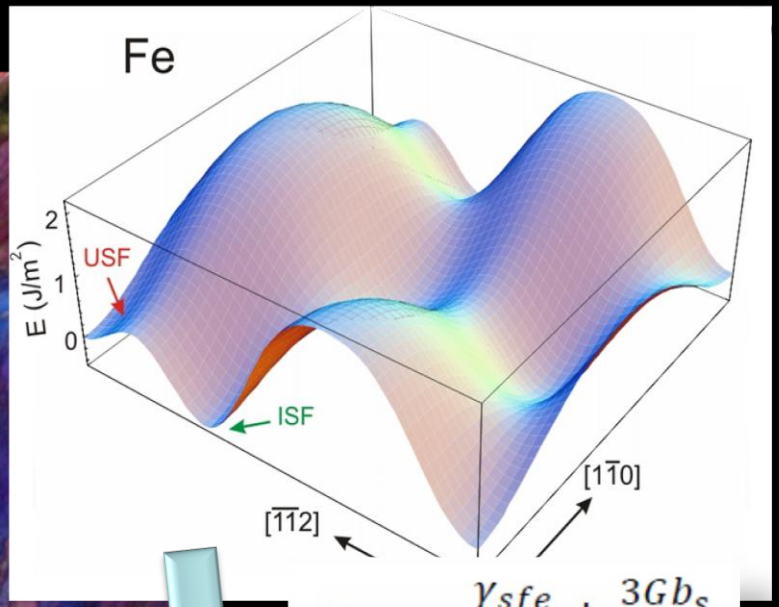


Ab-initio methods for the design of high strength steels

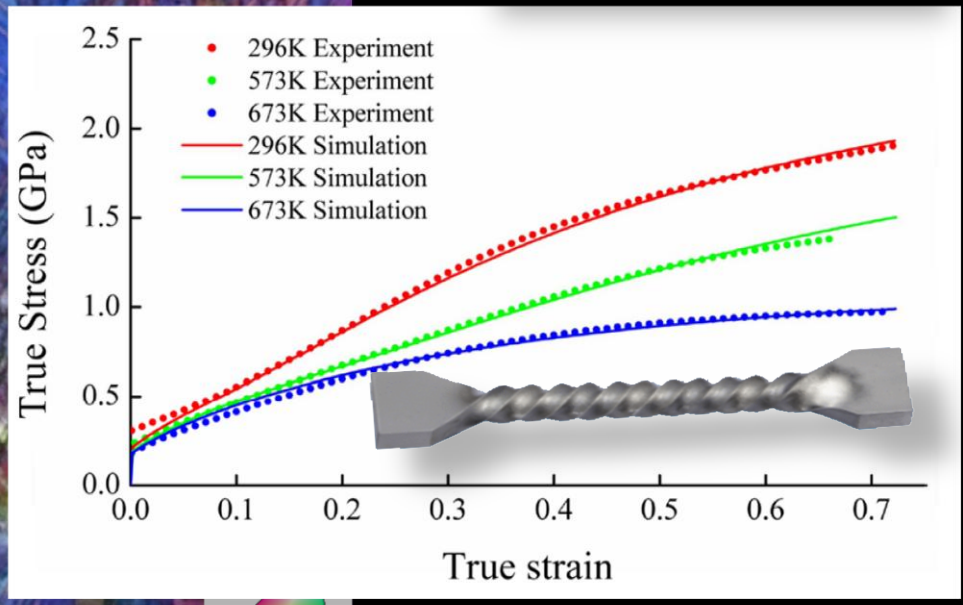








$$\tau_{tw} = \frac{\gamma_{sfe}}{3b_s} + \frac{3Gb_s}{L_0}$$



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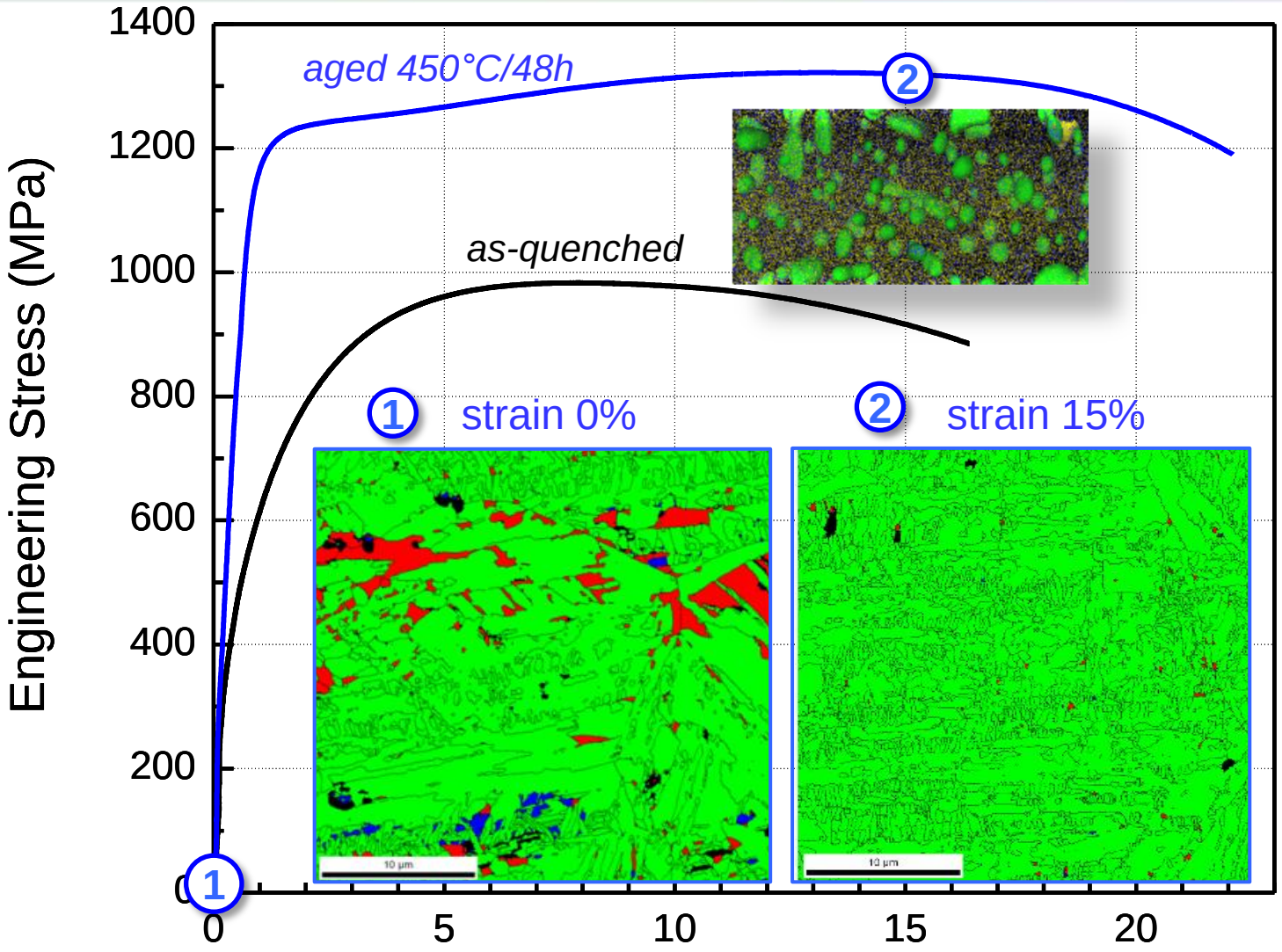
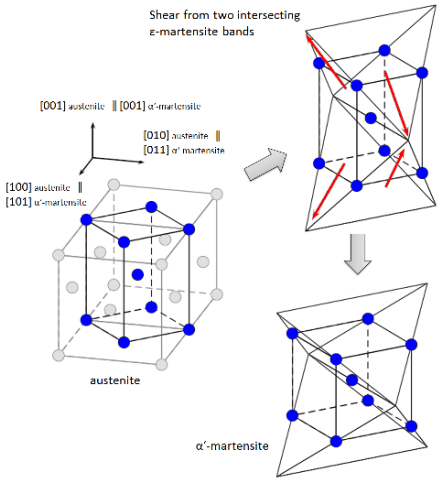
Raabe: Adv. Mater. 14 (2002)

Effect of aging on ductility



Precipitation hardening

increase of γ austenite fraction during aging



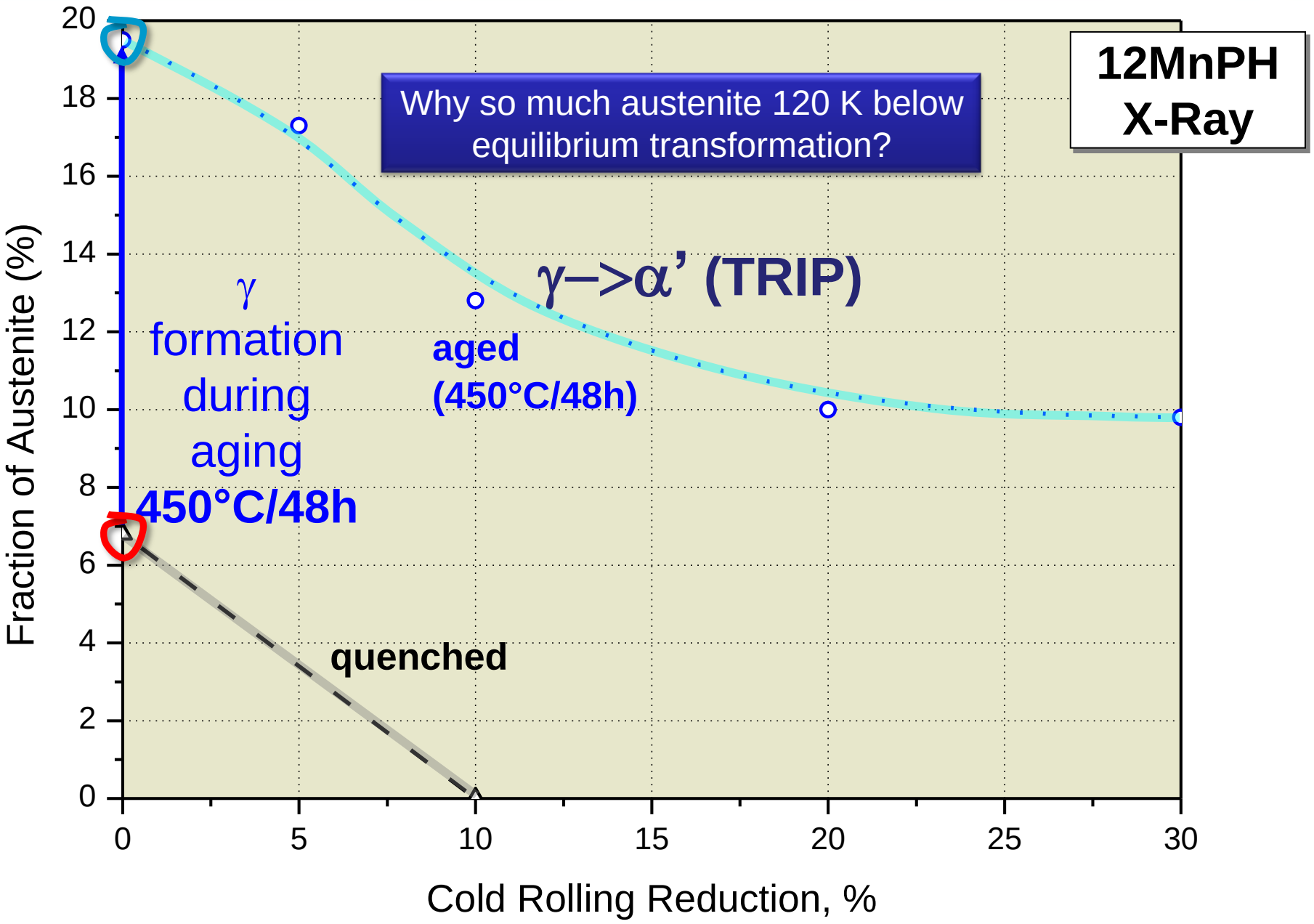
α-Fe (Martensite)

γ-Fe (Austenite), vol. fraction 15-20%

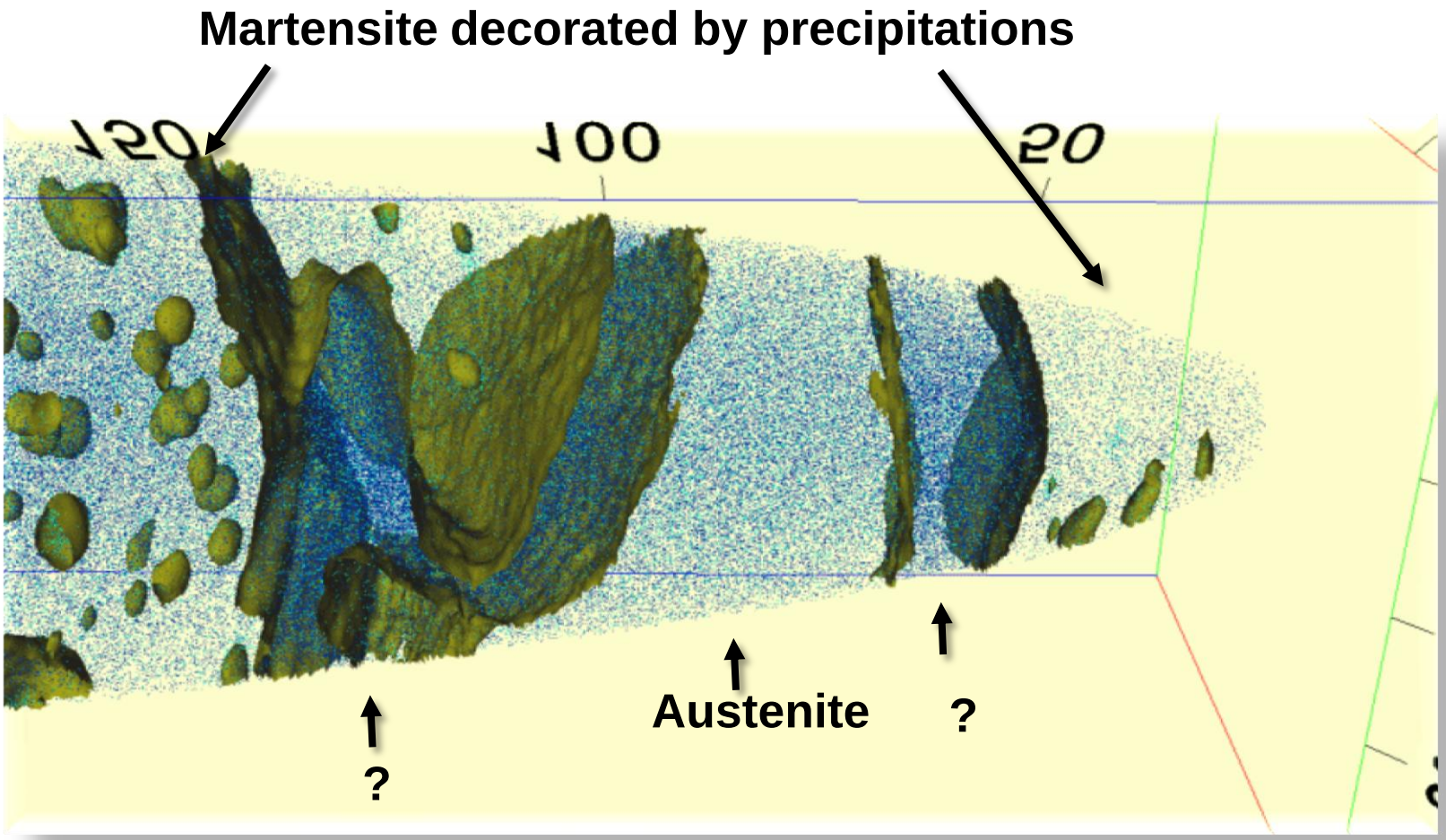
C	Ni	Mo	Ti	Al	Mn	Fe
0.01	2.0	1.0	1.0	0.15	12	bal.

D. Raabe et al. Scripta Materialia 60 (2009) 1141

Effect of cold rolling after aging



APT results: Atomic map (12MnPH aged 450°C/48h)



Mn atoms
Ni atoms
Mn iso-concentration: 18 at.%

C	Ni	Mo	Ti	Al	Mn	Fe
0.01	2.0	1.0	1.0	0.15	12	bal.

70 million ions
Laser mode
(0.4nJ, 54K)

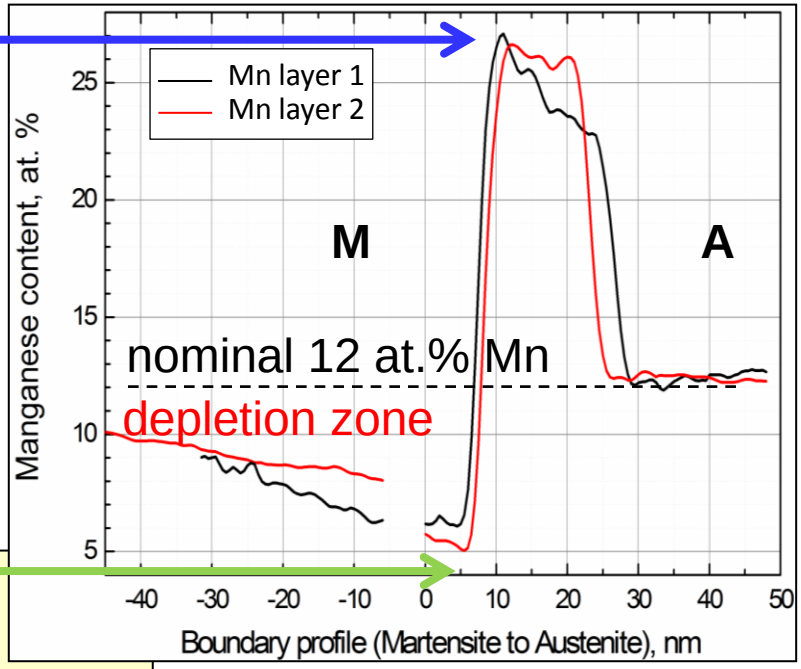
Aging-induced austenite reversion

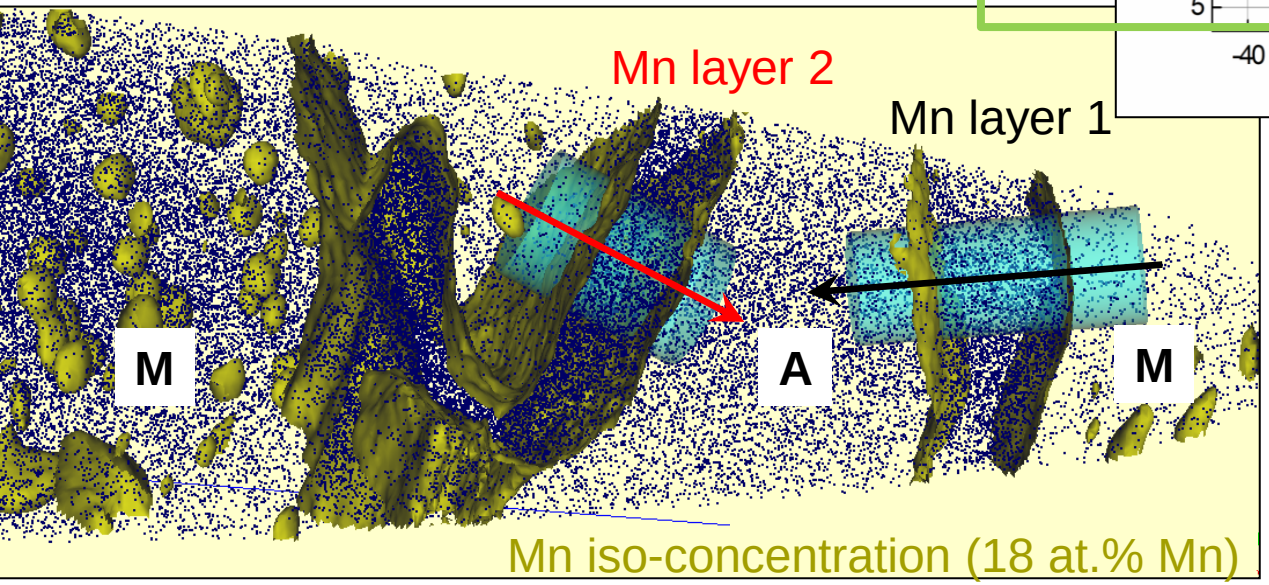
Thermo-Calc ⇒

equilibrium Mn-conc.:

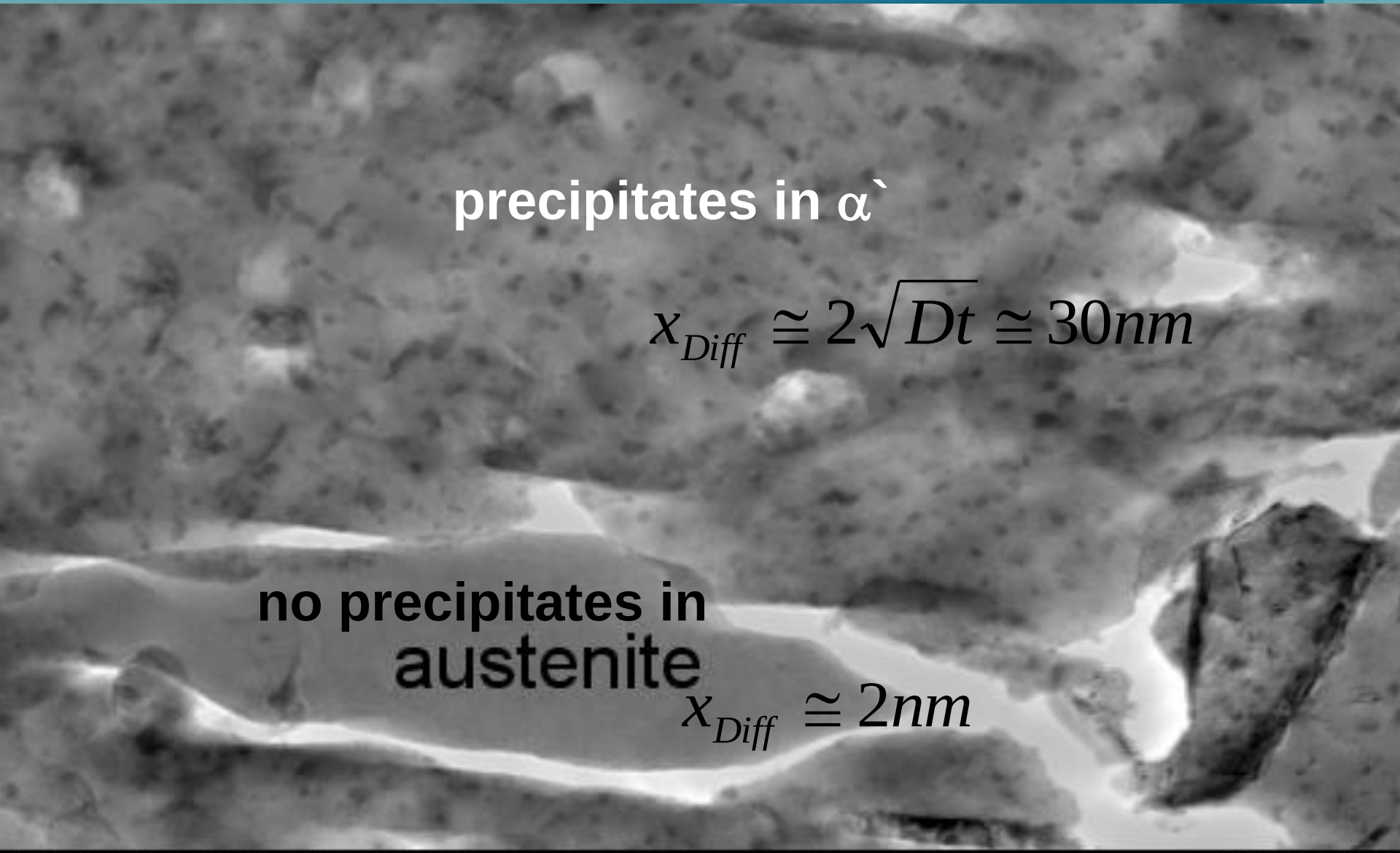
27 at. % Mn in austenite (A)

3 at. % Mn in ferrite (martensite) (M)





12MnPH after aging (48h 450°C)



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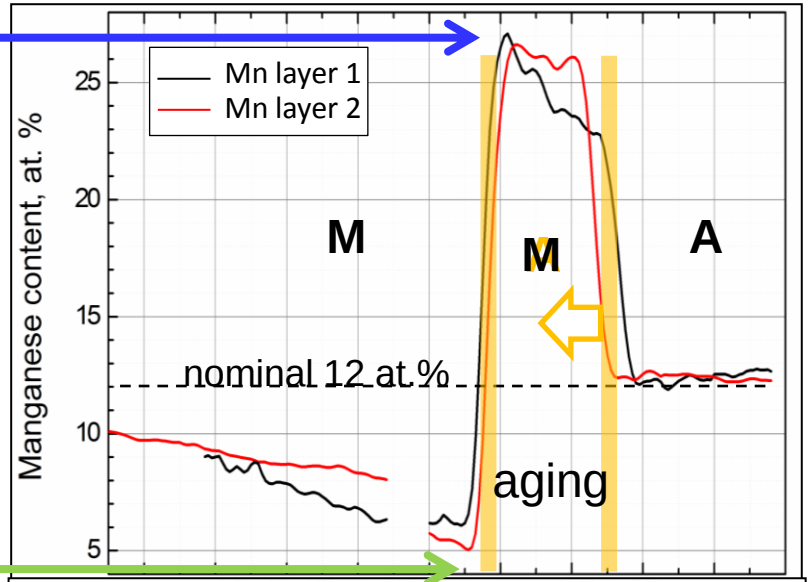
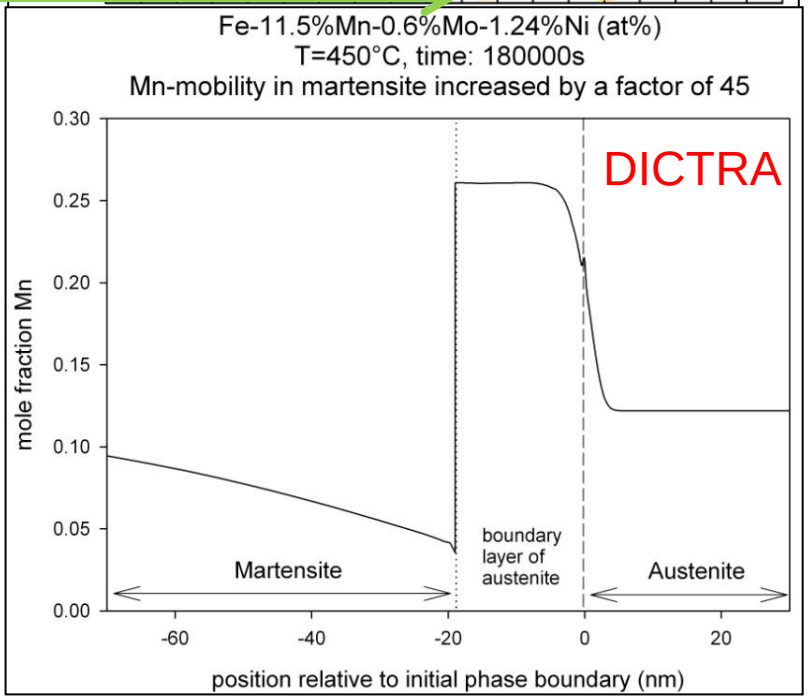
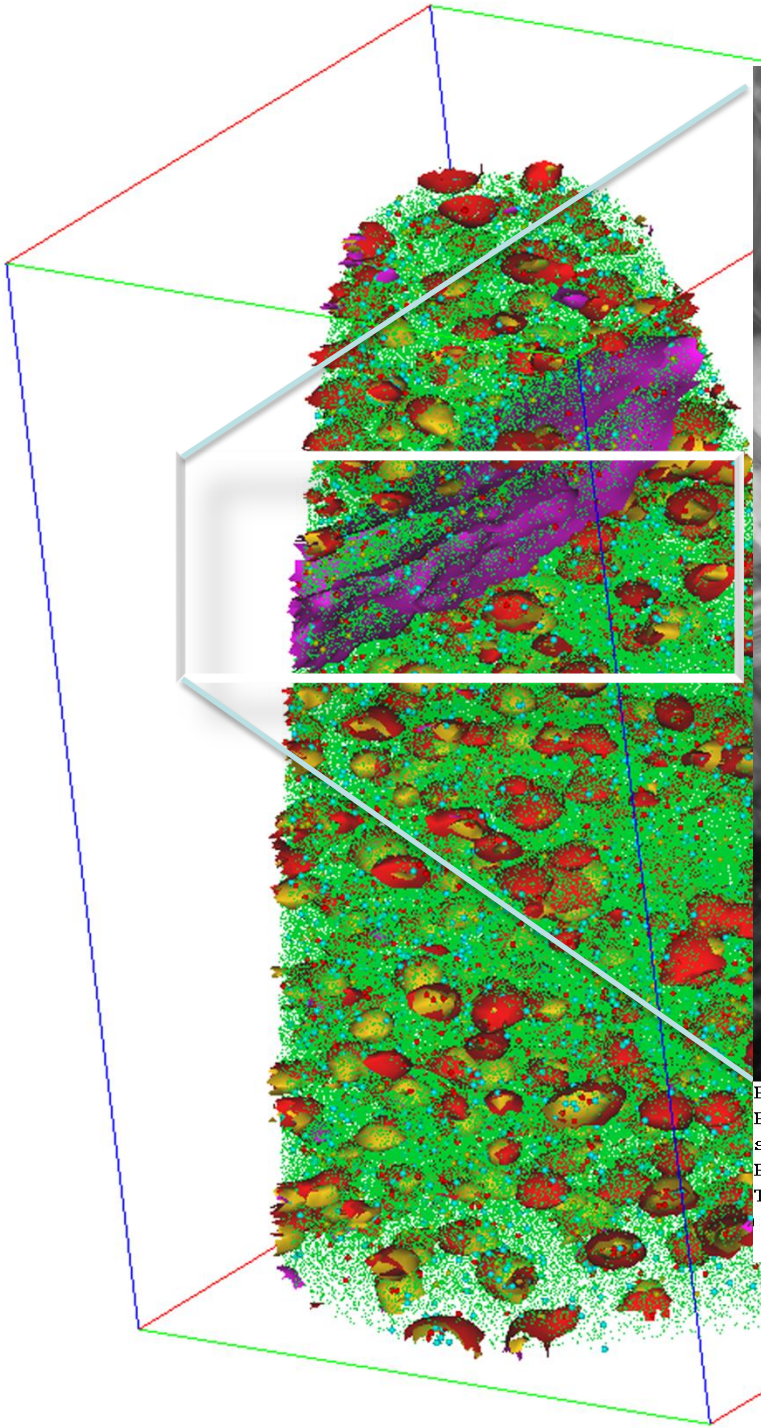
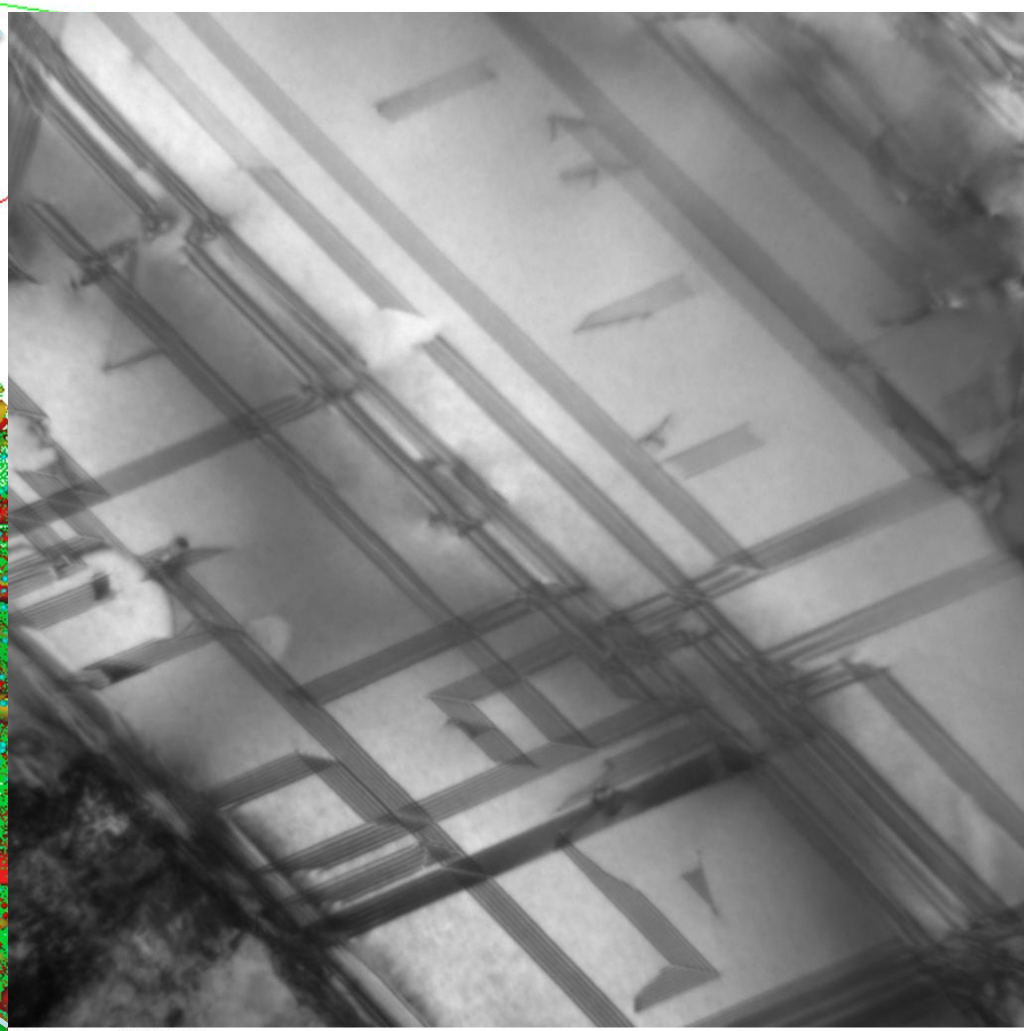




Excellent agreement between experiment & simulation !





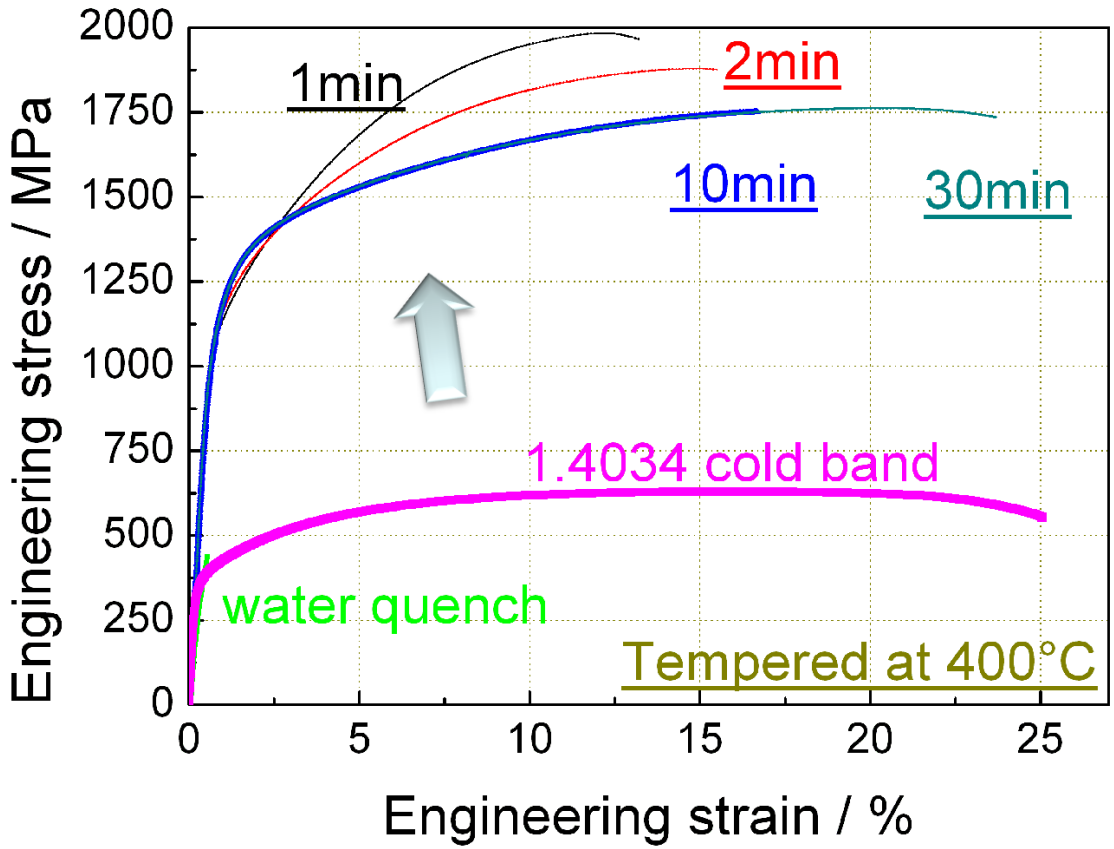
PR_proben003.tif
PR13 65h@450 C
stacking faults
Print Mag: 49500x @ 100 mm
TEM Mode: Imaging

100 nm
HV=200,0kV
Direct Mag: 44000x
X:-107.789 Y: 194.272
MPI f r Eisenforschung - CM20

10 nm

Martensite relaxation & aging & nanoscale austenite reversion

650 MPa to 2 GPa

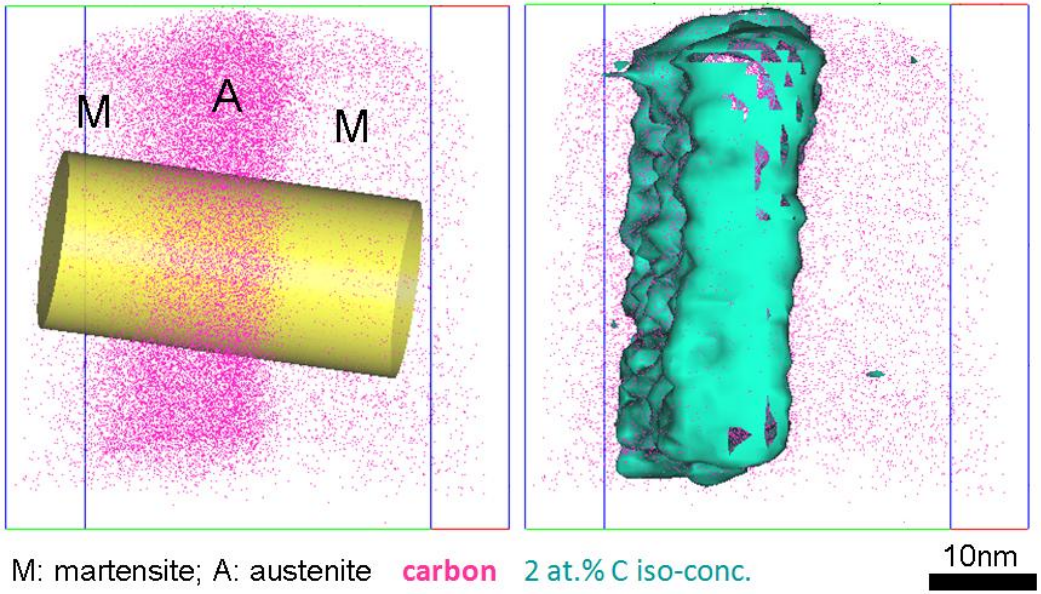


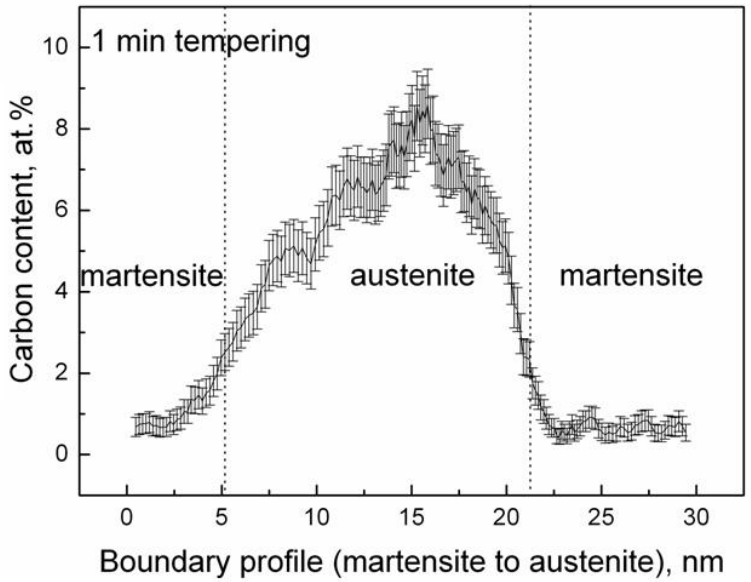
400°C aging: Ms-relaxation + prec. (aging) + austenite reversion

Fe-13.6Cr-0.44C (wt.%)

Martensite relaxation & aging & nanoscale austenite reversion

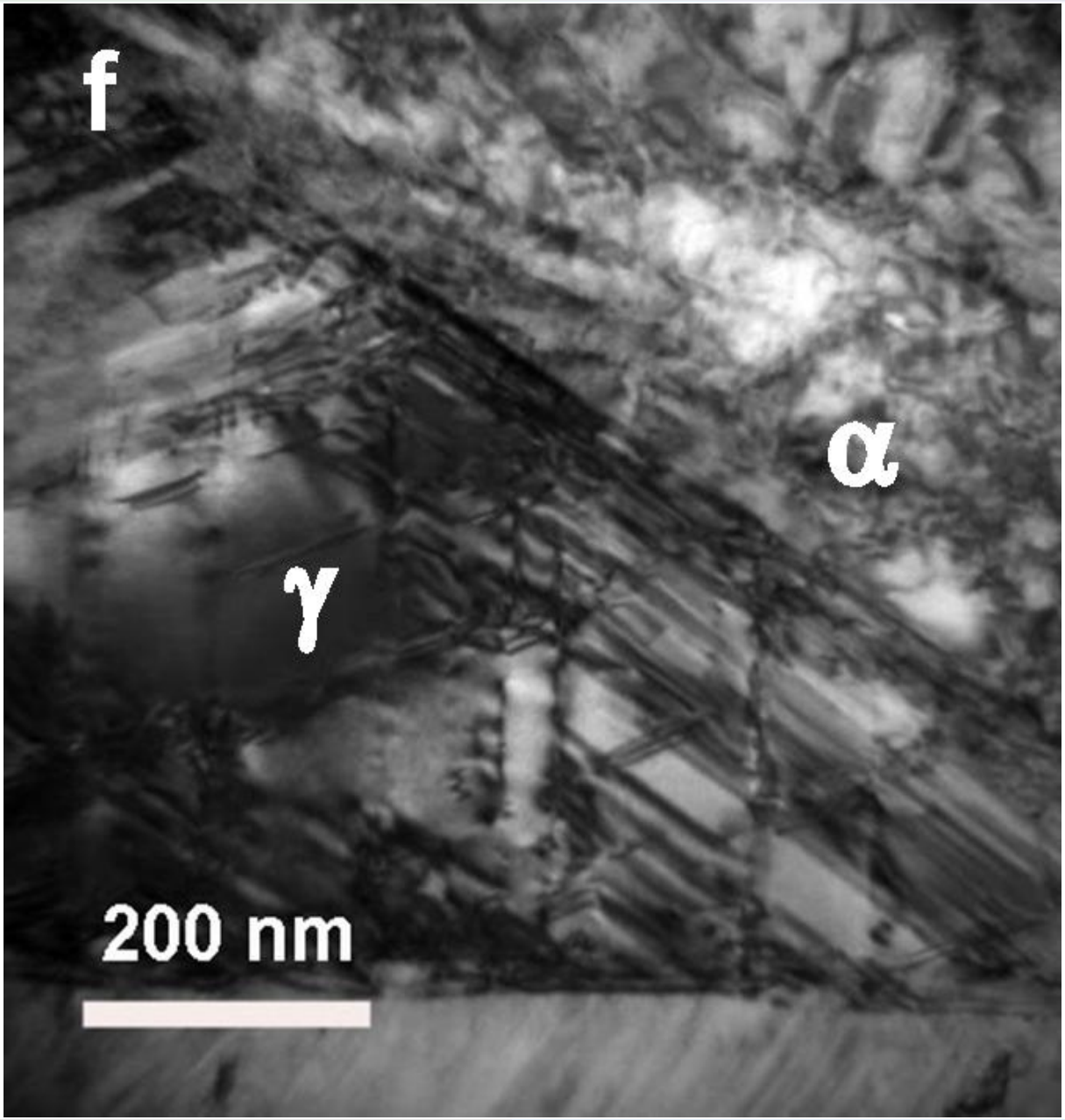
at 5.45 at.% C, austenite forms at 400°C





Microstructure development

400° C
1min



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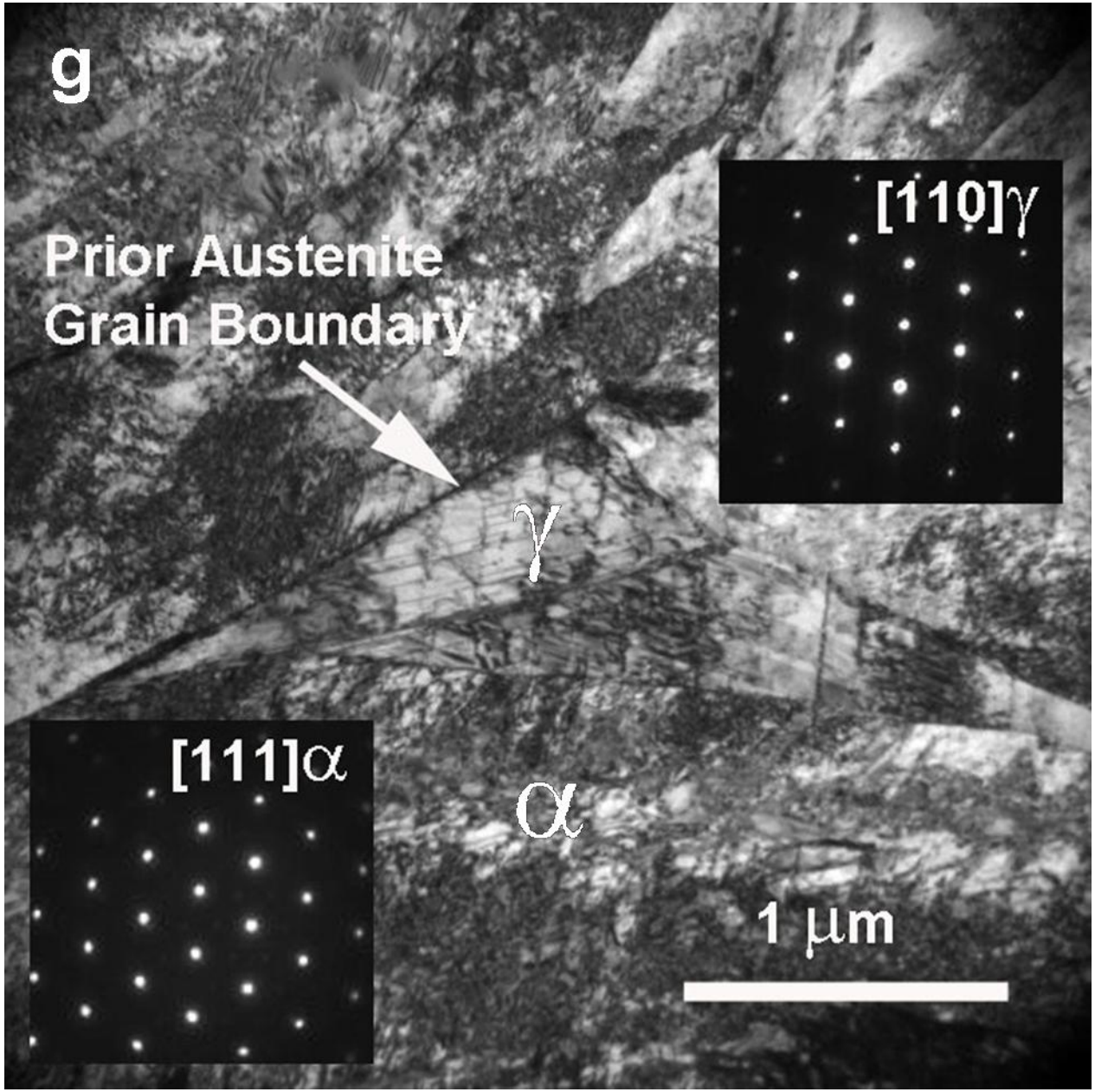
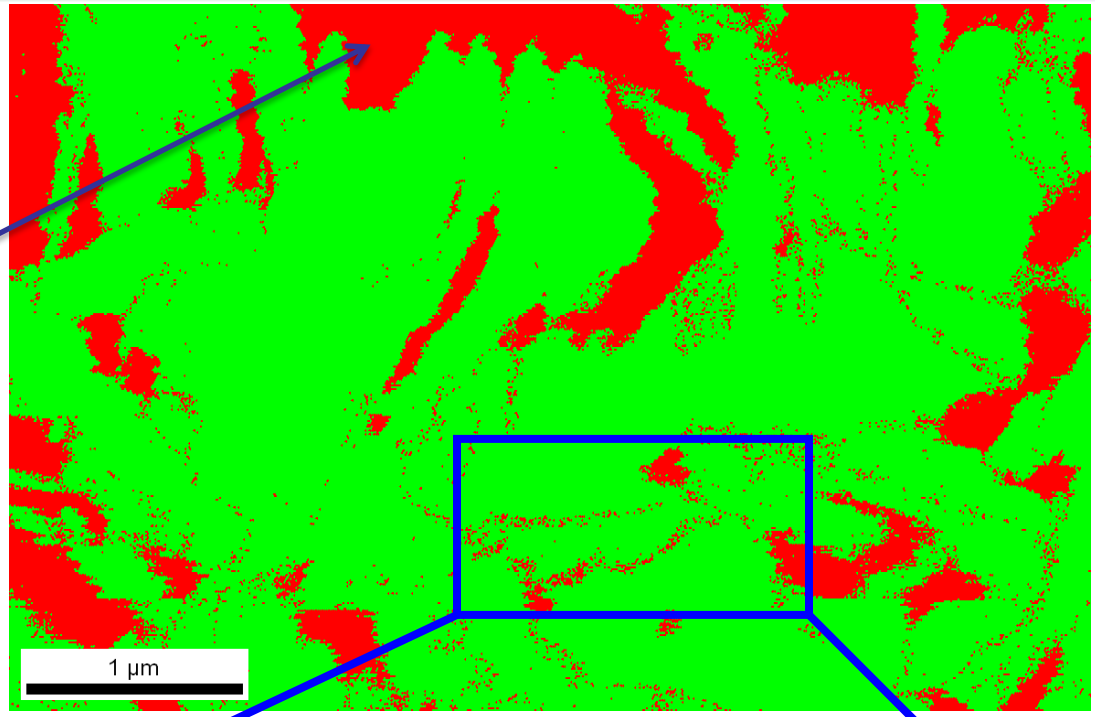


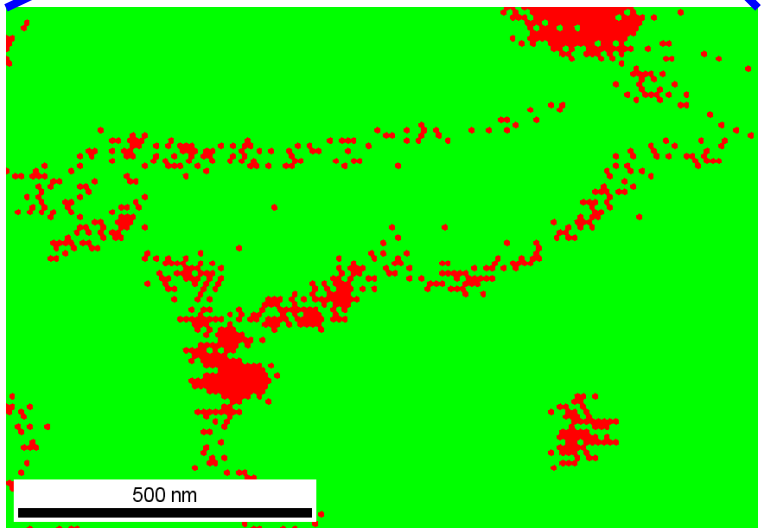
Self-repair steels

Retained austenite



Phase
Iron - Gamma
Iron - Alpha

Reversed austenite



Self-repair steels