Atomistic understanding of hundred thousand tons: the new steel story

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Self-organized nanostructuring by selective phase transformation

Motivation for nanostructuring alloys via self-organization:

Properties of alloys change profoundly at nanoscale (mech. properties)

Self organization essential for nanostructuring large quantities: e.g. steels: 1.4 Billion t/a; aluminum: 24 Million t/a; titanium: 150 Thousand t/a

Can be applied to many metallic alloy systems that are the backbone of modern societies

Complexity of engineering alloy design, manufacturing, use

Design alloys

Solidification

Processing

Great products

Knowledge-based
(ab-initio, DFT, GGA)

'Rapid' solidification
(of 100 tons)

TMP - induced
nanostructures

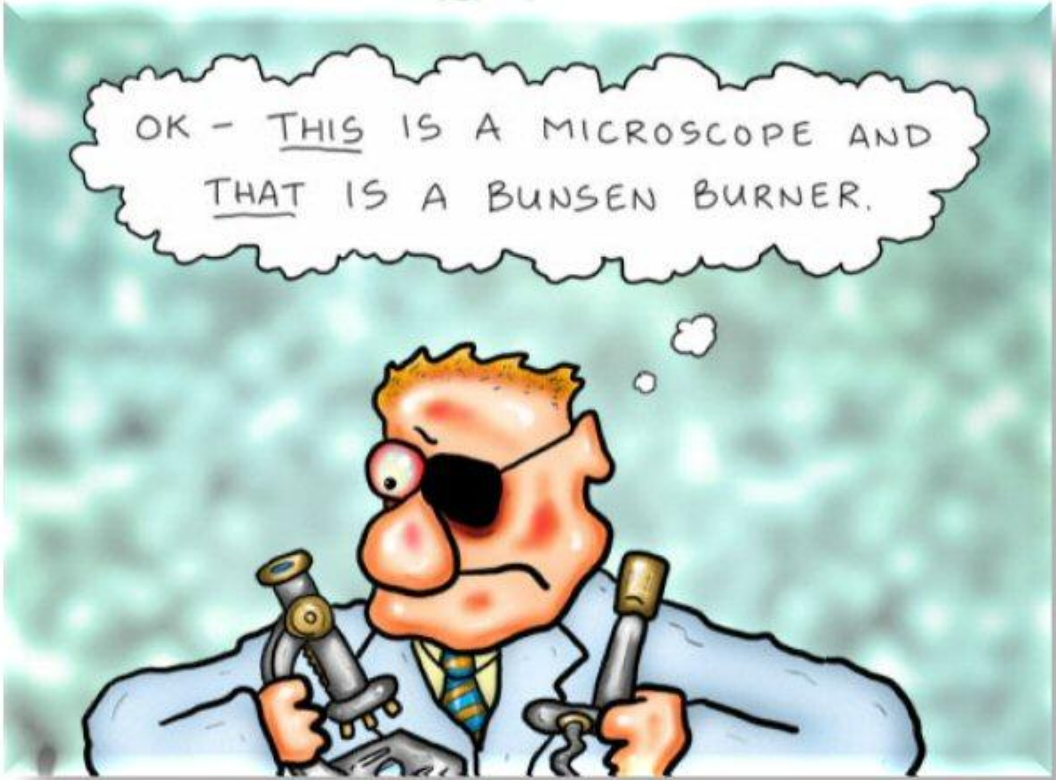
Design complexity

Get the right tools for the job:

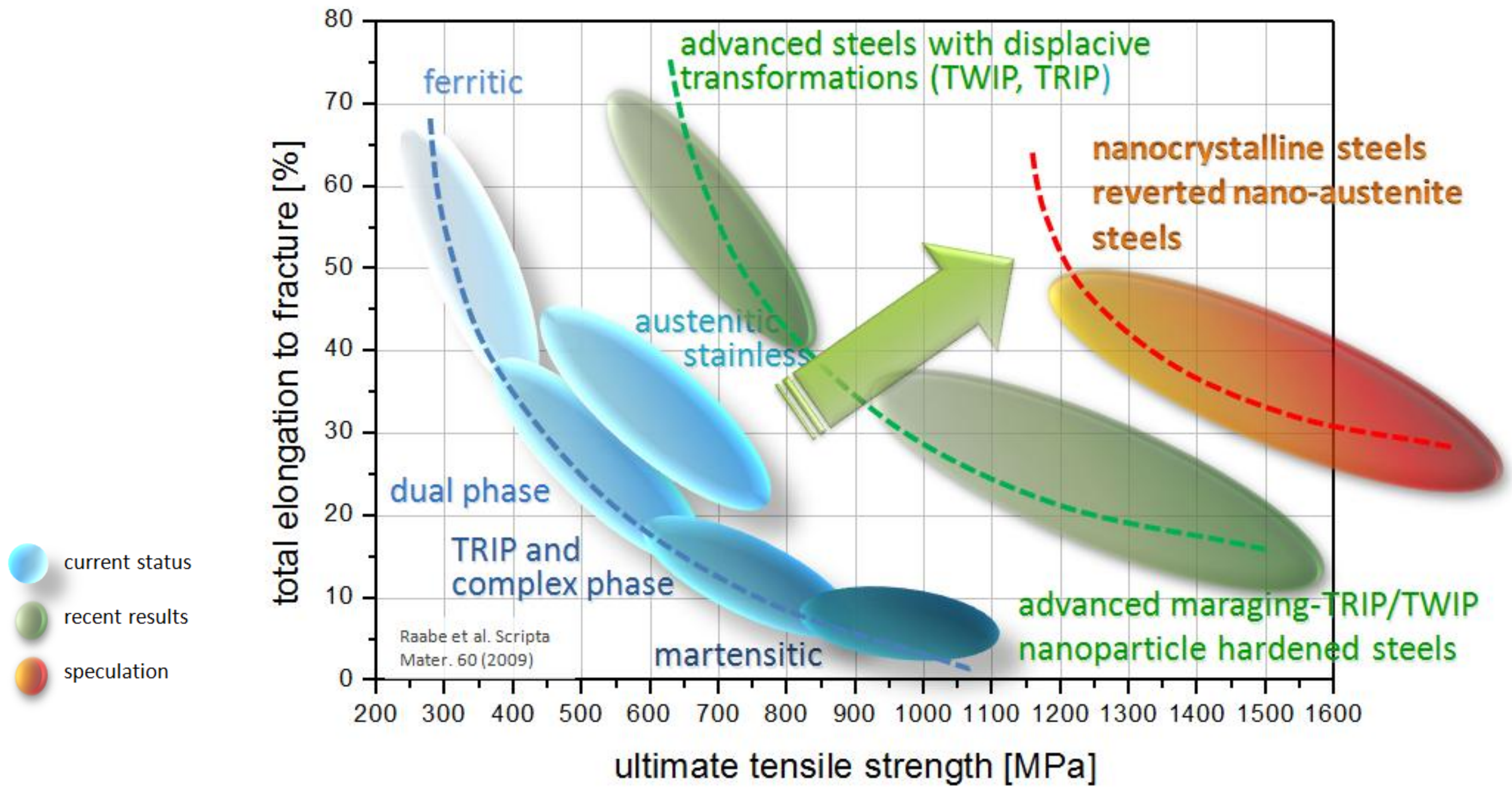
Models, characterization, new mechanisms, synthesis

things that don't work

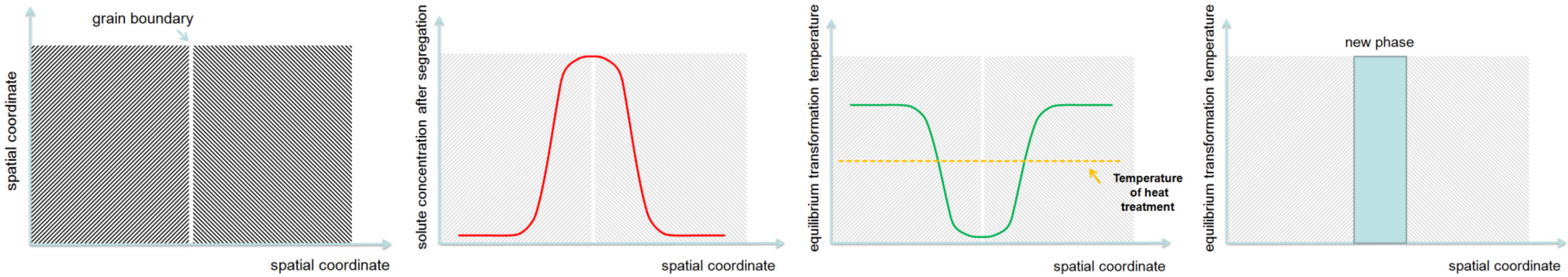
things that work



From atomistic understanding towards designing new materials



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



Driving force for solute decoration

- Gibbs adsorption isotherm: equilibrium segregation
- Non-equilibrium segregation (additional point defects)
- Kinetic freezing

Hetero-Interfaces   Homophase-Interfaces

Dmitrieva et al. Acta Mater 59 (2011)

Compositions in mass%: new lean maraging steels

Steel	C	Ni	Co	Mo	Ti	Al	Mn	Fe
Maraging	0.01	18	12	4	1.6	0.15	0.05	Balance
09MnPH	0.01	2	-	1	1.0	0.15	9	Balance
12MnPH	0.01	2	-	1	1.0	0.15	12	Balance
15MnPH	0.01	2	-	1	1.0	0.15	15	Balance

Low carbon: ductile martensite

Precipitation Hardenable

Mn (+Ni): austenite (TRIP)

Vacuum induction melting

Annealing

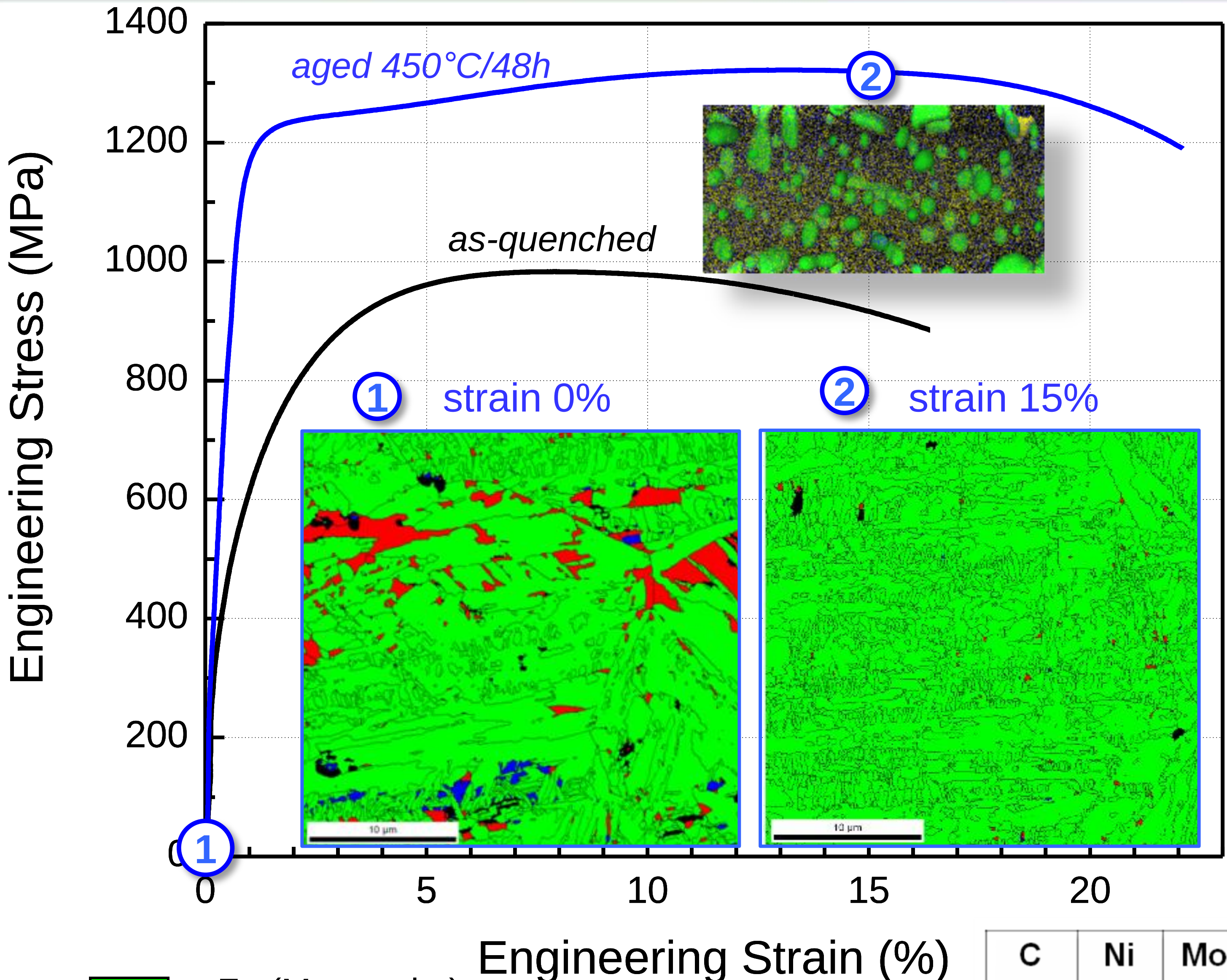
Hot deformation

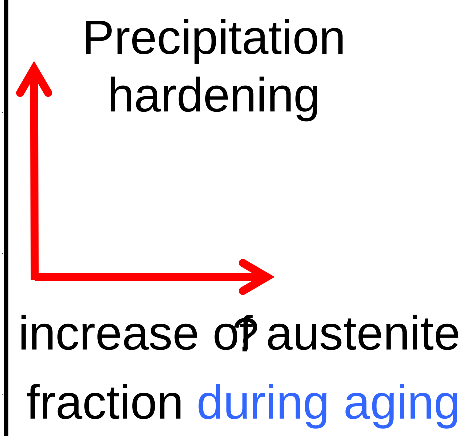
Solution heat treatment

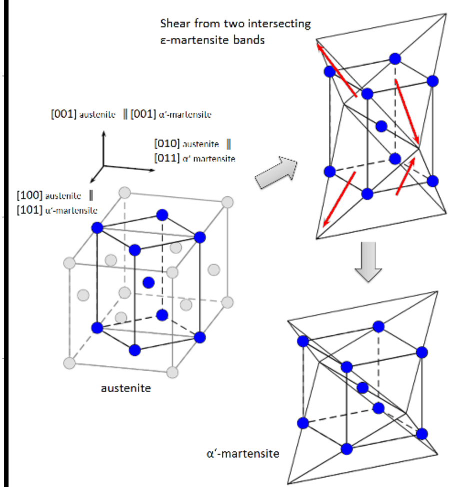
Quenching ⇨ Martensite + retained austenite

Aging (450°C) “Maraging“ retained + new austenite

Effect of aging on ductility



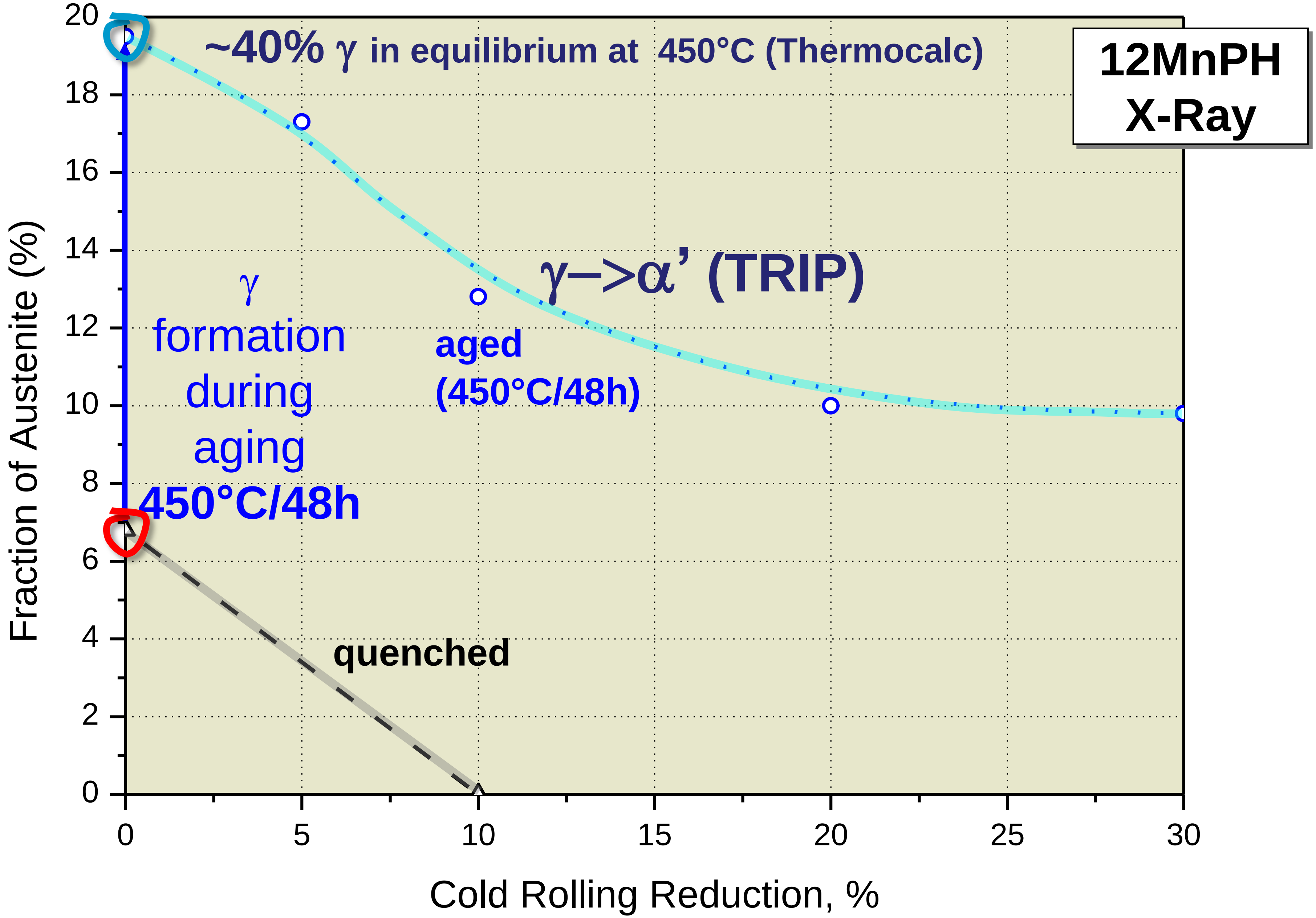




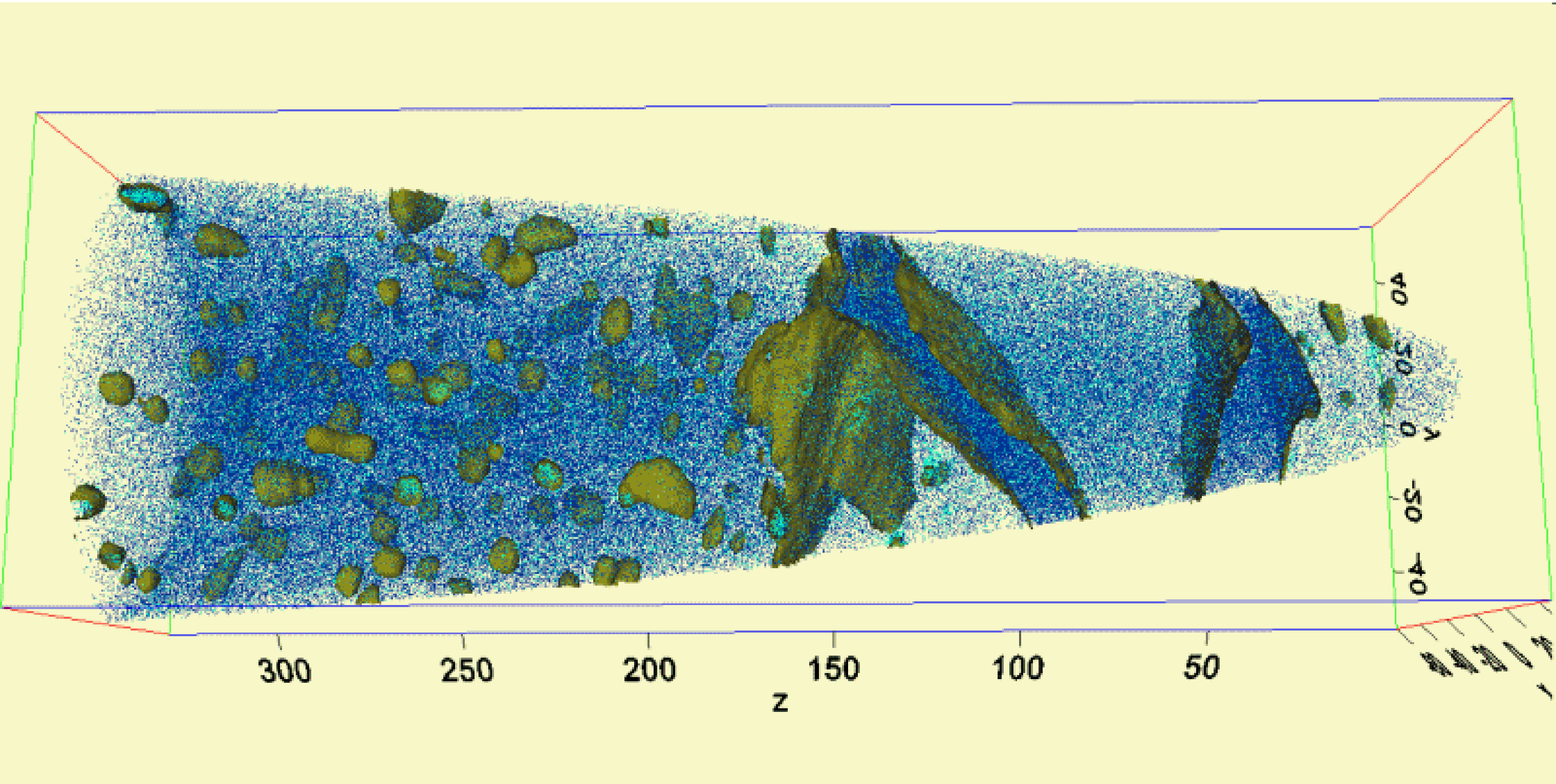
α-Fe (Martensite)
γ-Fe (Austenite), vol. fraction 15-20%

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

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)

Dmitrieva et al. Acta Mater 59 (2011)

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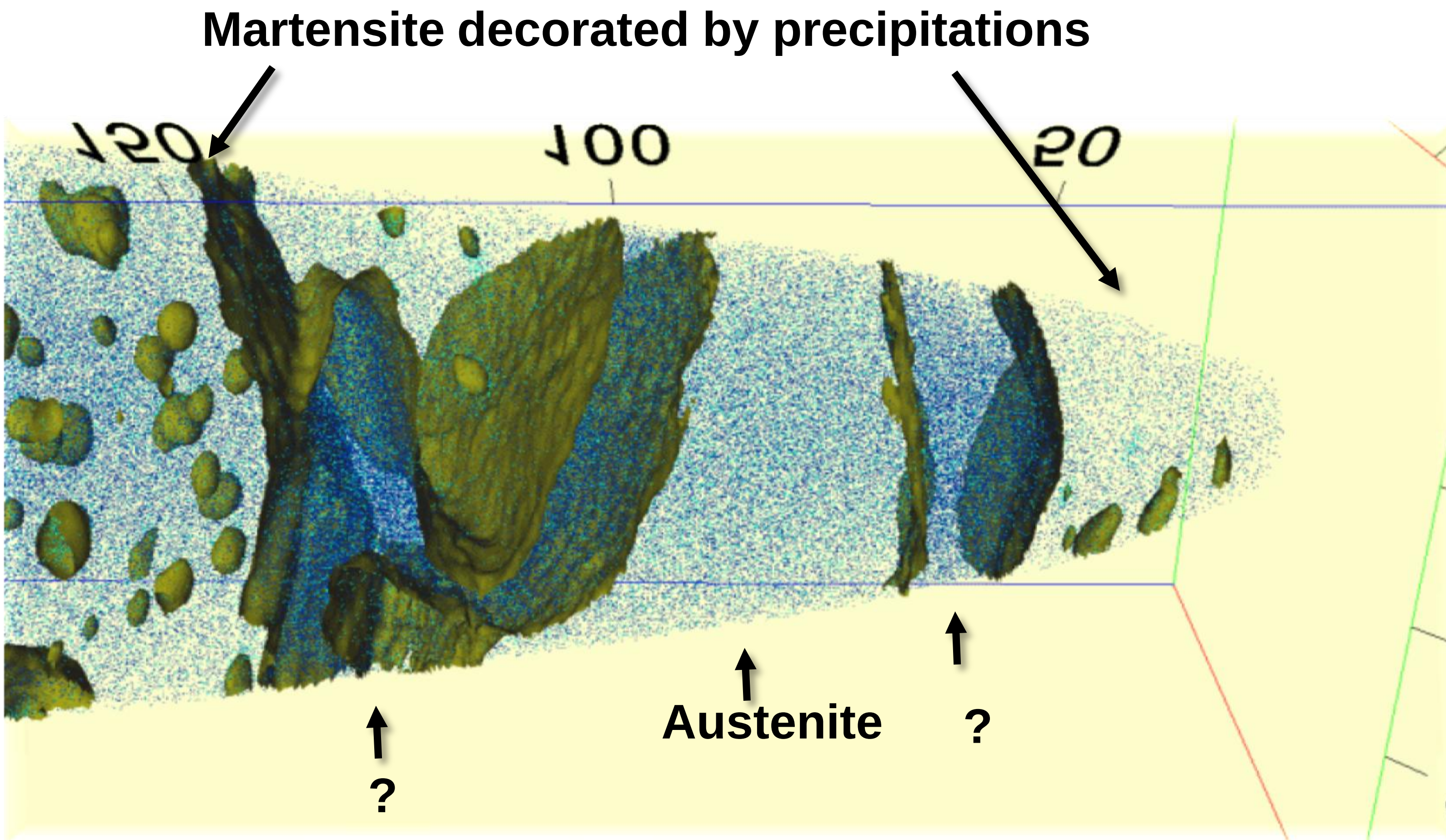

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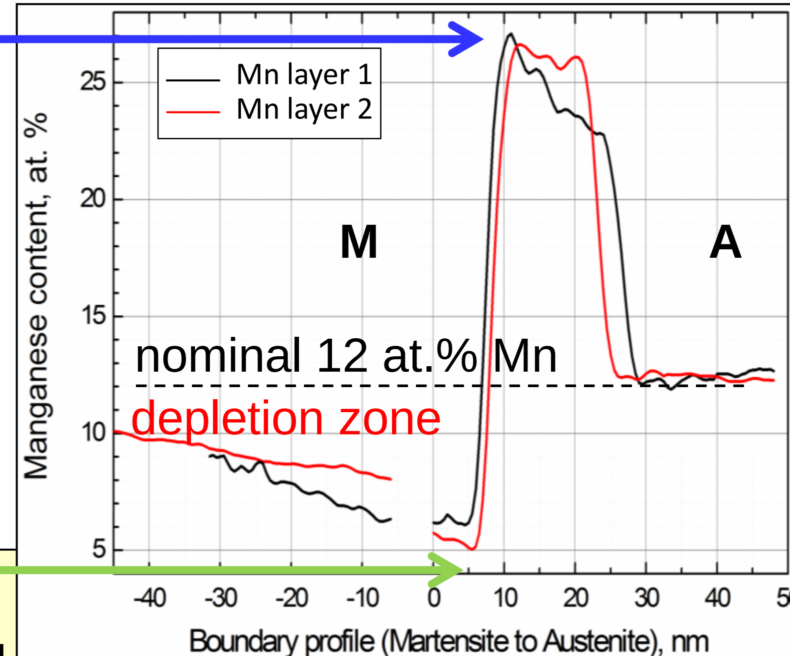
Aging-induced austenite reversion

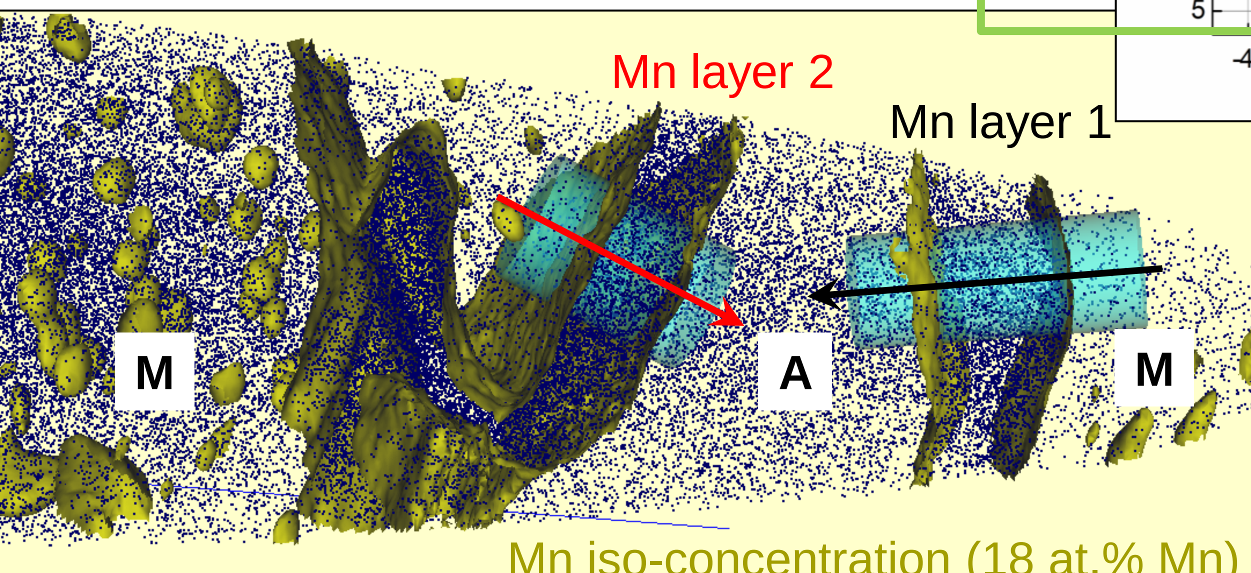
Thermo-Calc ⇒

equilibrium Mn-conc.:

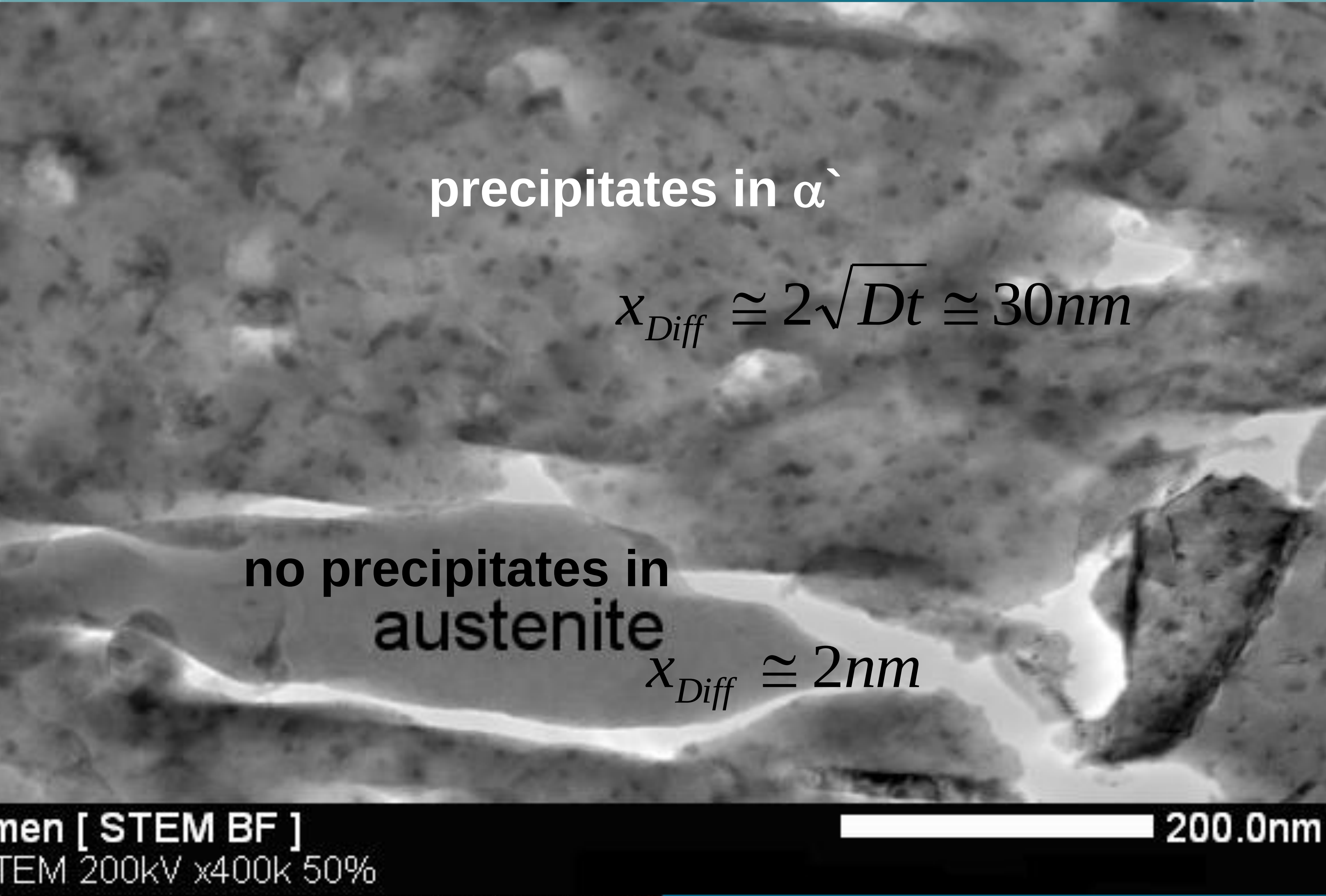
27 at. % Mn in austenite (A)

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





12MnPH after aging (48h 450°C)



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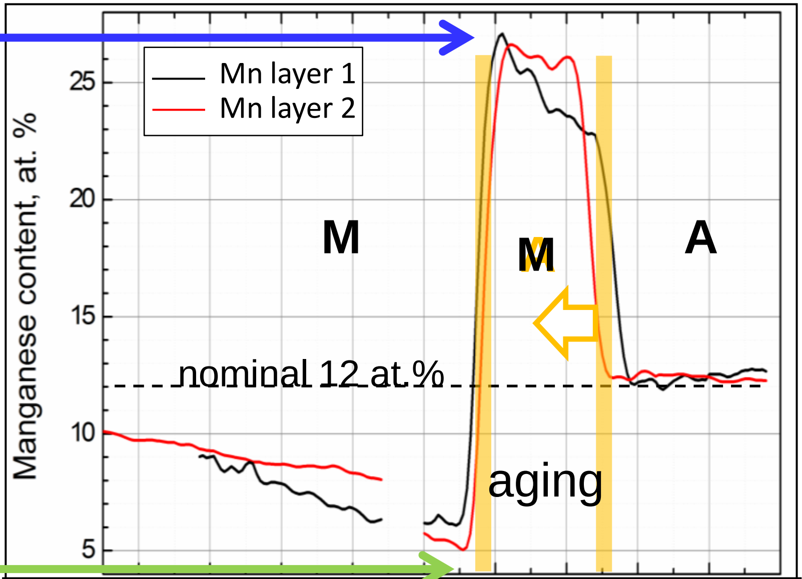
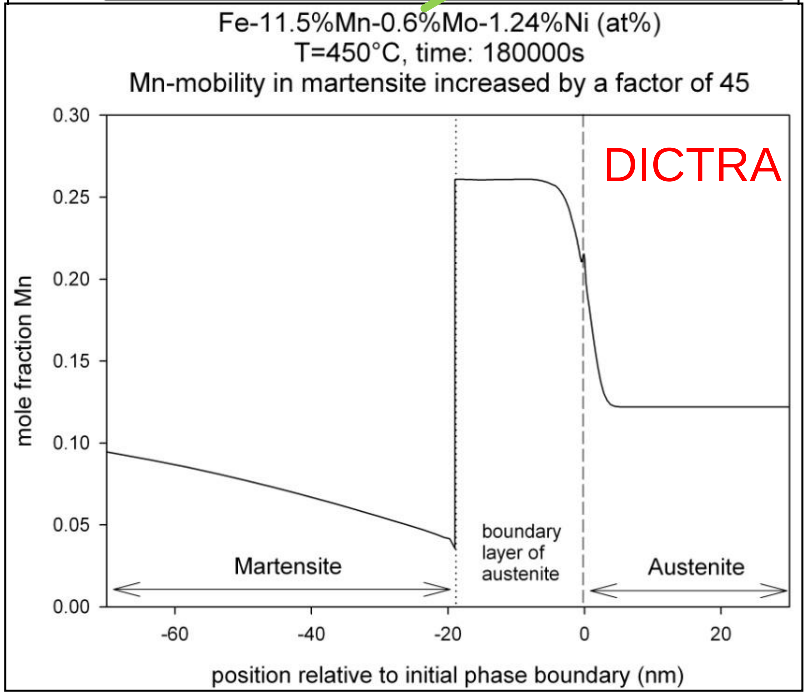
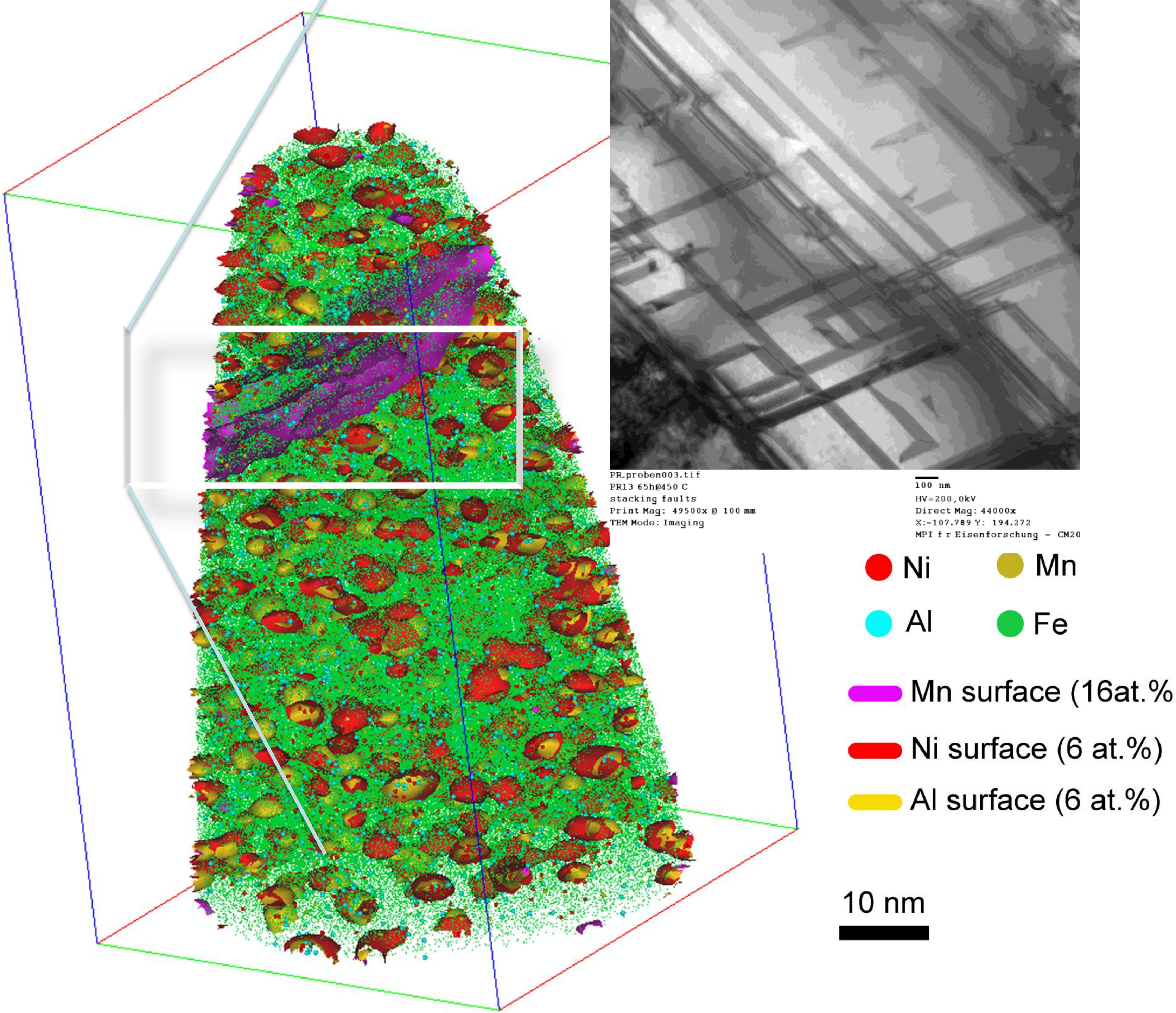
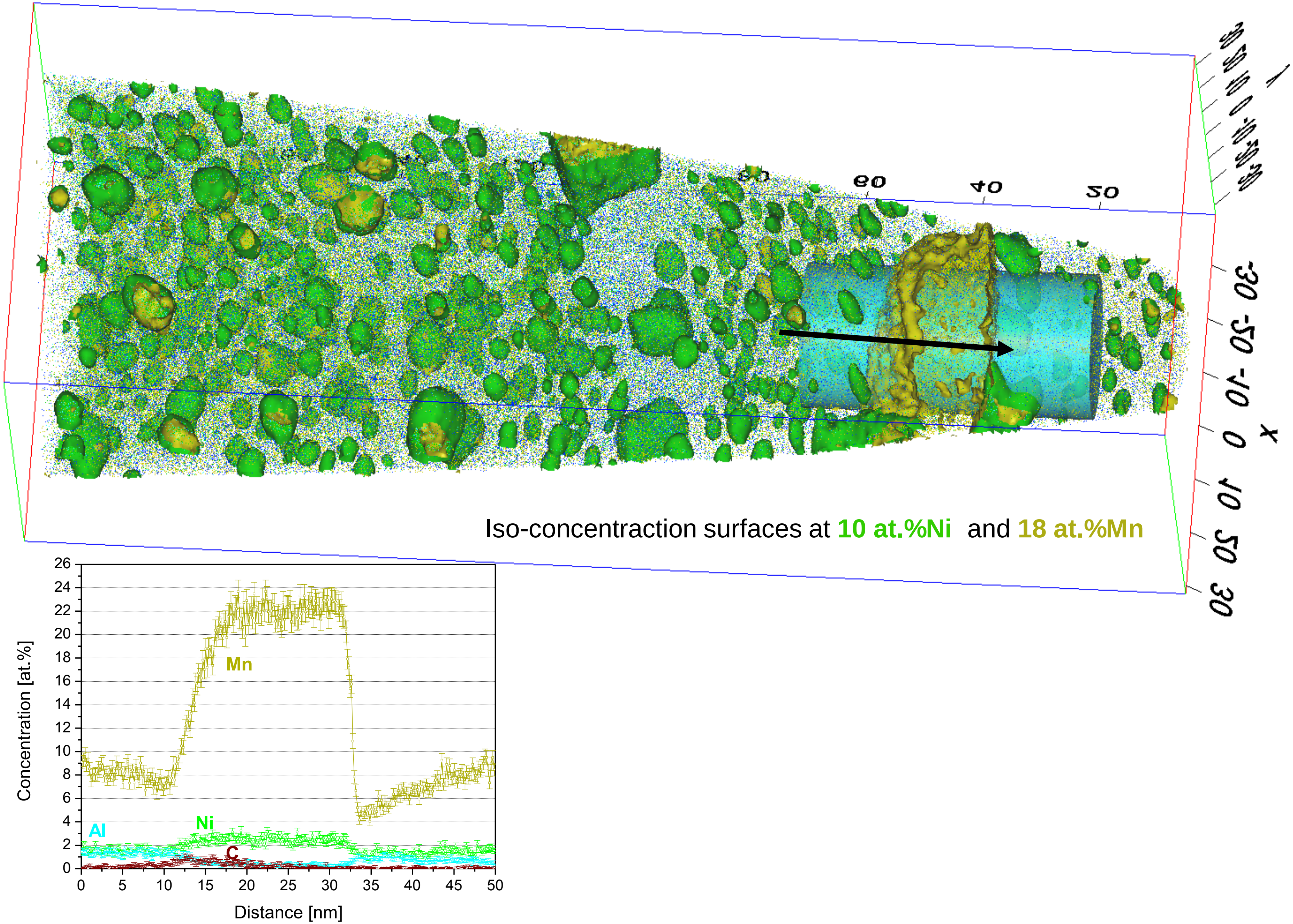




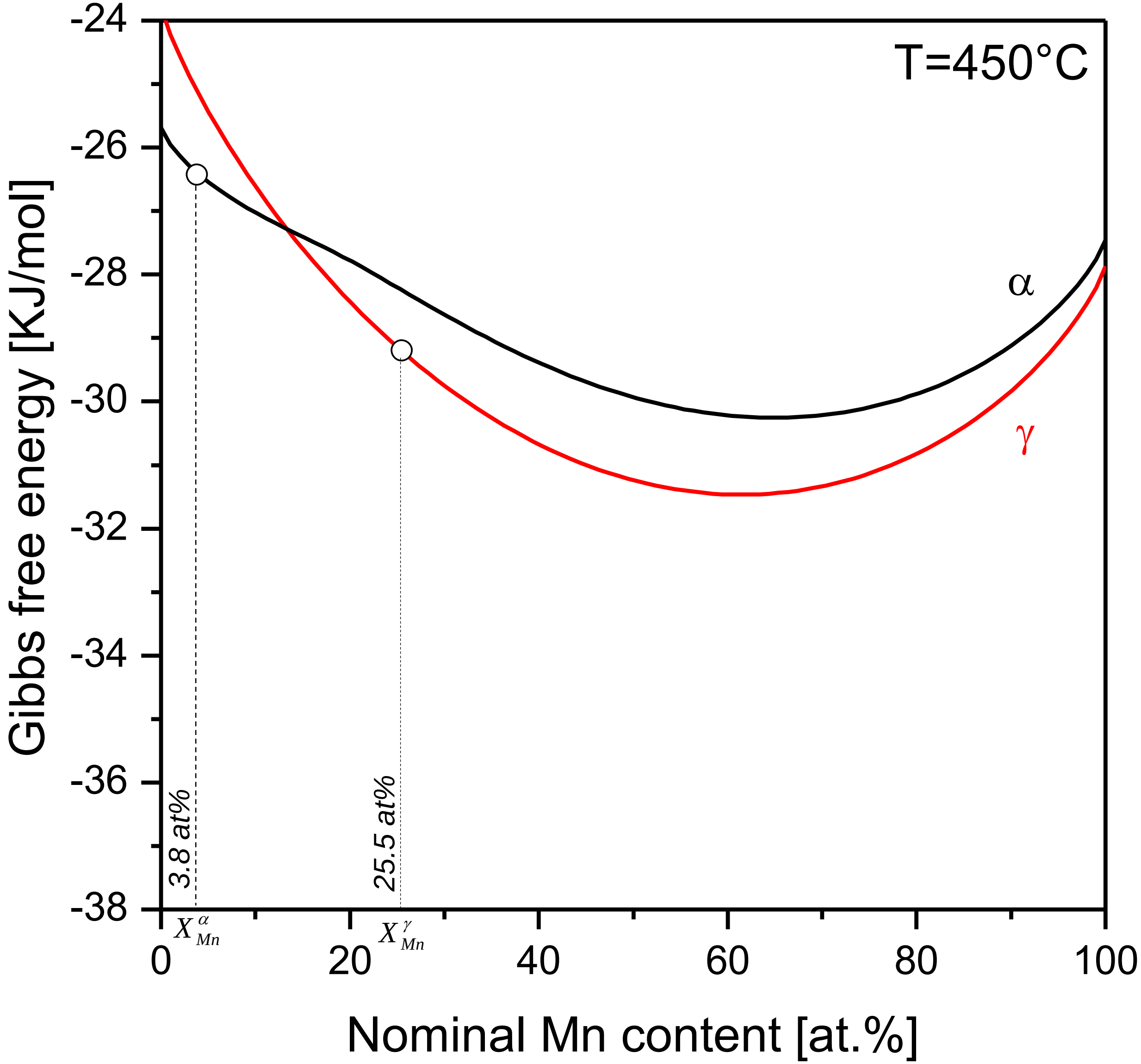
Excellent agreement between experiment & simulation !

Kinetic freezing and associated austenite reversion !


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
Ni
Mn
Al
Fe
Mn surface (16at.%)
Ni surface (6 at.%)
Al surface (6 at.%)
10 nm


Iso-concentration surfaces at 10 at.%Ni and 18 at.%Mn
Concentration [at.%]
Distance [nm]
Mn
Ni
Al
C

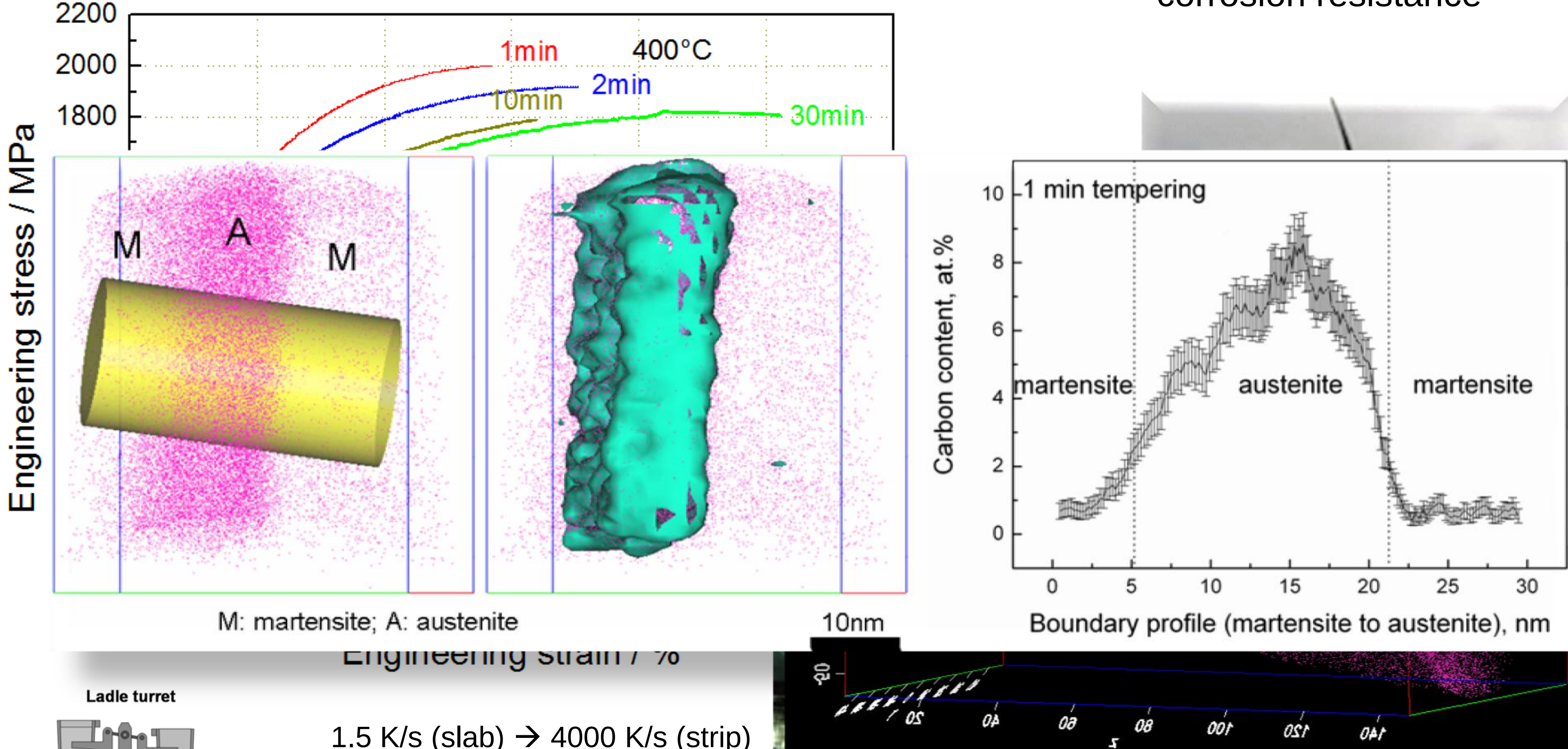
Fe-Mn system. G curves at 450°C



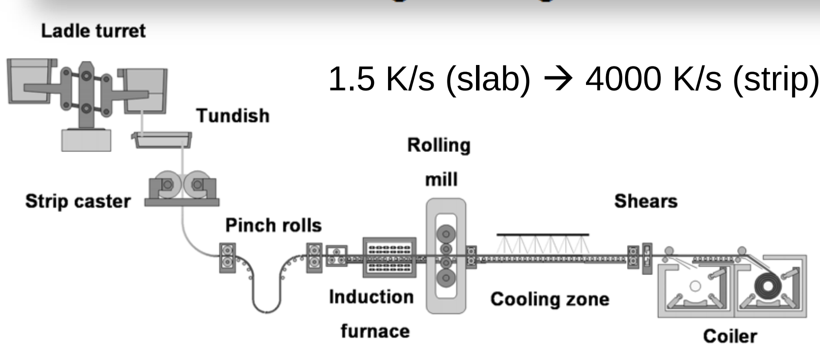
Martensite relaxation & aging & nanoscale austenite reversion

from 650 MPa to 2 GPa (SAME alloy: Fe 13 Cr > 0.3 C)
Aged martensite: Ms-relaxation + prec. (aging) + austenite reversion

Ultra high strength and corrosion resistance



1.5 K/s (slab) → 4000 K/s (strip)

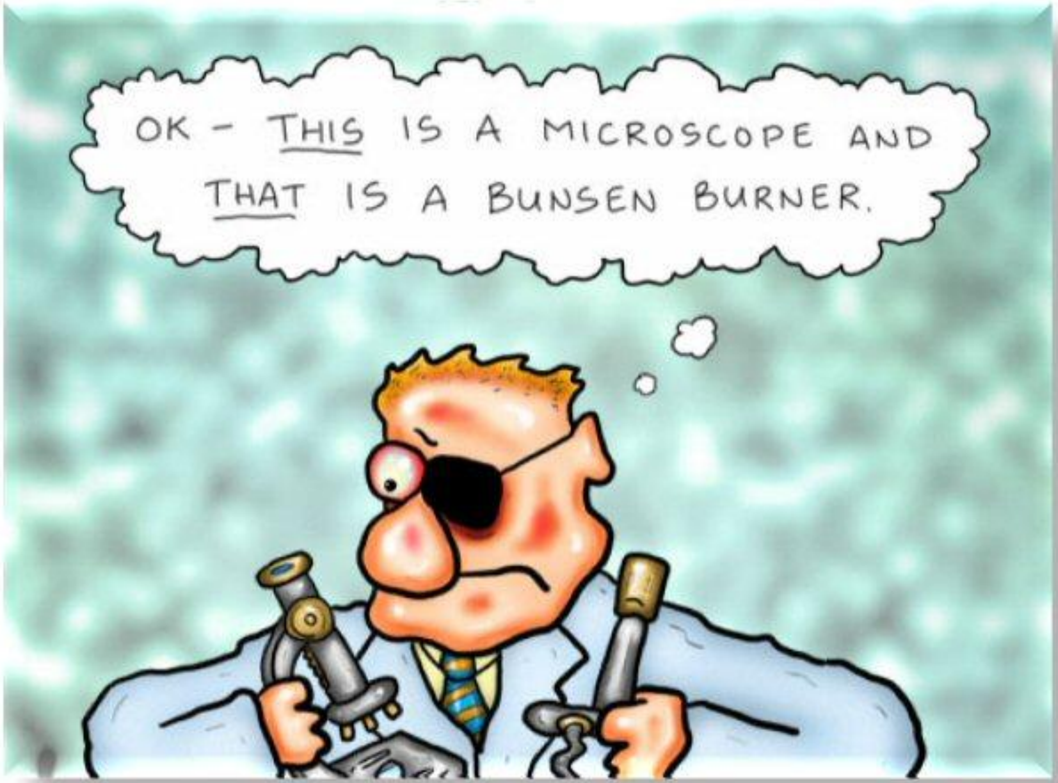


Get the right tools for the job:

Models, characterization, new mechanisms, synthesis

things that don't work

things that work



Combinatorial approaches to structural materials design

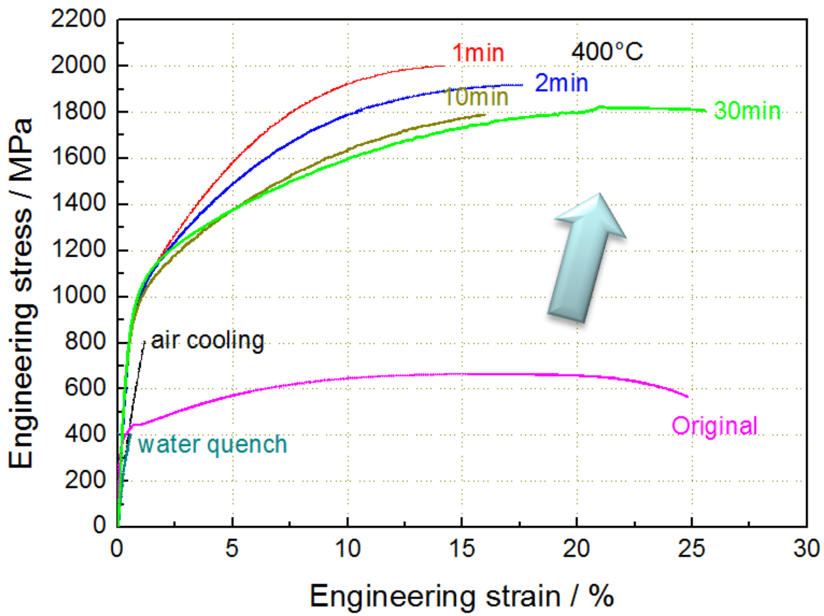
Challenge: How to obtain large numbers of mechanical data sets for new structural metallic alloys:

systematic and fast variations in:
composition
TM processing
Heat treatment
Mechanical testing
weldability

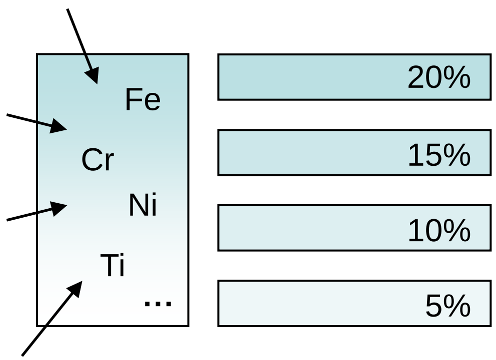
Conventional high-throughput methods do not work for structural materials:

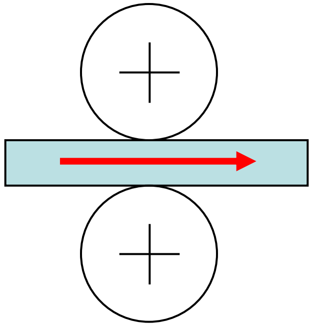
correlation length scales relevant for mechanical properties > thin film thickness

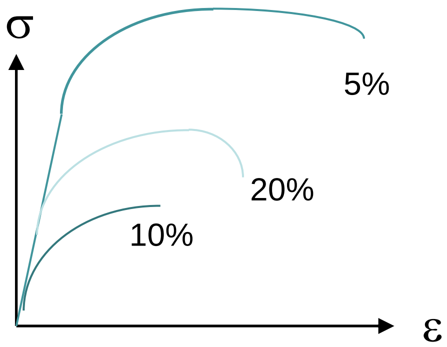
correlation length scales created during processing, hence,
! SAME COMPOSITION ! but different processing



Combinatorial approaches to structural materials design







1. Generating of bulk specimens:

• Rapid change of (chemical) composition between single specimens

• Large variation of element-combinations (base materials)

• Fast / easy production (effort, speed, post processing)

• Few specific effects (e.g.porosity, dispersed oxides) desired

2. Thermomechanical treatment:

• Generate „appropriate“ microstructure representative for applications

• Ensure comparability of results to conventional methods

• Minimise / eliminate specific effects of generating method (cast microstructure etc.)

3. Material testing:

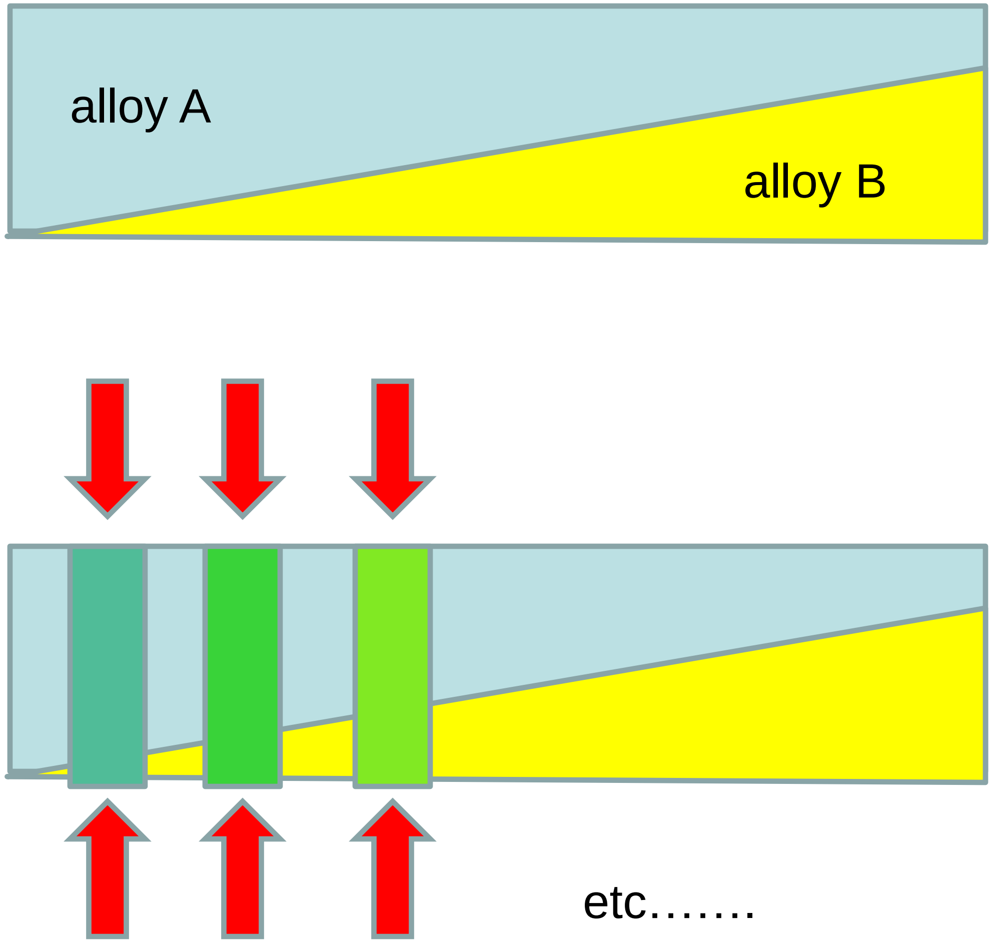
• Mainly tensile test for quick „fingerprinting“ (screening)

• Additional testing? (Flexible generating method for different sample dimensions)

High throughput alloy design

step 1

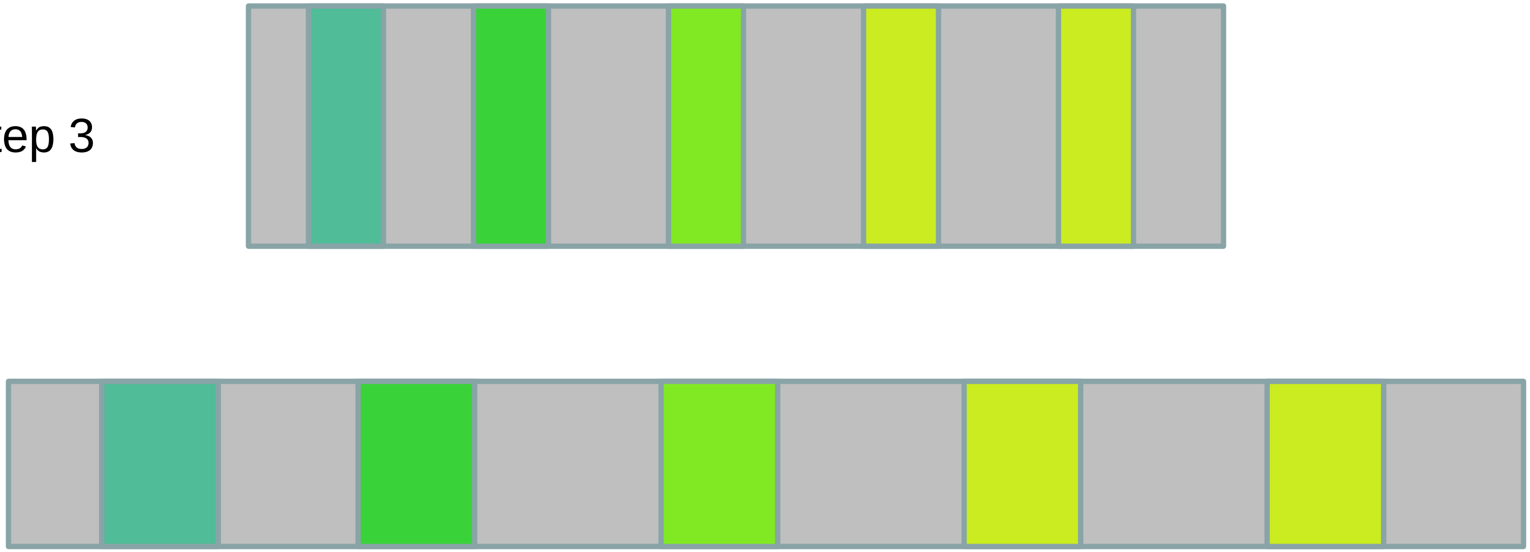
step 2



local melting
(inductive, LASER, electron beam, resistive welding, etc)

High throughput alloy design

step 3

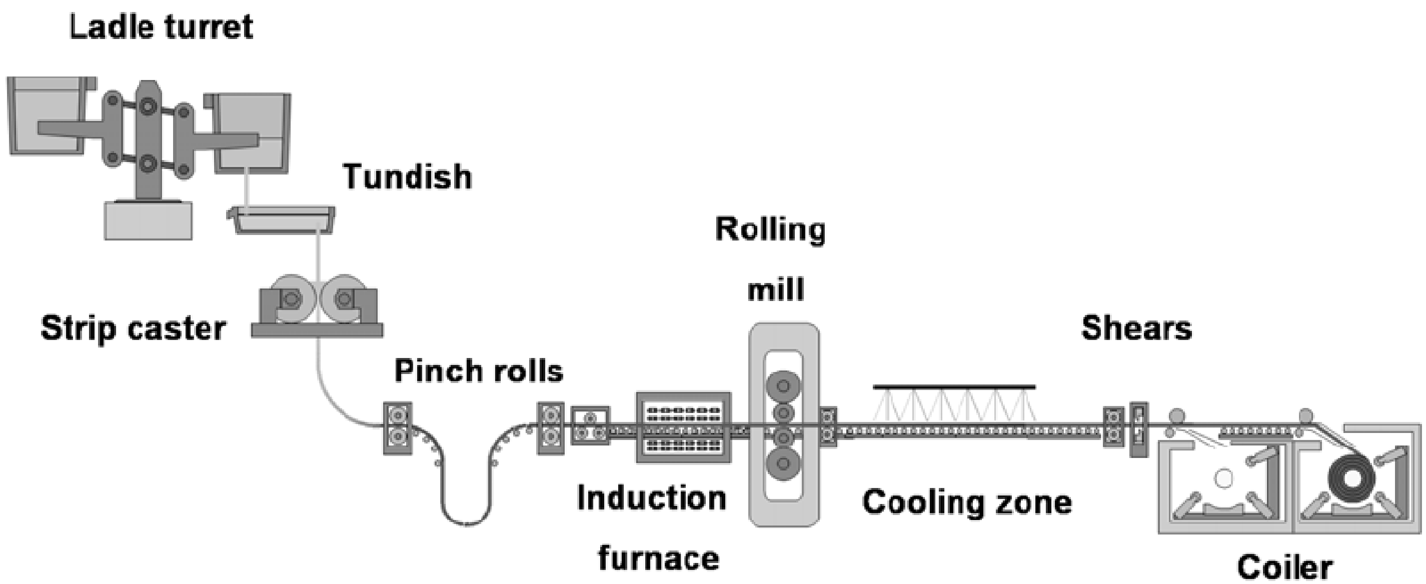


Thermomechanical treatment (e.g. rolling, annealing, etc: design microstructure after the solidified primary structure

step 4

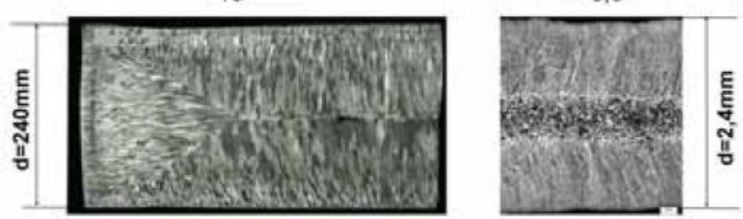
machining and mechanical testing (hardness not good enough: need tensile tests)

Combinatorial approaches to structural materials design



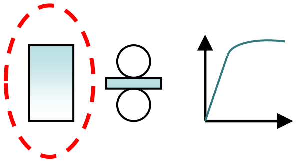
	Slab casting	Thin strip casting
Casting speed (m/min)	0,9 - 2,2	40 -100
Solidification rate (mm/s)	0,1	5
Heat flux density (MW/m²)	1,0 - 2,5	5 -14
Solidification time (s)	10^3	<0,5

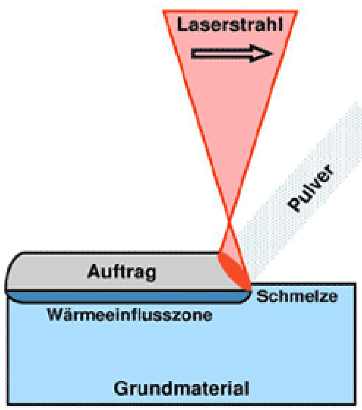
Solidification structure
(AISI 304)



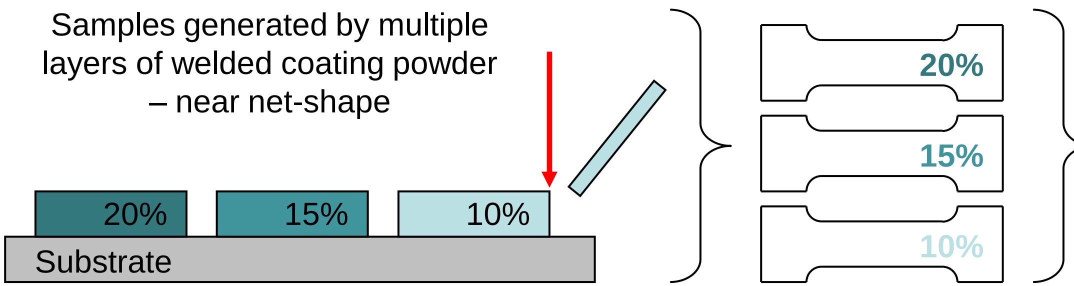
Rapid Alloy Prototyping – Development of High Troughput Methods

1. Laser-powdercoating (welding)





Samples generated by multiple layers of welded coating powder – near net-shape



→ Thermo mech. treatment