Nanostructuring of 100 thousand tons

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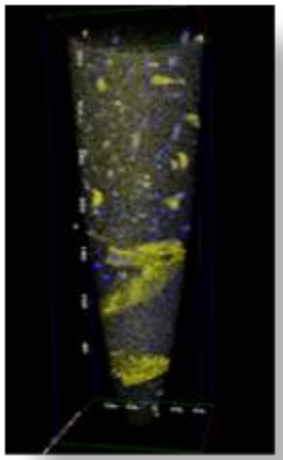

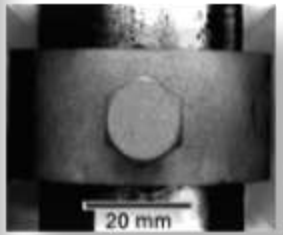

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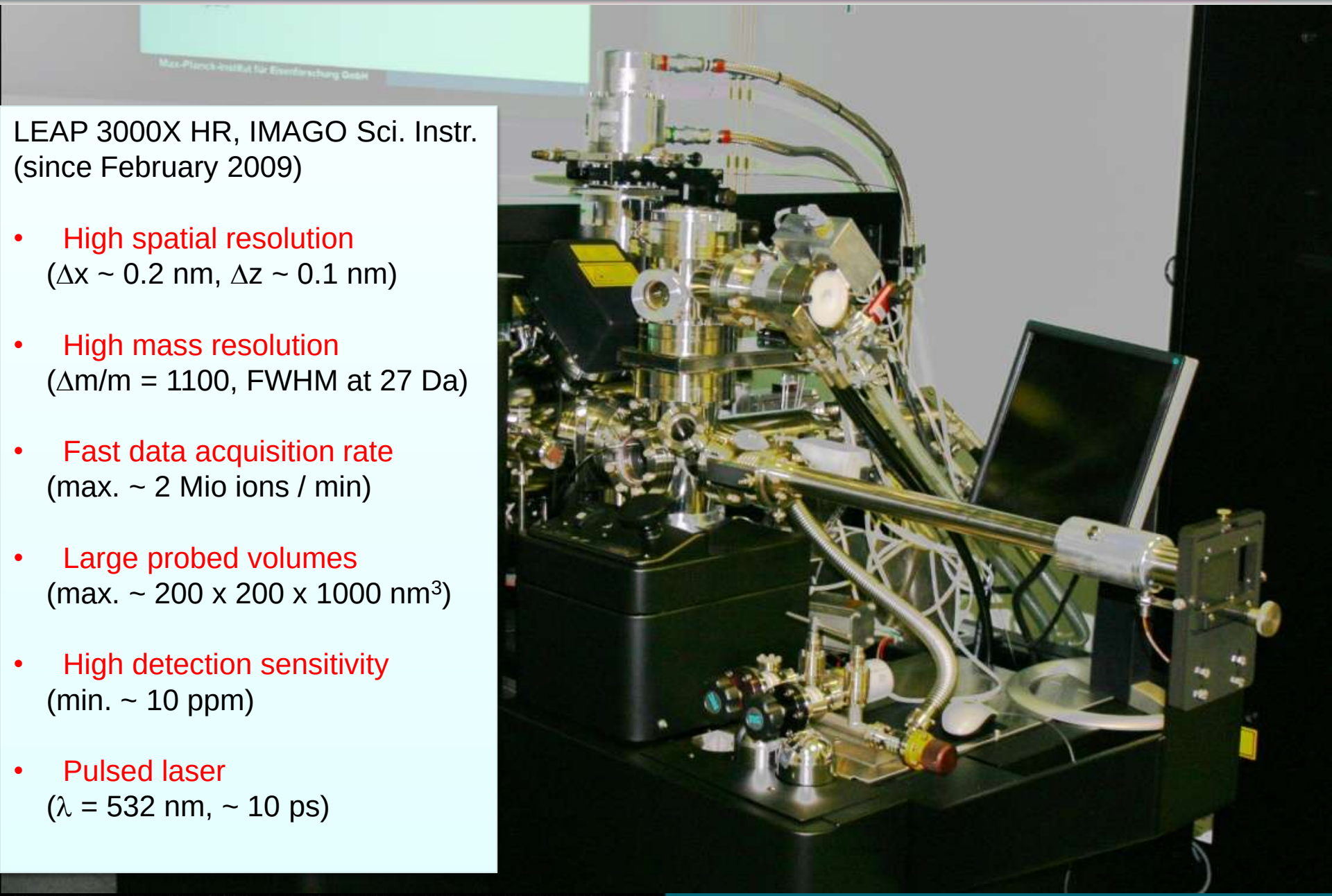
Nanostructures in 100 thousand tons

- Agitation: metallic alloys in 10 minutes
- Self-organized nanostructuring: partitioning, kinetic freezing, adsorption isotherm

The Düsseldorf Local Electrode Atom Probe (LEAP) Laboratory



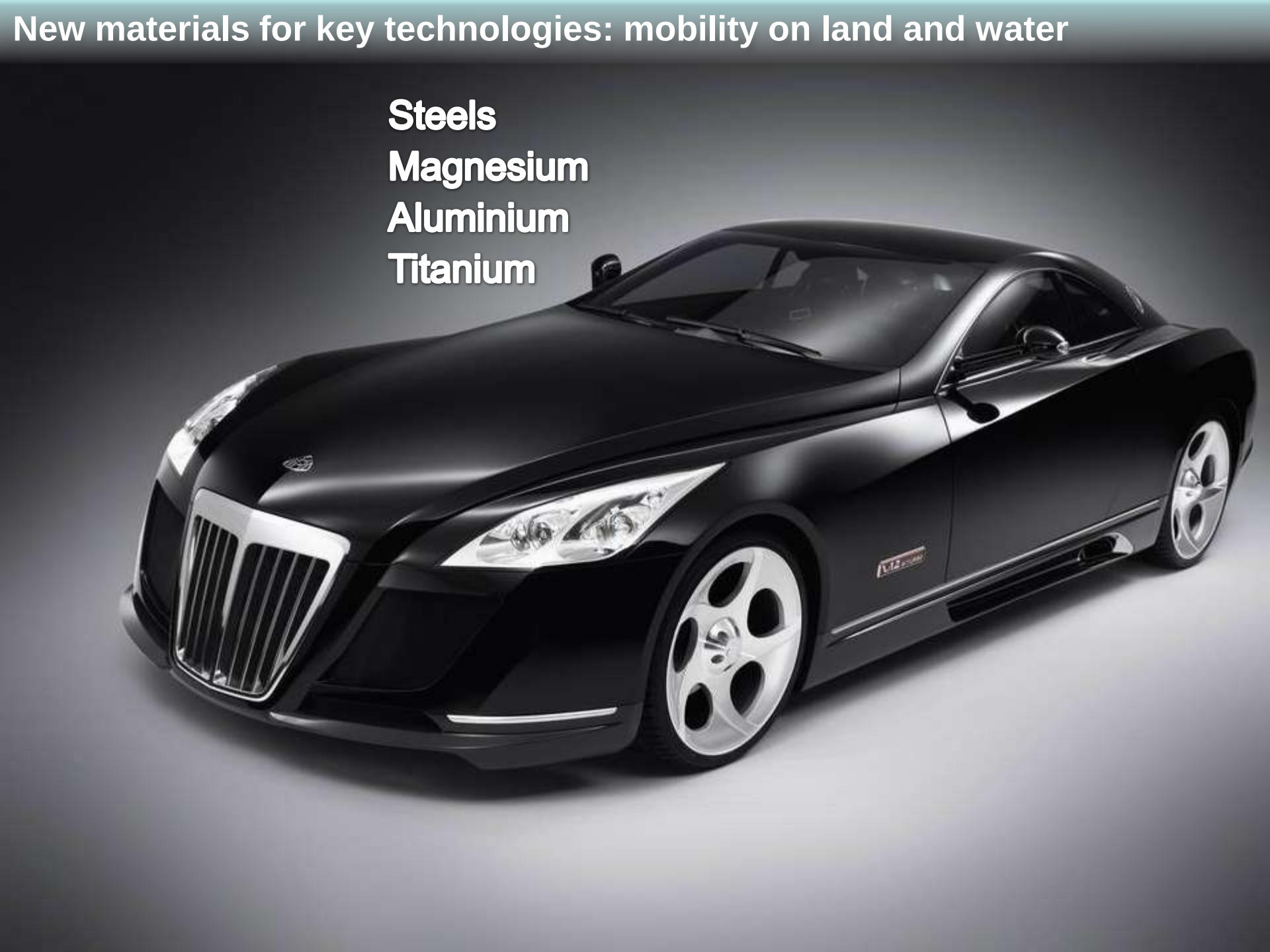
LEAP 3000X HR, IMAGO Sci. Instr. (since February 2009)

- High spatial resolution
  (Δx ~ 0.2 nm, Δz ~ 0.1 nm)
- High mass resolution
  ($\Delta m/m$ = 1100, FWHM at 27 Da)
- Fast data acquisition rate
  (max. ~ 2 Mio ions / min)
- Large probed volumes
  (max. ~ 200 x 200 x 1000 nm^3)
- High detection sensitivity
  (min. ~ 10 ppm)
- Pulsed laser
  (λ = 532 nm, ~ 10 ps)

New materials for key technologies: Aero-space

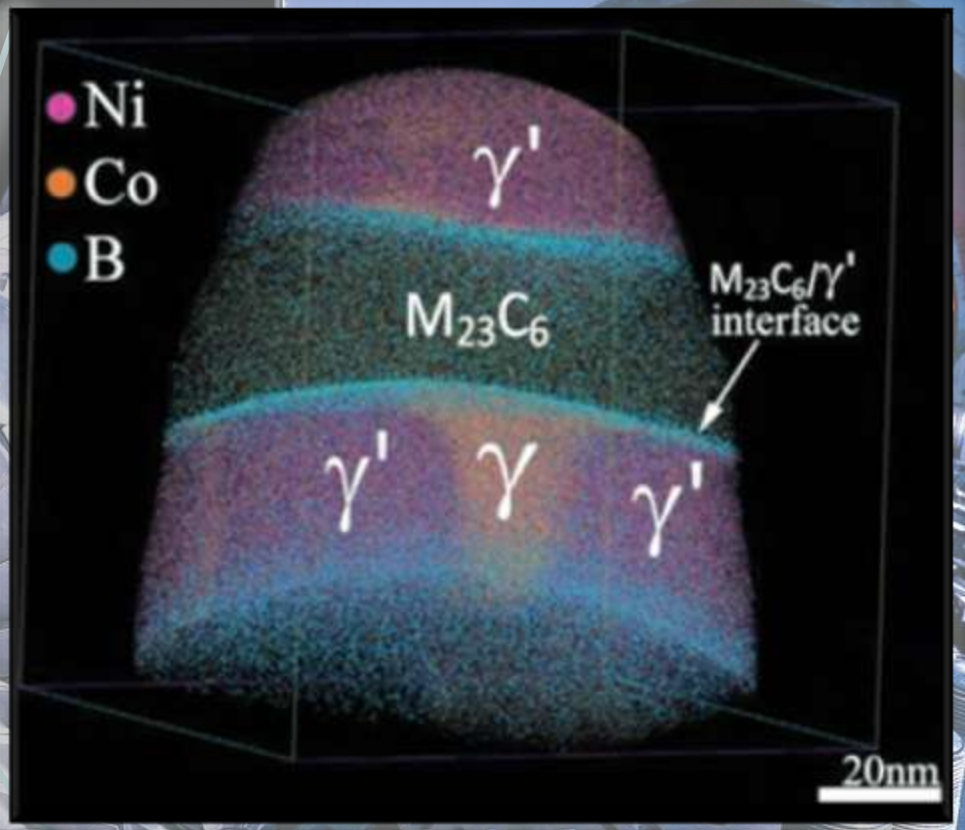
Titanium
Aluminium
Magnesium
Nickel
Steels
Intermetallics

New materials for key technologies: mobility on land and water



New materials for key technologies: Power plants

- Steels
- Nickel
- Intermetallics

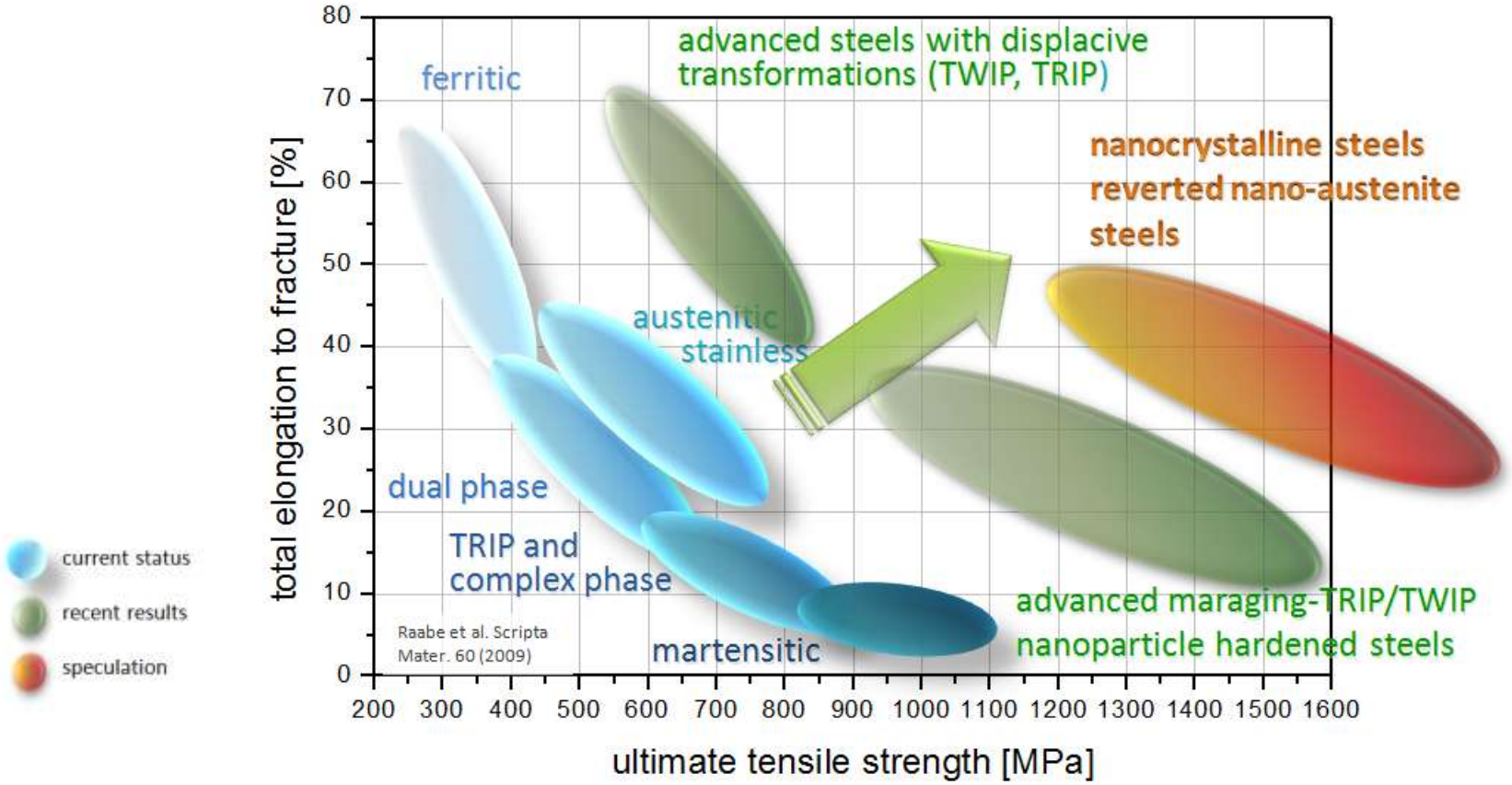


New materials for key technologies: Green energy

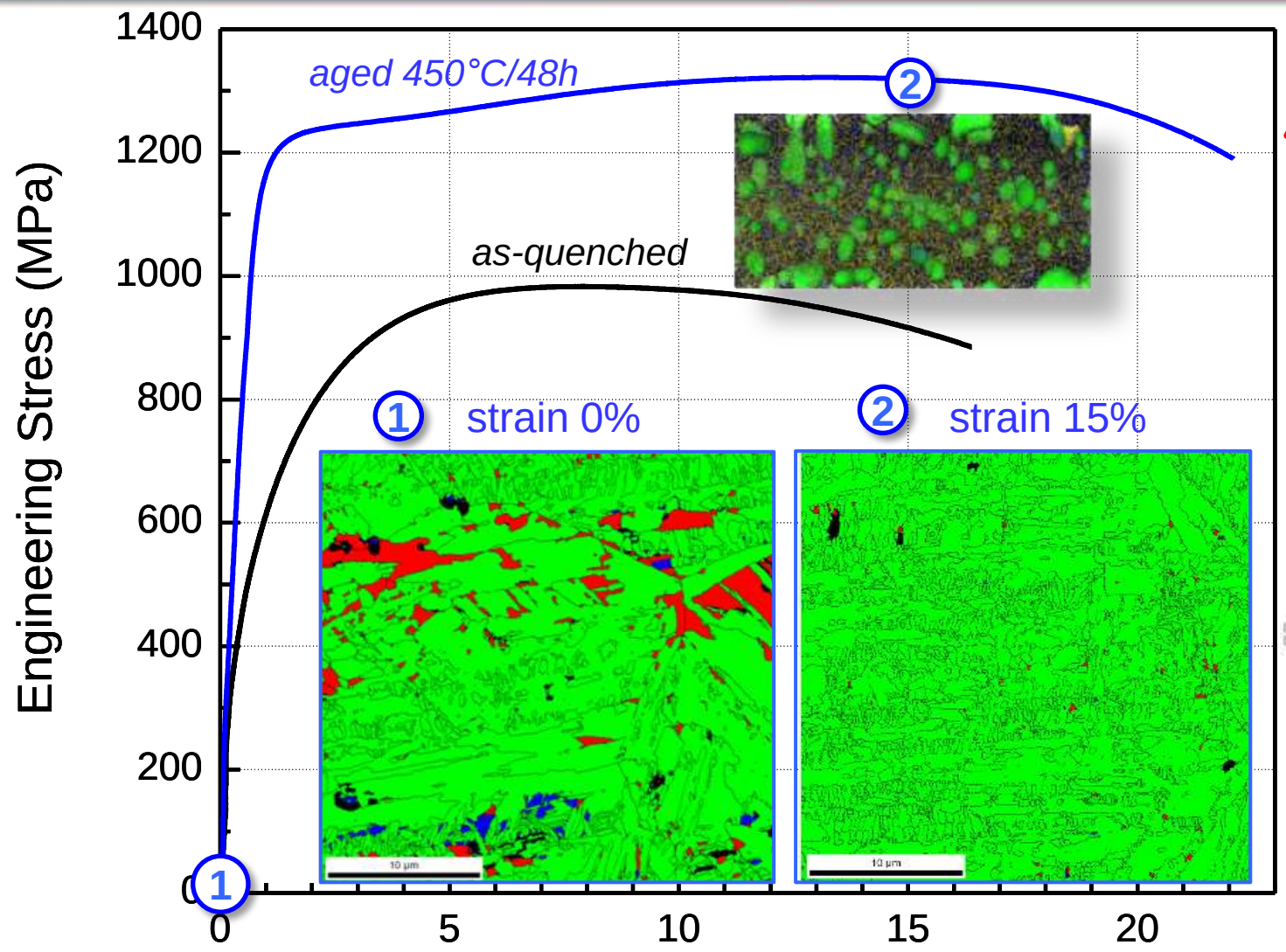
New materials for key technologies: Health

TITANIUM
MAGNESIUM
COPPER
STEELS

From atomistic understanding towards designing new materials

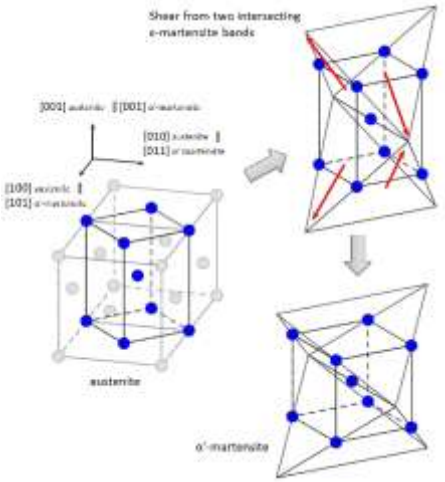


Effect of aging on ductility



Precipitation hardening

increase of γ austenite fraction during aging

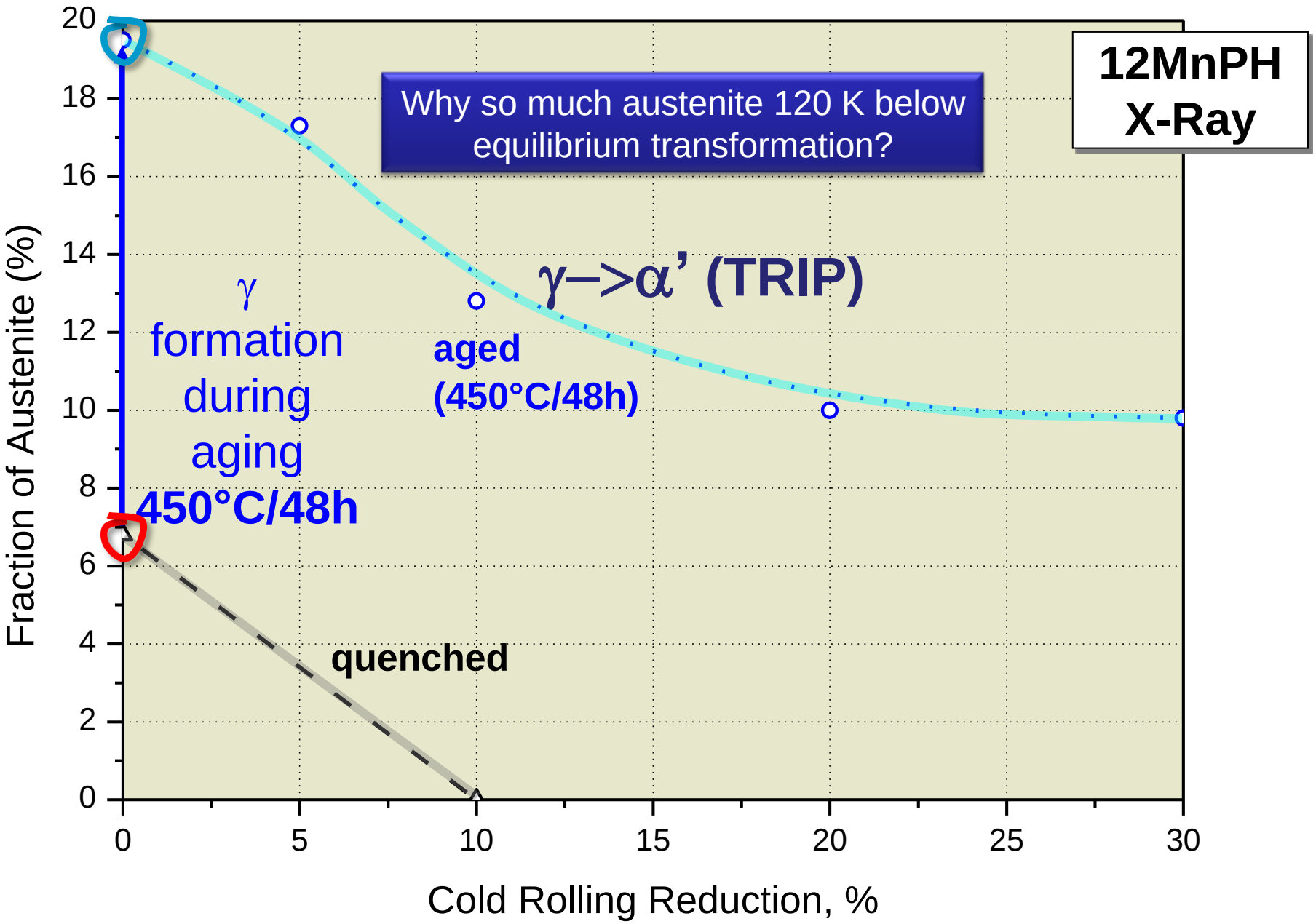


α-Fe (Martensite)

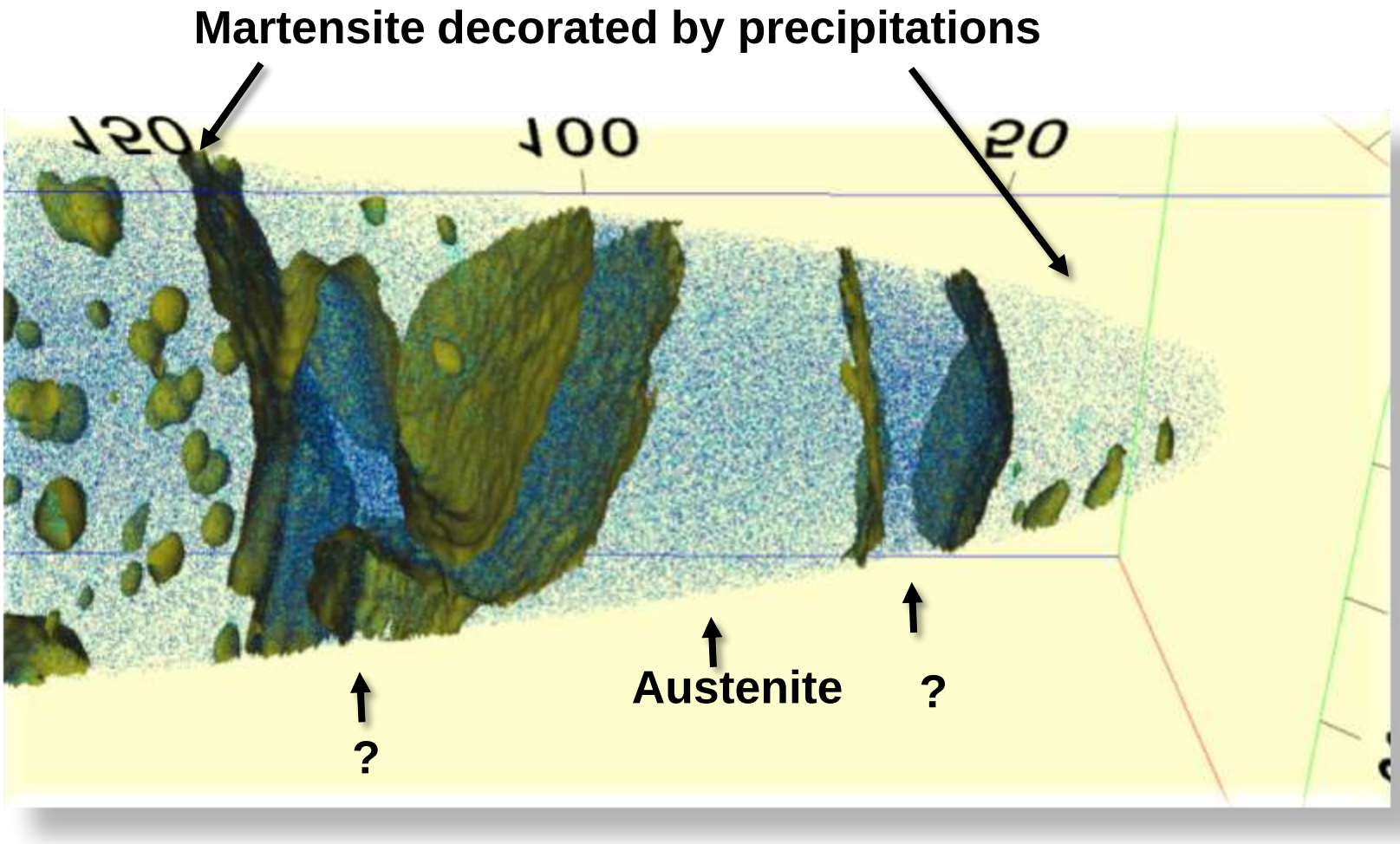
γ-Fe (Austenite), vol. fraction 15-20%

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

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)

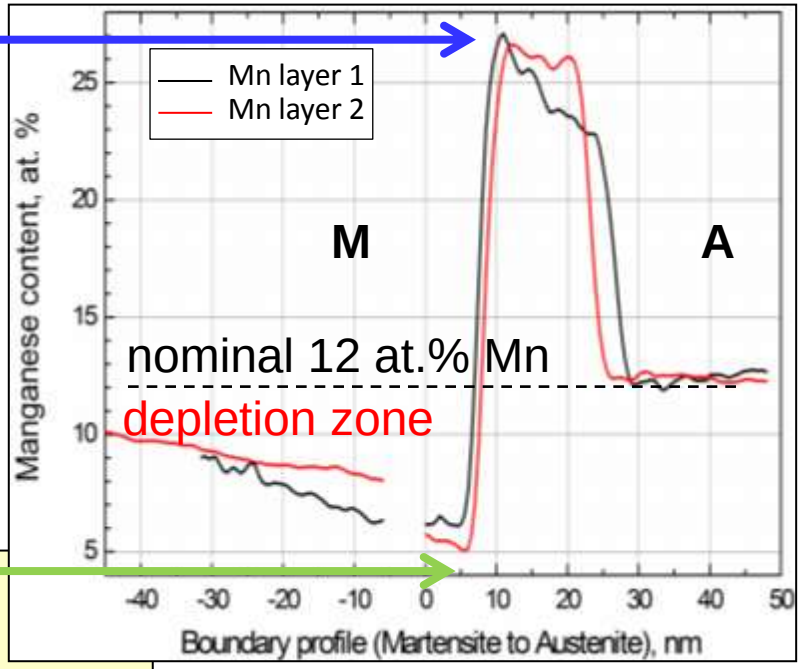
Aging-induced austenite reversion

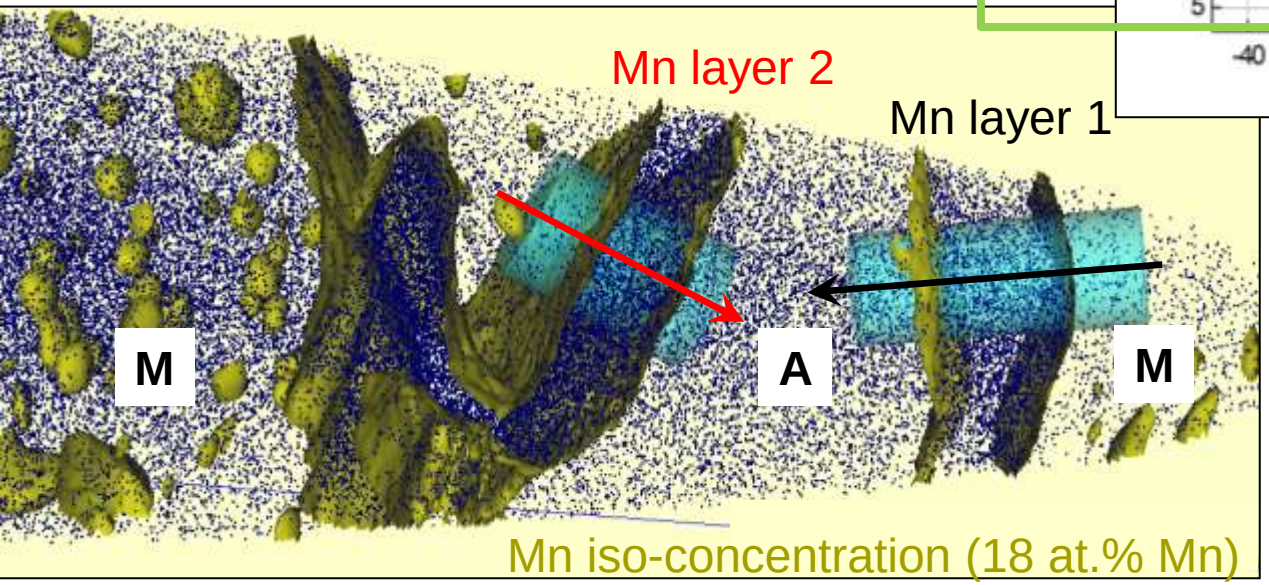
Thermo-Calc ⇒

equilibrium Mn-conc.:

27 at. % Mn in austenite (A)

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





Aging-induced austenite reversion

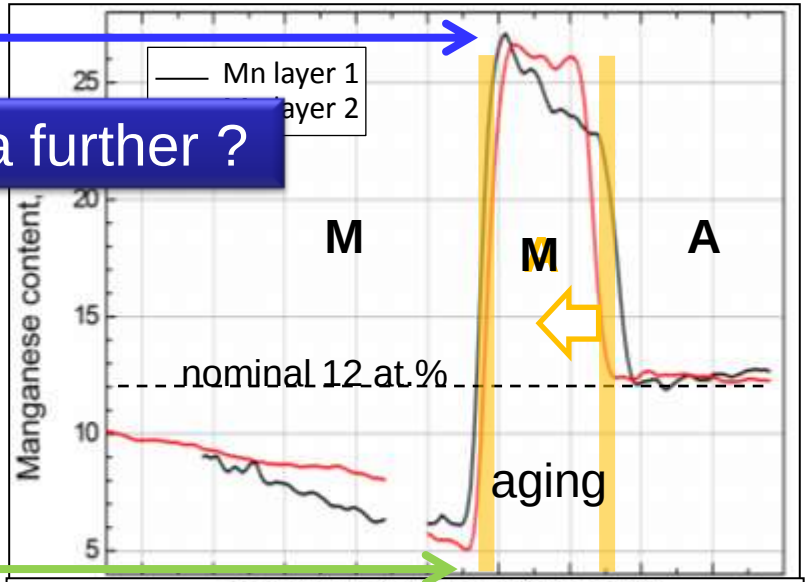
Thermo-Cal

equilibrium Mn-conc.:

27 at. % Mn in austenite (A)

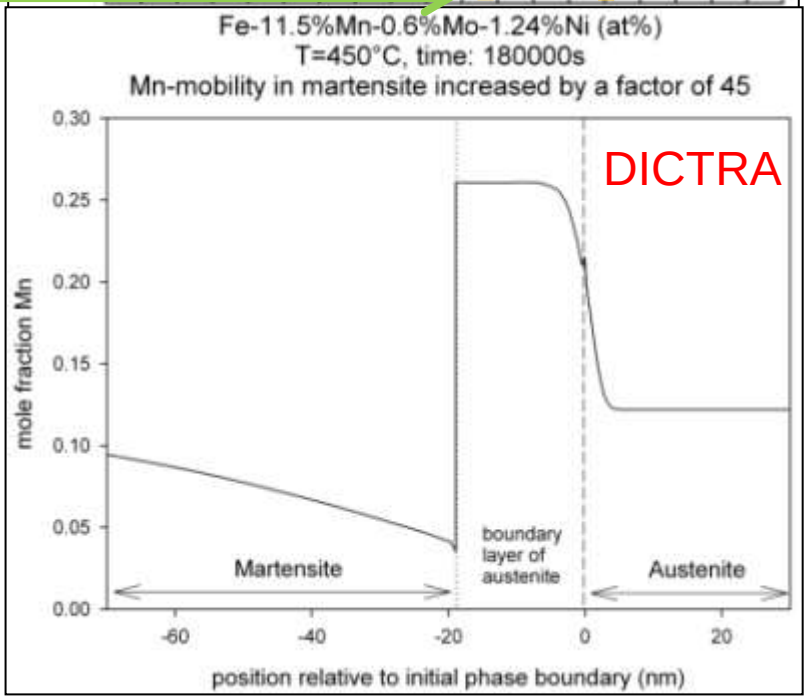
3 at. % Mn in ferrite (martensite) (M)

Can I push this idea further ?



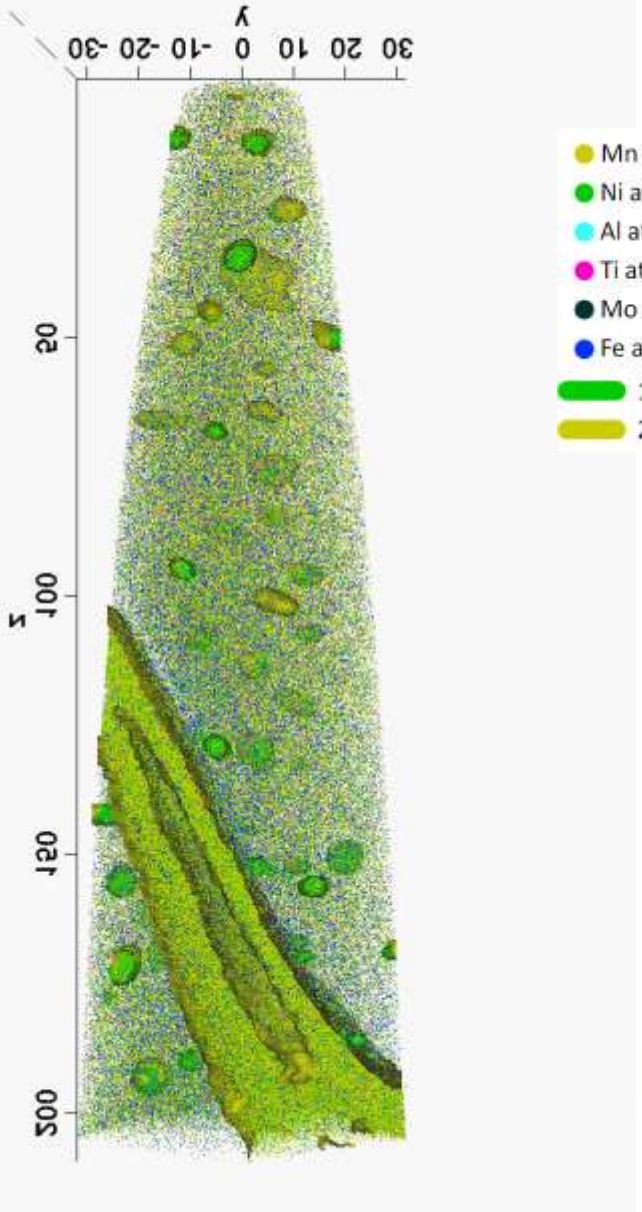
Excellent agreement between experiment & simulation !

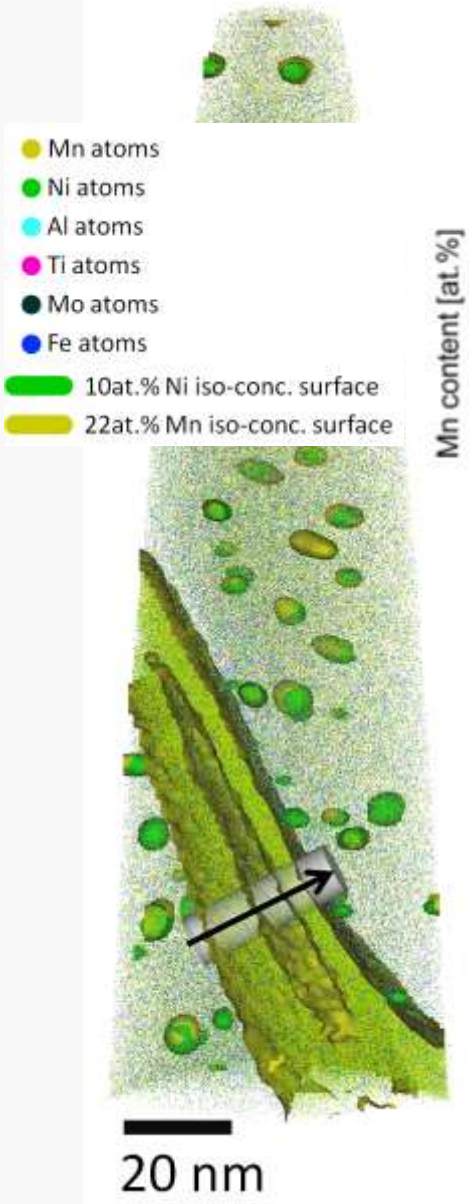
Kinetic freezing and associated austenite reversion !



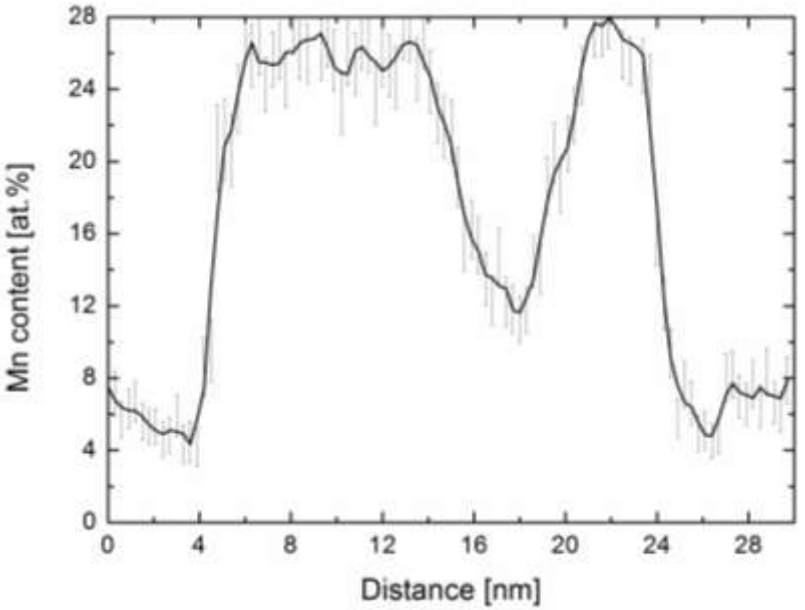
Dmitrieva et al. Acta Mater 59 (2011)

Growth of retained austenite 450°C/48h. 12MnPH





1D. Conc. Profile - Manganese

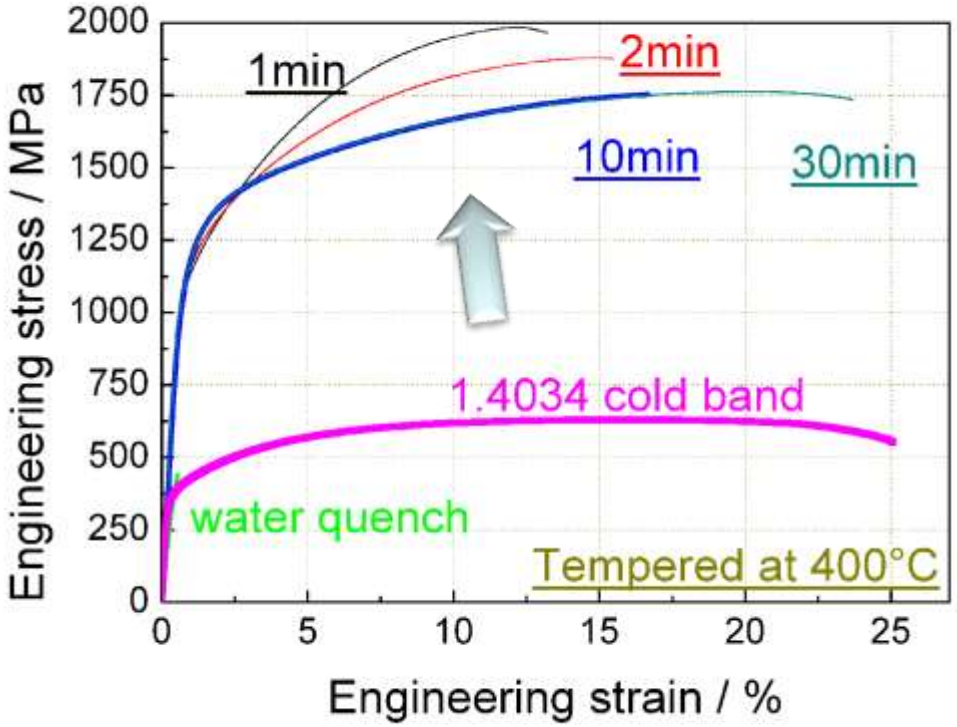


C	Ni	Mo	Ti	Al	Mn	Fe
0.01	2.0	1.0	1.0	0.15	12	bal.

Martensite relaxation & aging & nanoscale austenite reversion

650 MPa to 2 GPa

Ultra high strength and corrosion resistance

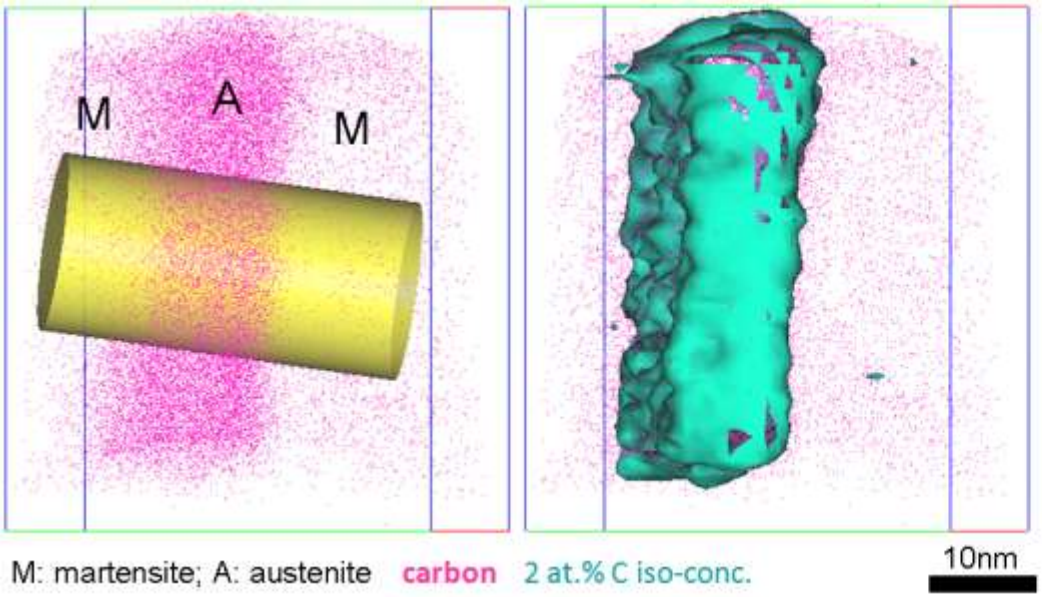


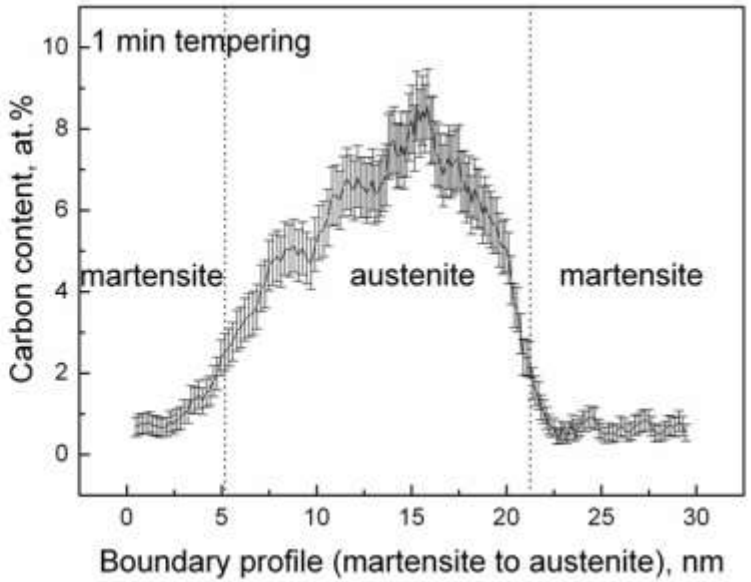
400°C aging: Ms-relaxation + prec. (aging) + austenite reversion

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

Martensite relaxation & aging & nanoscale austenite reversion

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

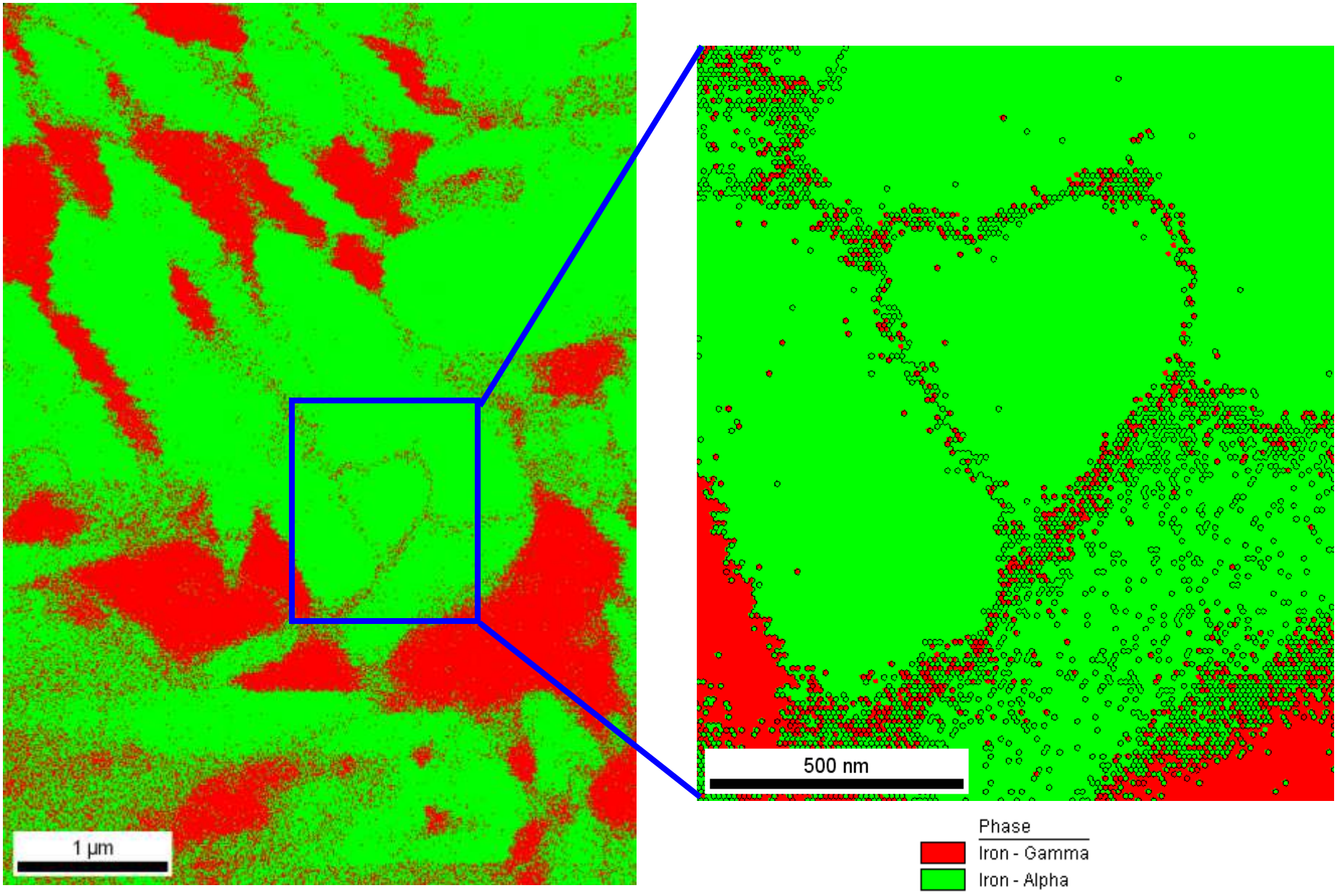




C has ‘/\’ shape in austenite layer: inheritance from austenite, Gibbs adsorption isotherm;
C on martensite grain boundaries

C has ‘V’ shape in austenite layer: austenite reversion through partitioning and kinetic freezing

Self-repair steels



Answering societies' grand challenges with complex alloys

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

Specifically, **metallic materials** occupy key roles
(energy, transportation, health, safety, infrastructure)

Our mission: Designing new metallic alloys from first principles

- Multiscale simulation
- Multiscale characterization starting from the atomic scale
- Synthesis, processing, testing