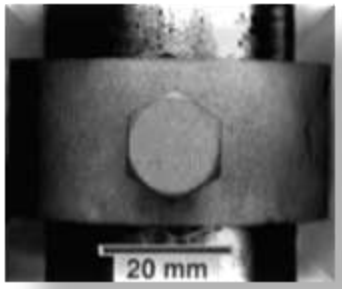
Designing Nanostructured Metallic Bulk Alloys via First Principles Simulations and Atomic Scale Characterization: The Basis of Modern Manufacturing

D. Ponge, J. Millan, L. Yuan, S. Sandlöbes, P. Choi, M. Herbig, J. Wittig, G. Inden, M. Friak, T. Hickel, J. Neugebauer, D. Raabe

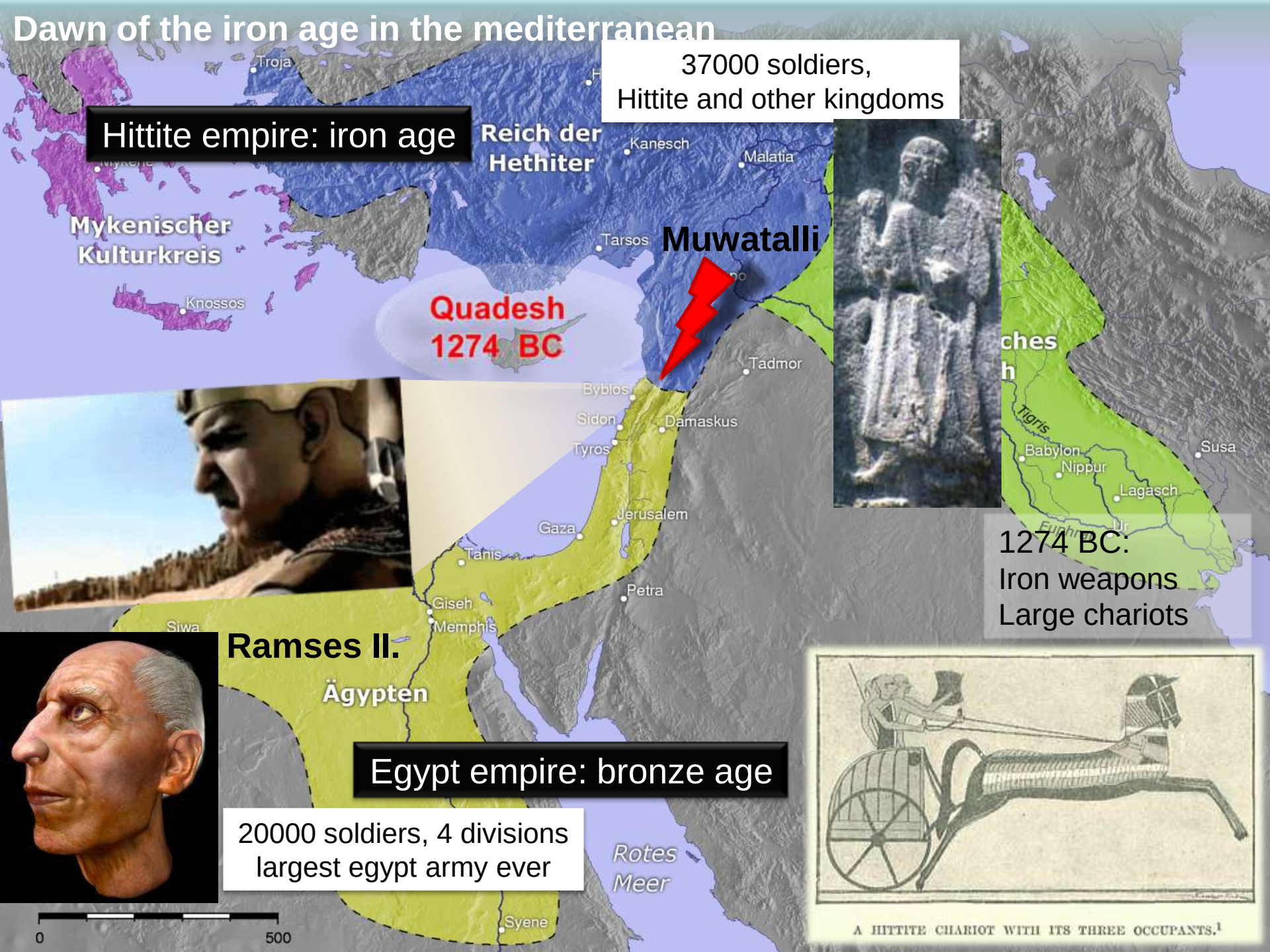
Max-Planck-Institut
für Eisenforschung GmbH
Düsseldorf, Germany
WWW.MPIE.DE
d.raabe@mpie.de



Dawn of the iron age in the mediterranean

37000 soldiers,
Hittite and other kingdoms

Hittite empire: iron age

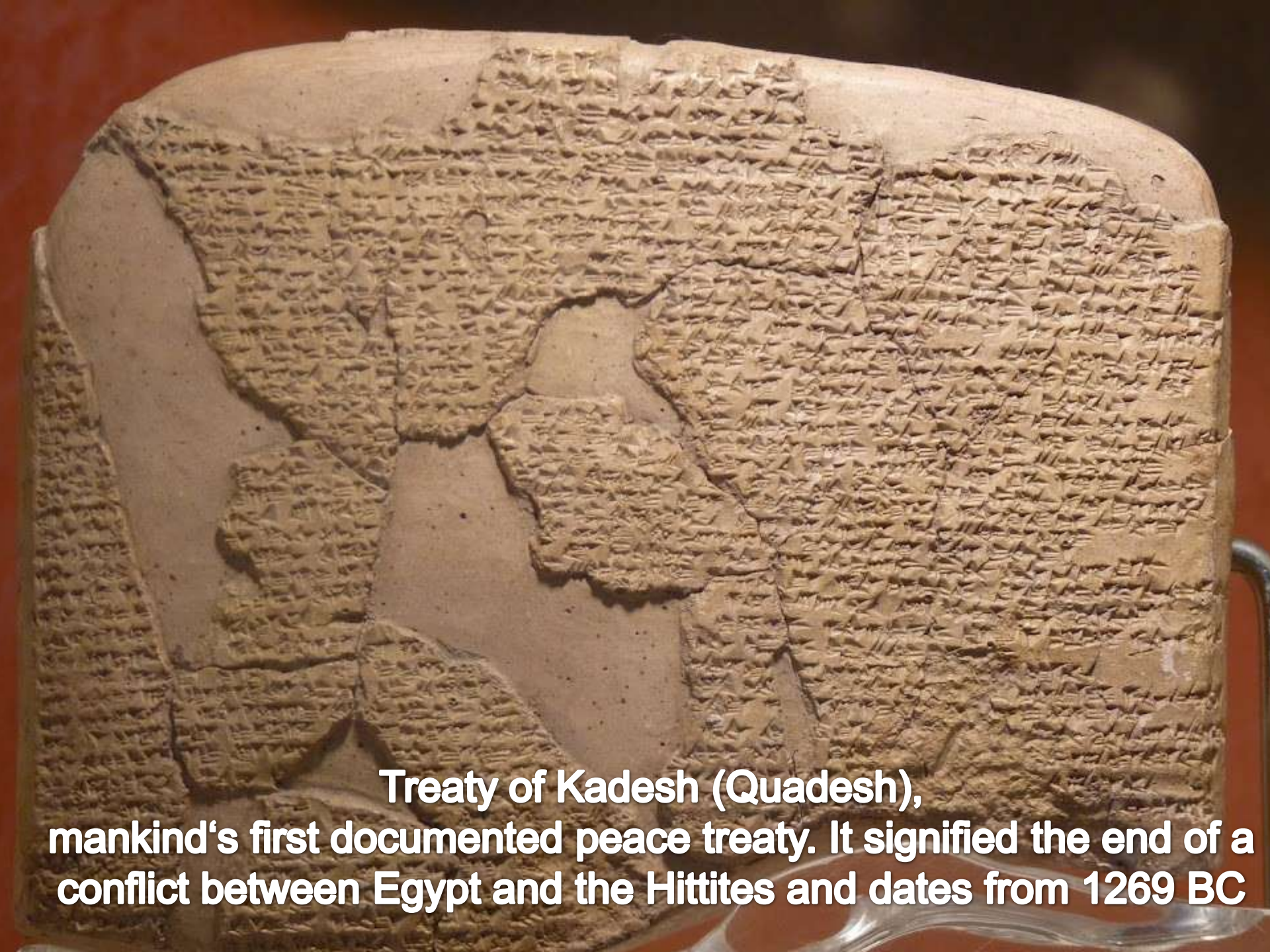


1274 BC:
Iron weapons
Large chariots

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

Overview

- **First principles guided design of structural alloys**
  - Mg-Li
  - Mg-Y
  - TWIP steel
  - Phase transformation at lattice defects

Mechanisms and properties

bulk

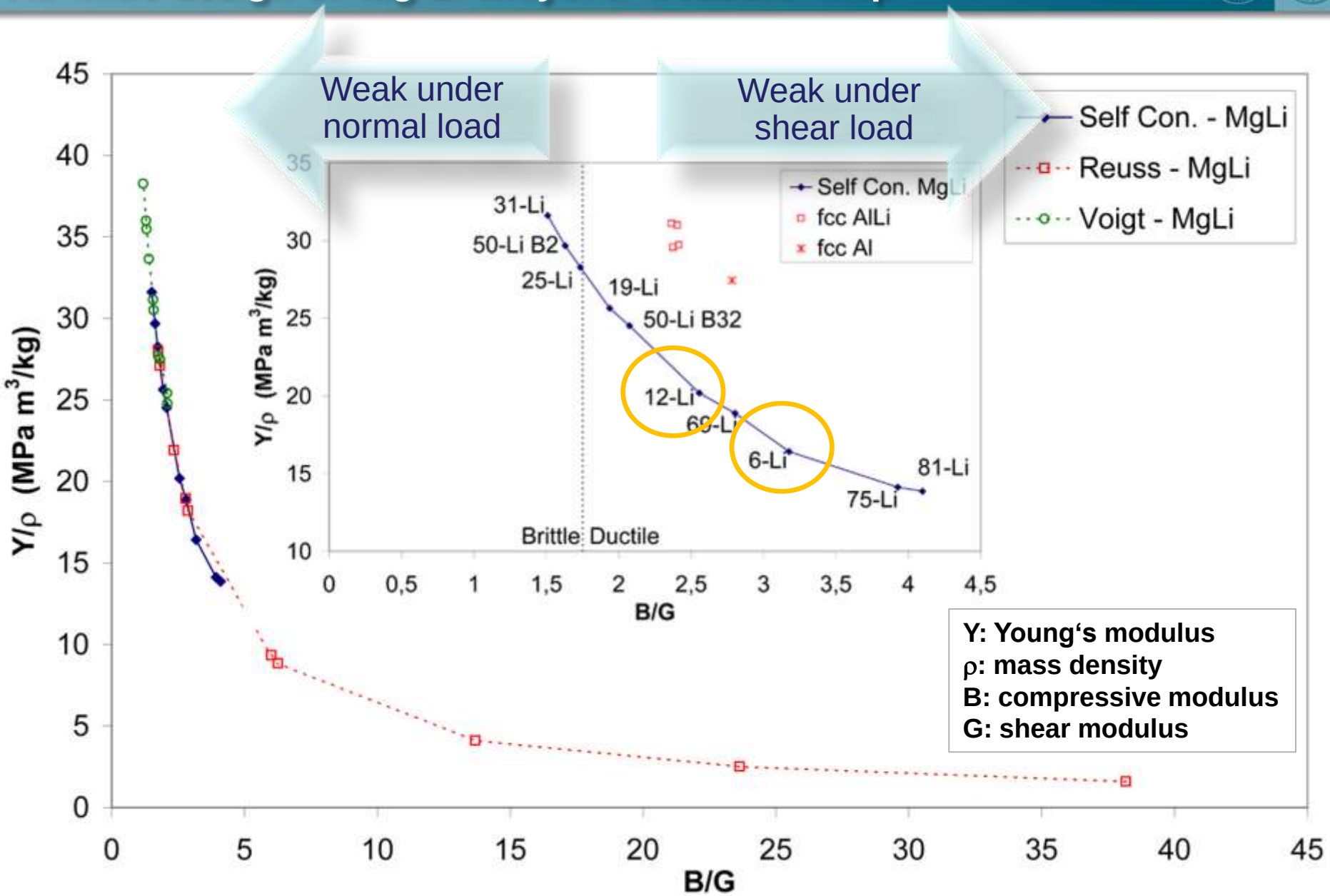
nano

- **RAP (Rapid Alloy Prototyping)**
  - Combinatorial design of bulk alloys
  - Density-reduced TRIPLEX steels

Processing and manufacturing

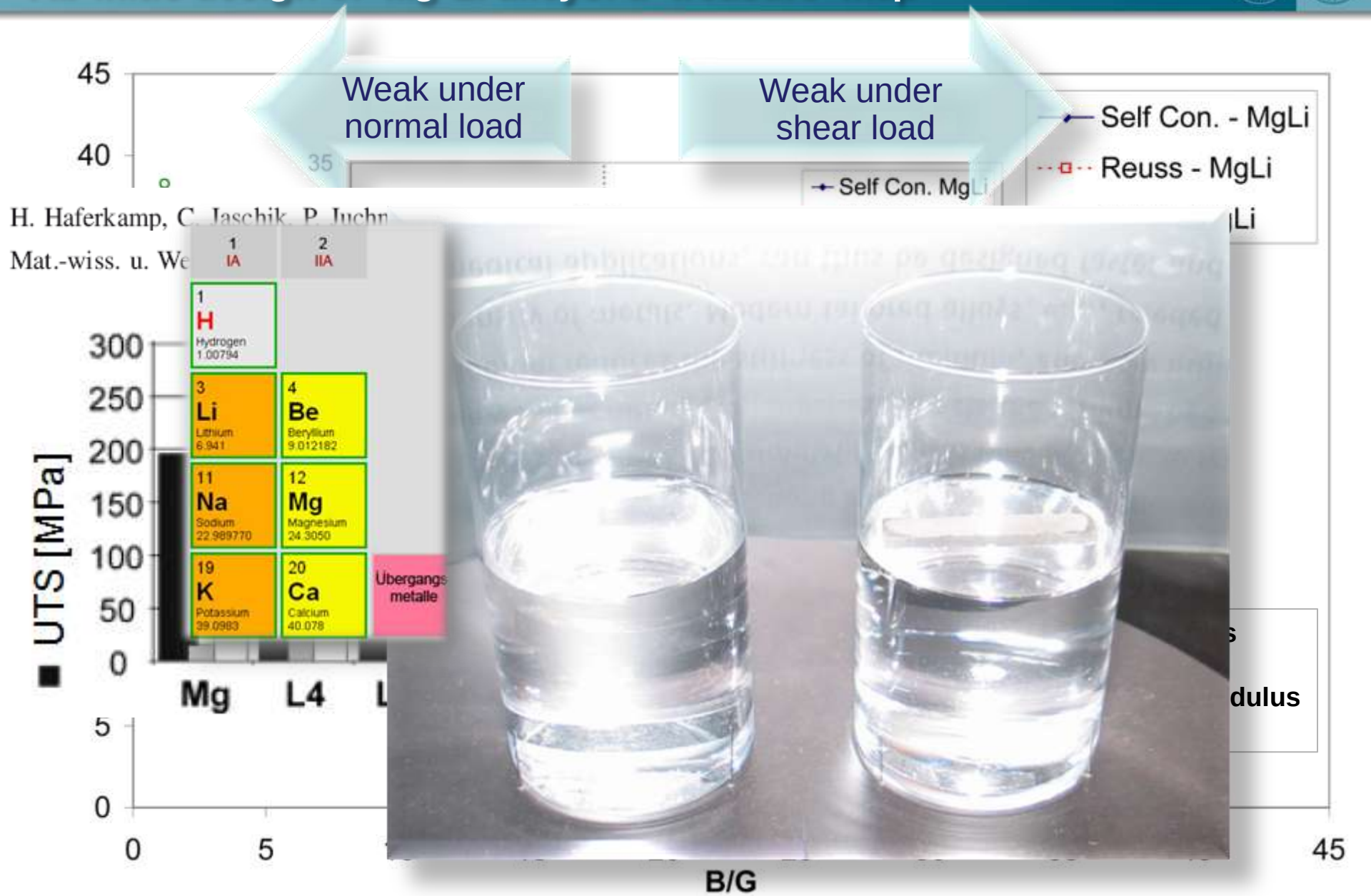
- **Conclusions**

Ab-initio design of Mg-Li alloys: a ‘treasure‘ map



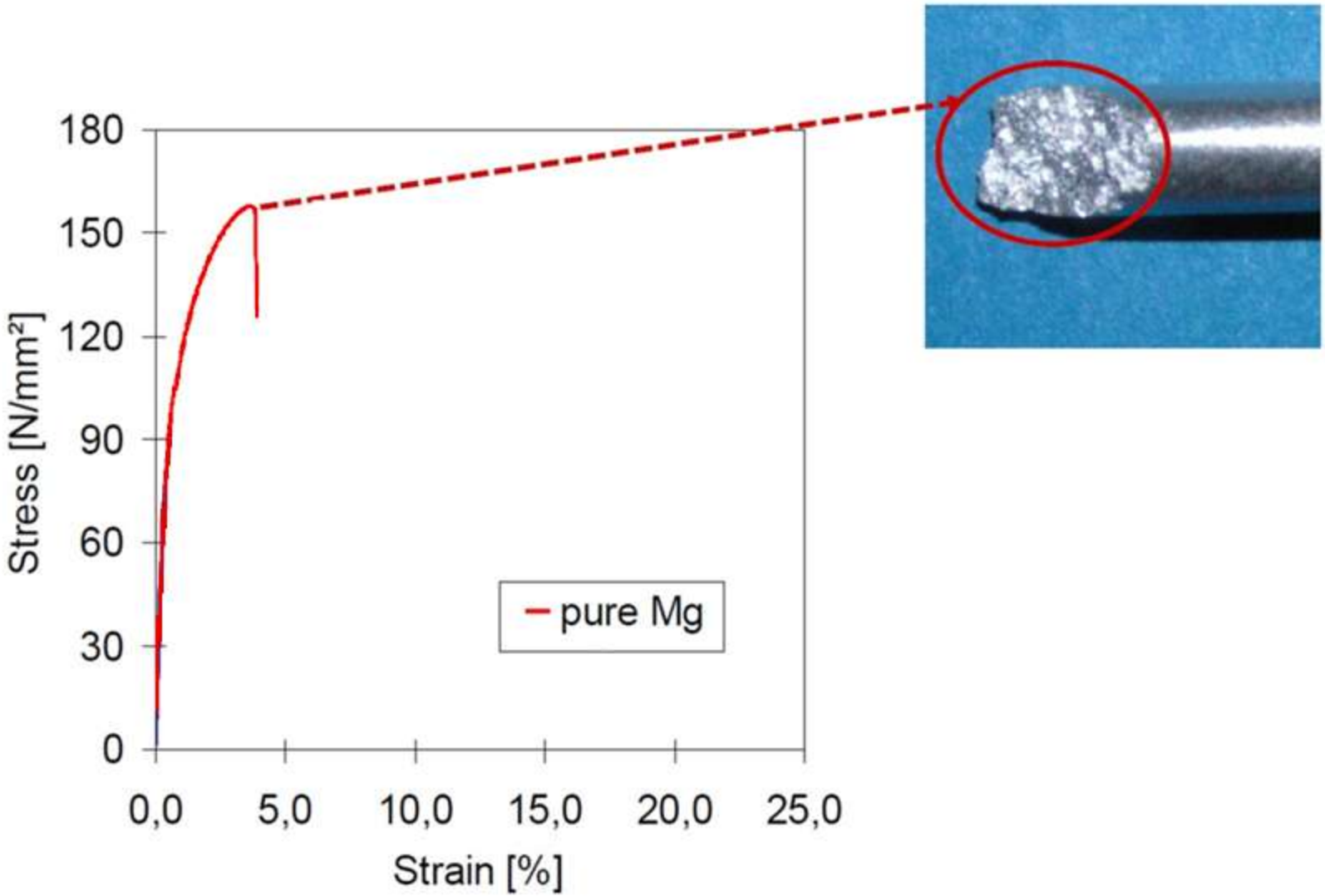
Counts et al.: phys. stat. sol. B 245 (2008) 2630

Ab-initio design of Mg-Li alloys: a ‘treasure‘ map



Counts et al.: phys. stat. sol. B 245 (2008) 2630

Mg vs. Mg-Y: > 5 times higher ductility at same stress level



Sandlöbes et al. Acta Materialia 60 (2012) 3011

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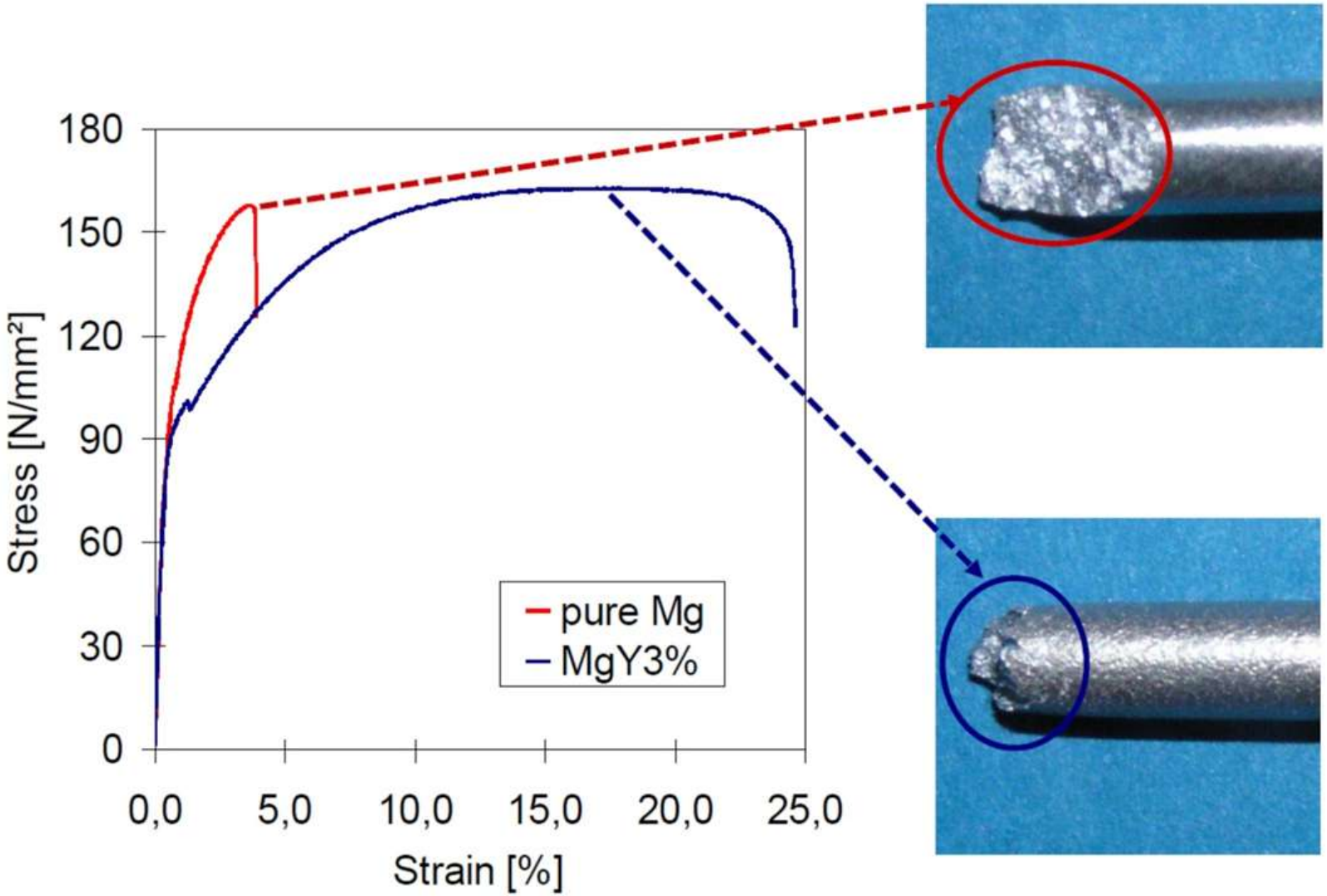

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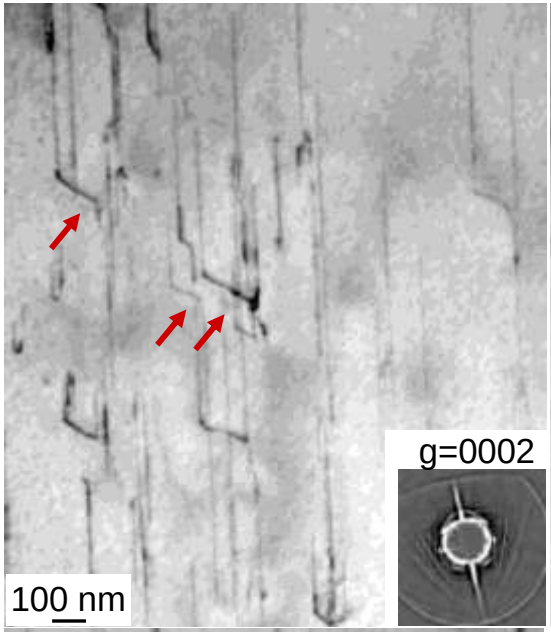
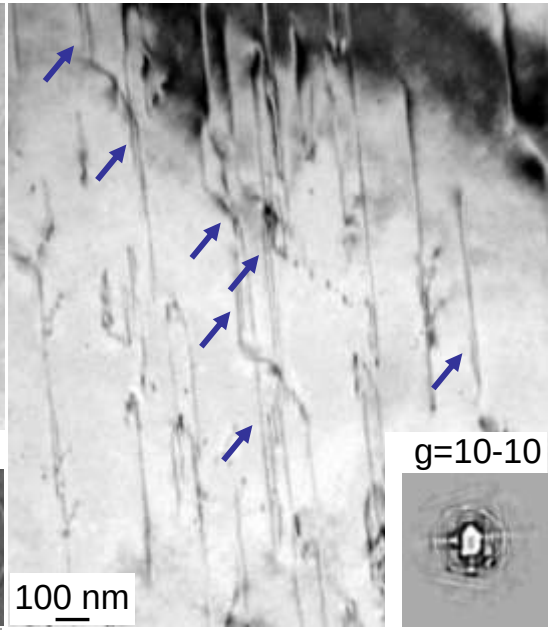
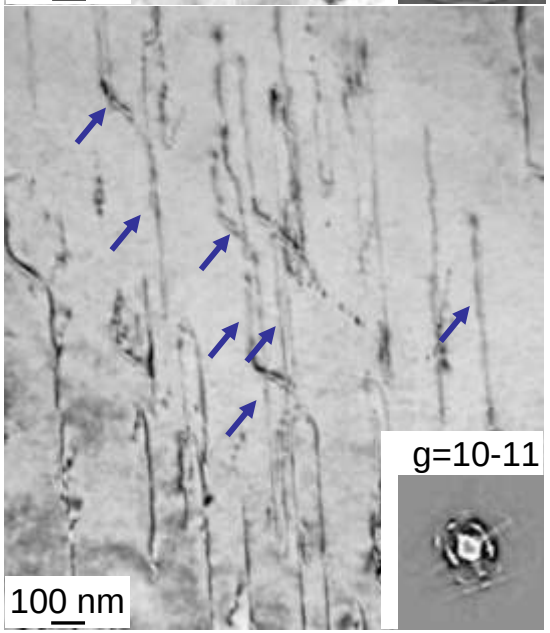
Deformation - dislocation activity







TEM images of <c+a> dislocations in Mg 3 wt-% Y (3.5 % CR)

- Red arrows: cross-slip events
- Blue arrows: dislocation dissociation on pyramidal planes

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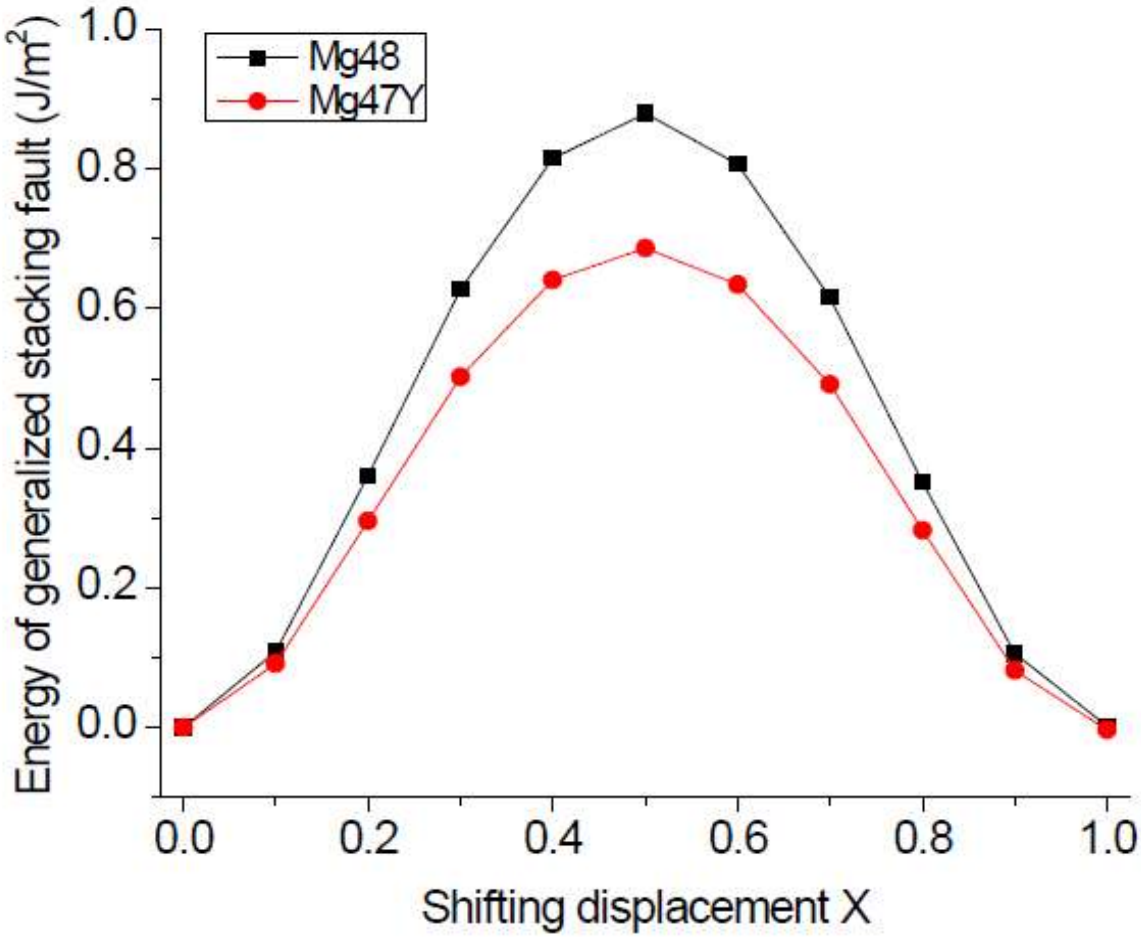
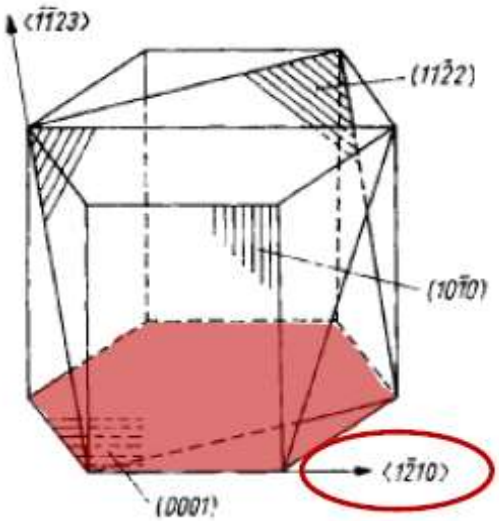
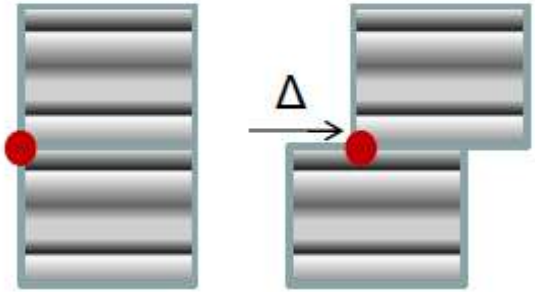
γ-surface calculations

{0001}<11-20>







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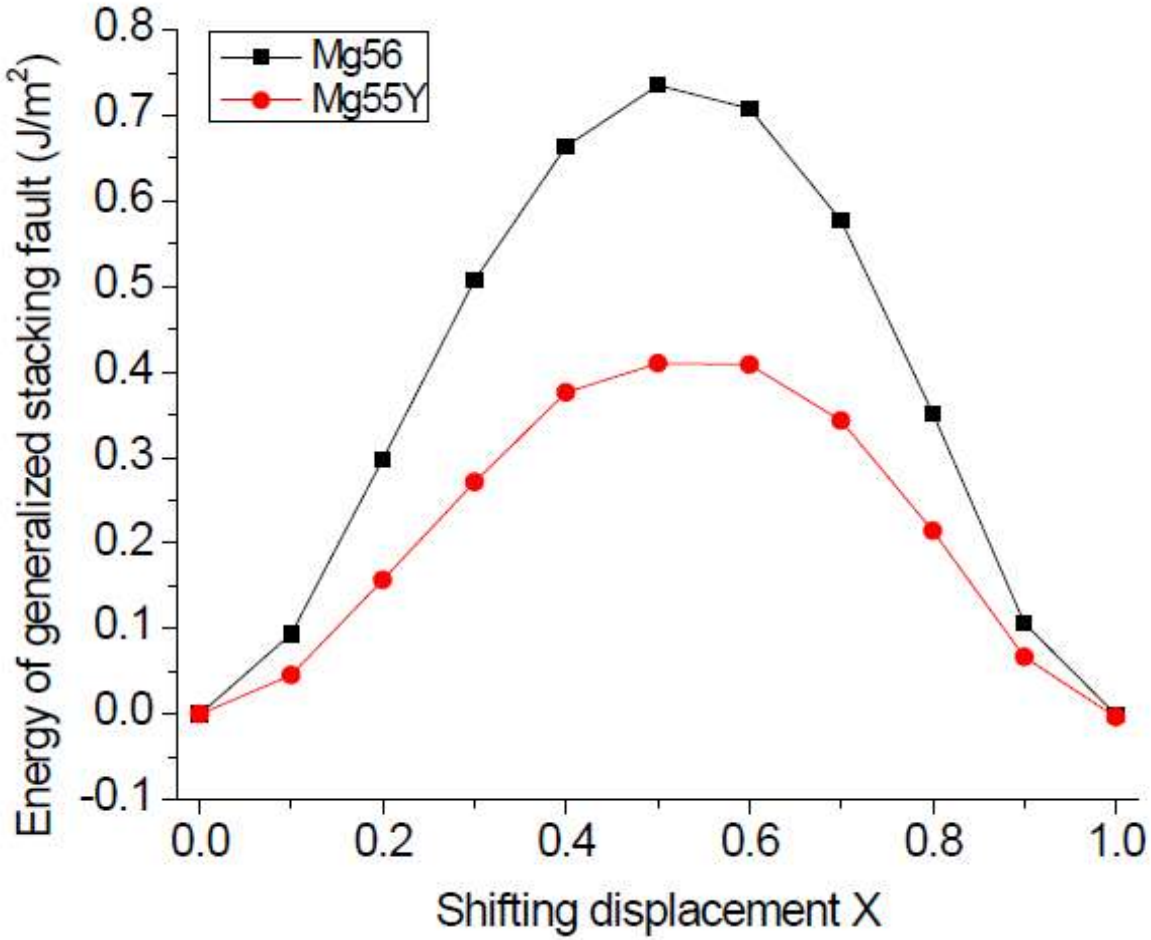
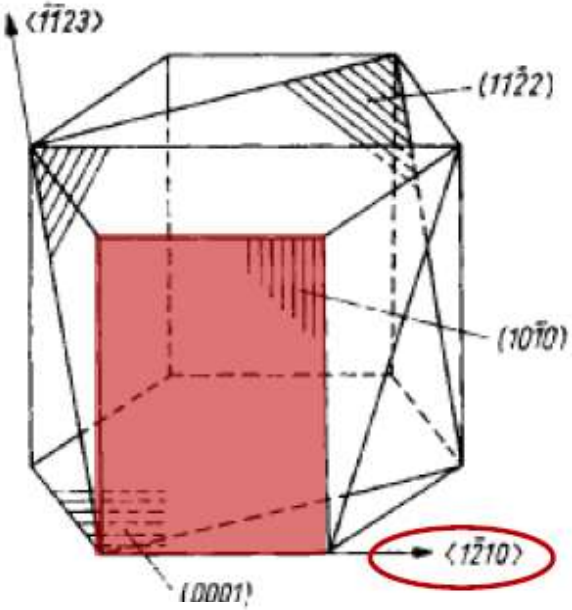
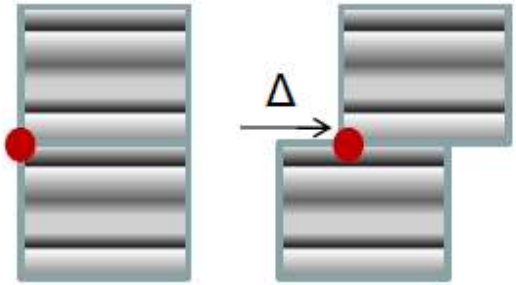
γ-surface calculations

{10-10}<11-20>







Sandlöbes et al. Acta Materialia 60 (2012) 3011

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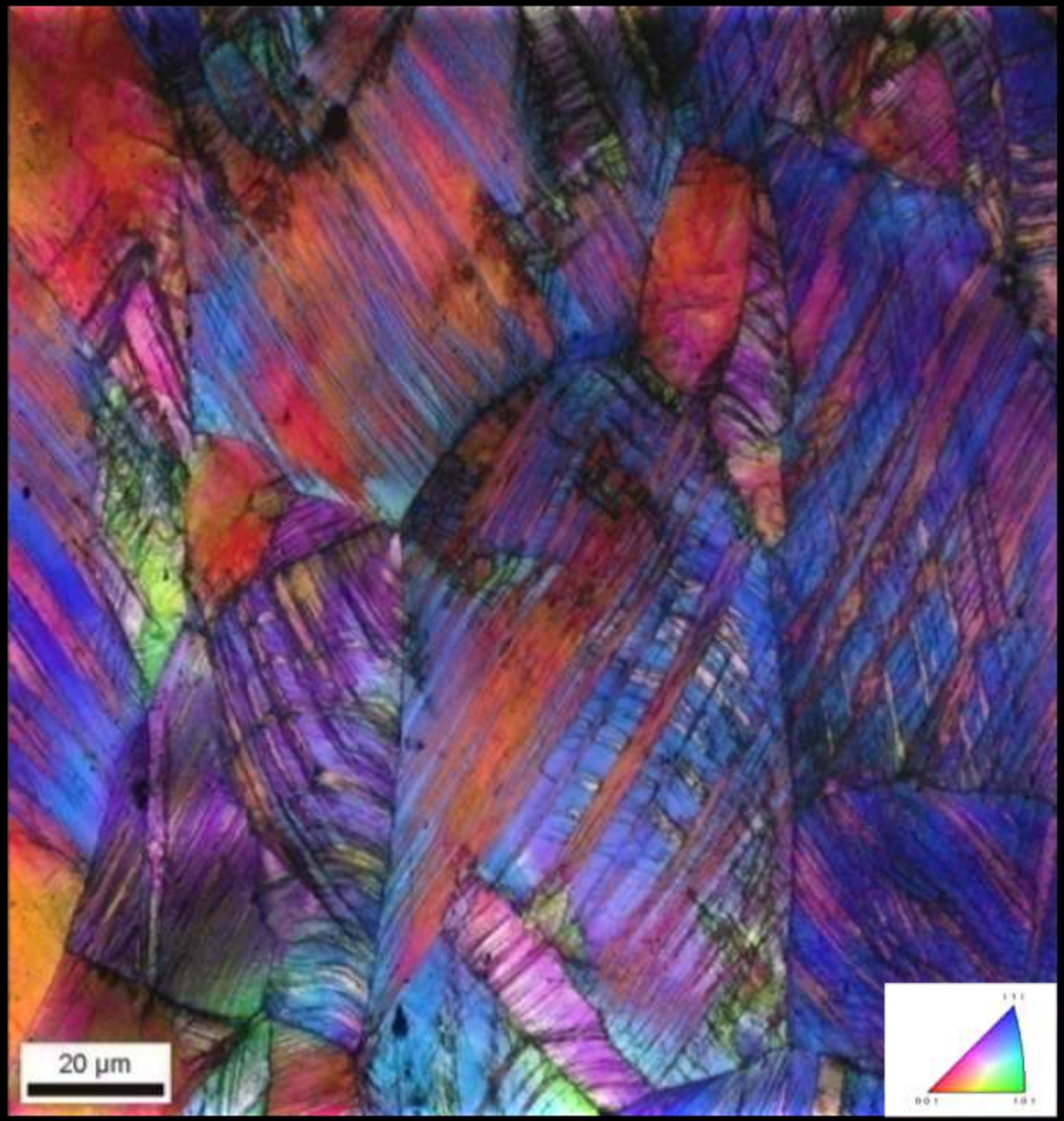
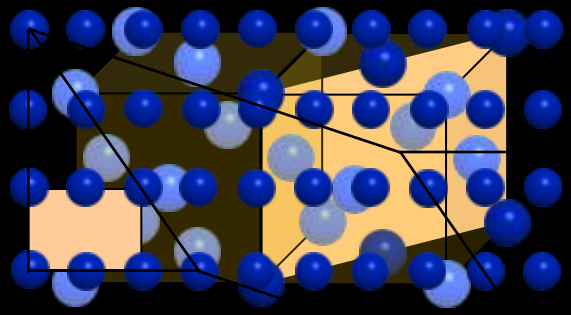
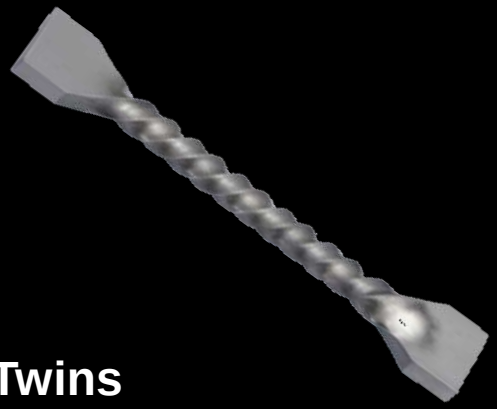
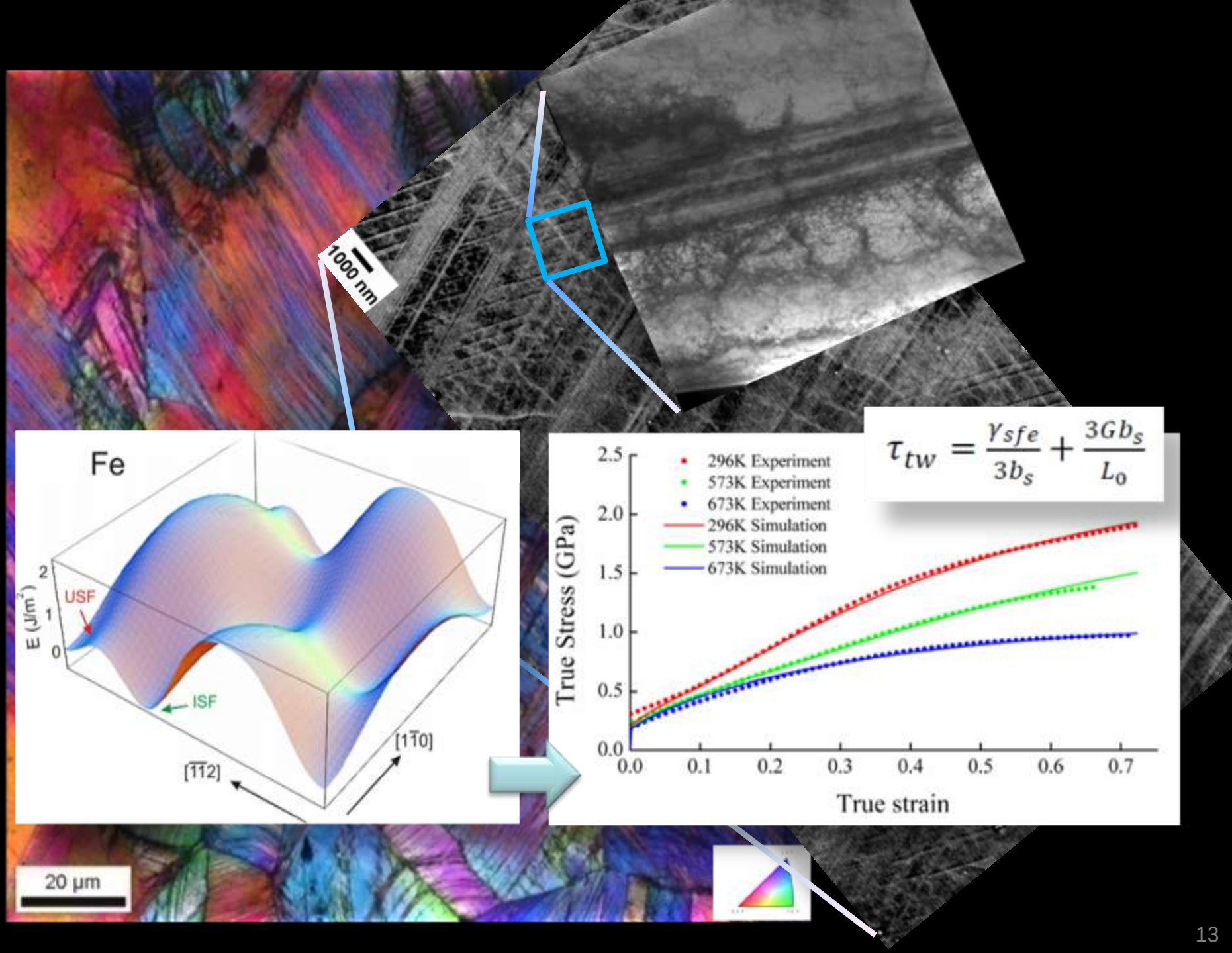
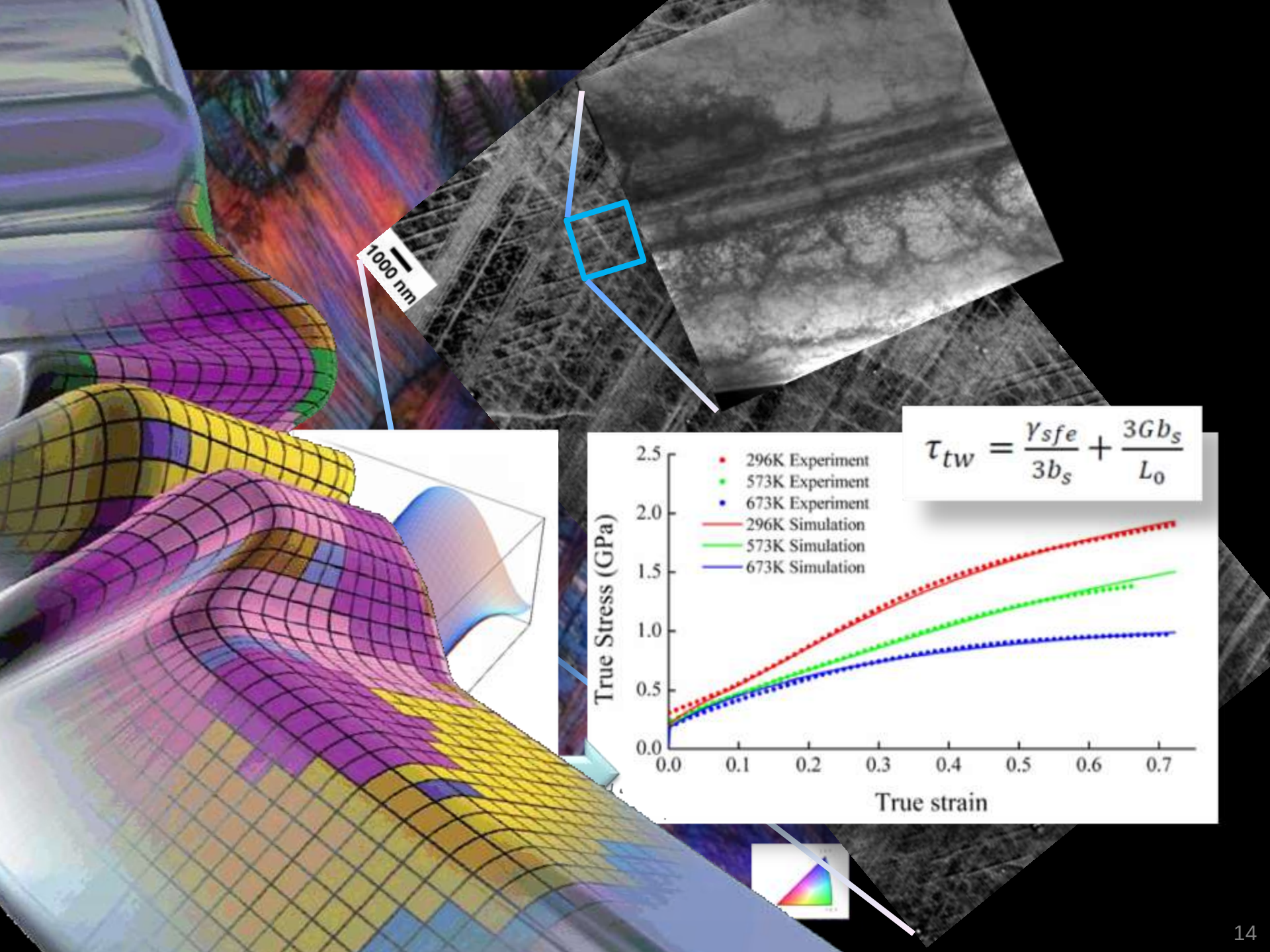




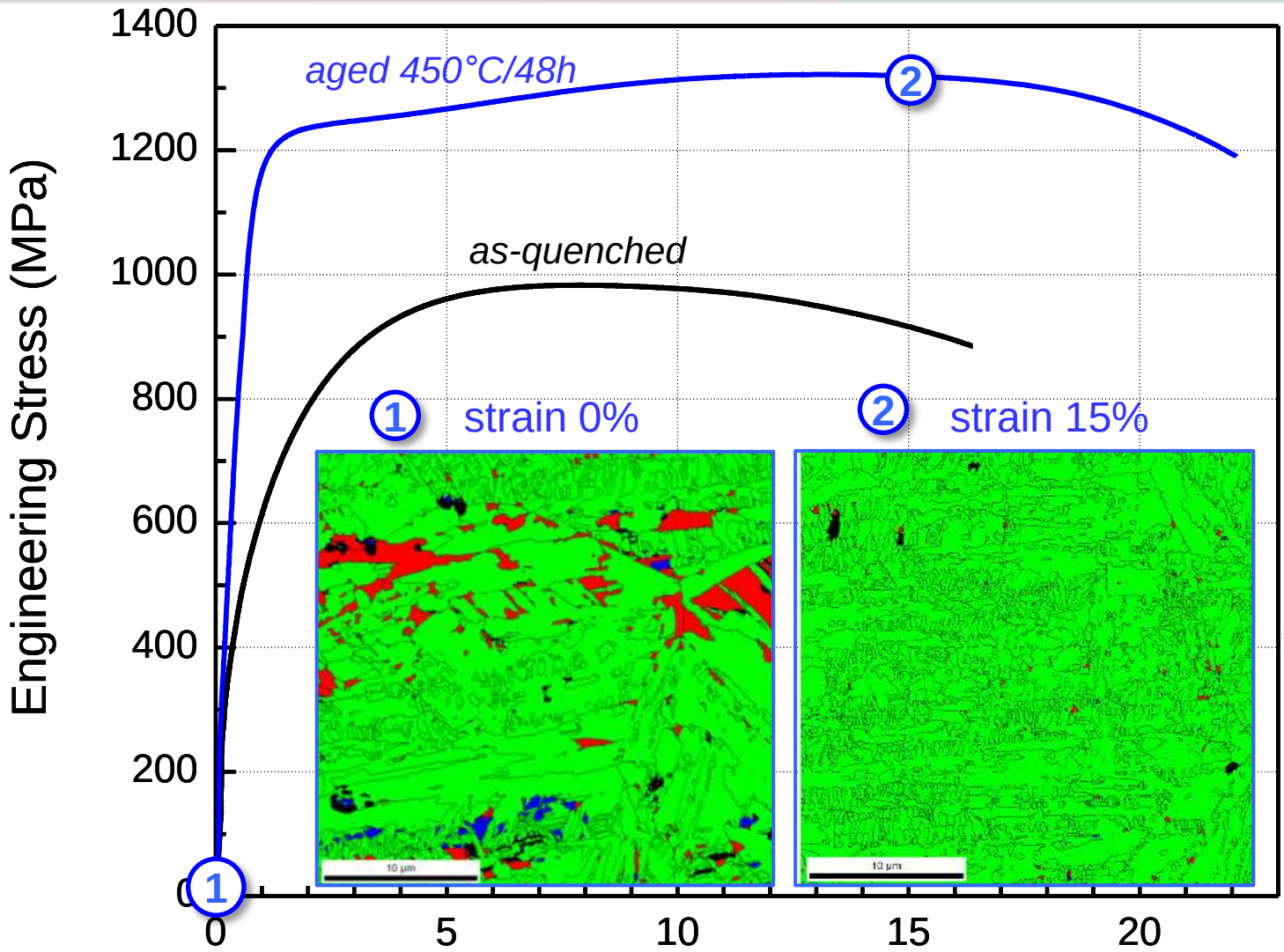


Twins
Double cross slip


1000 nm
Fe
E (J/m²)
USF
ISF
[1$\bar{1}$0]
[$\bar{1}\bar{1}$2]
20 µm
296K Experiment
573K Experiment
673K Experiment
296K Simulation
573K Simulation
673K Simulation
True Stress (GPa)
True strain
$\tau_{tw} = \frac{\gamma_{sfe}}{3b_s} + \frac{3Gb_s}{L_0}$

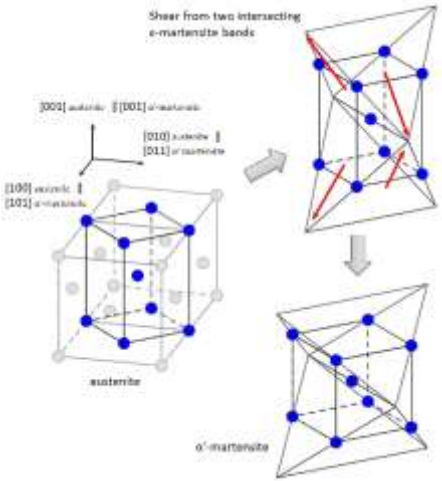

1000 nm
$\tau_{tw} = \frac{\gamma_{sfe}}{3b_s} + \frac{3Gb_s}{L_0}$
296K Experiment
573K Experiment
673K Experiment
296K Simulation
573K Simulation
673K Simulation
True Stress (GPa)
True strain
0.0
0.5
1.0
1.5
2.0
2.5
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7

Effect of aging on ductility



Precipitation hardening

increase of austenite fraction during aging



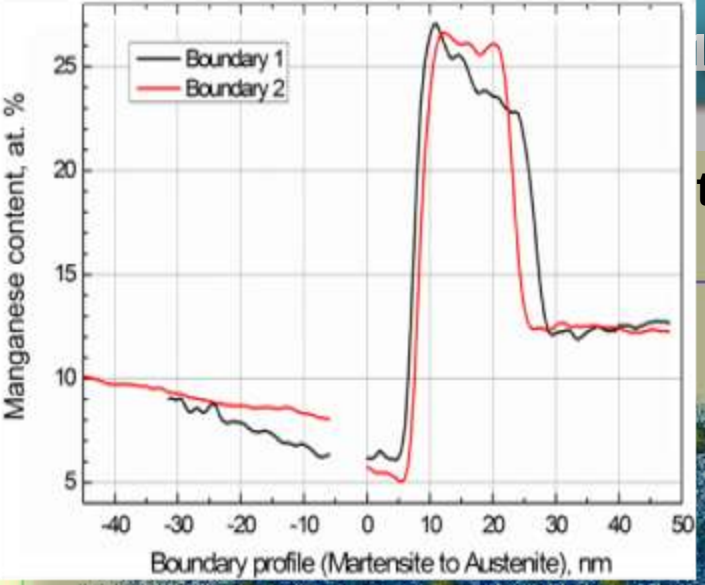
α-Fe (Martensite)

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

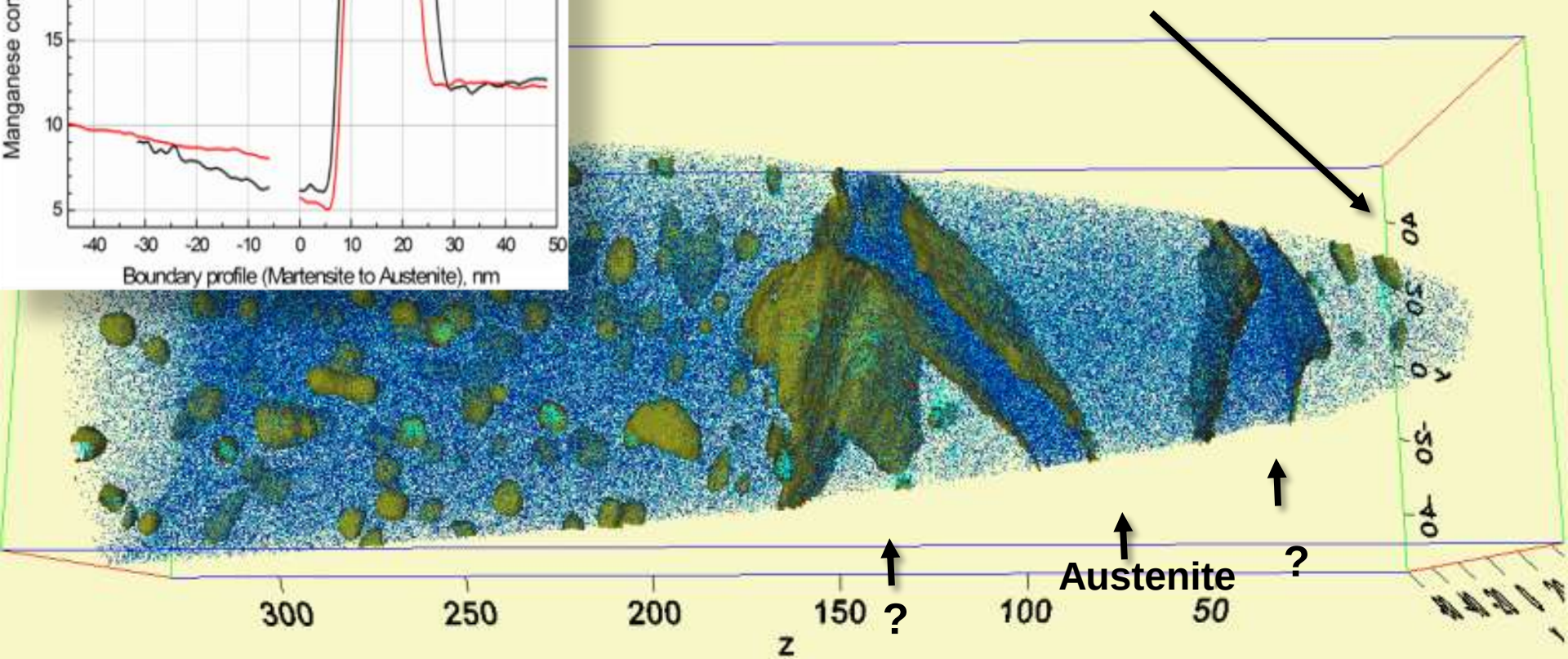
C	Ni	Mo	Ti	Al	Mn	Fe
0.01	2.0	1.0	1.0	0.15	12	bal.

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

12%Mn, aged 450°C/48h)



te decorated by precipitations



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

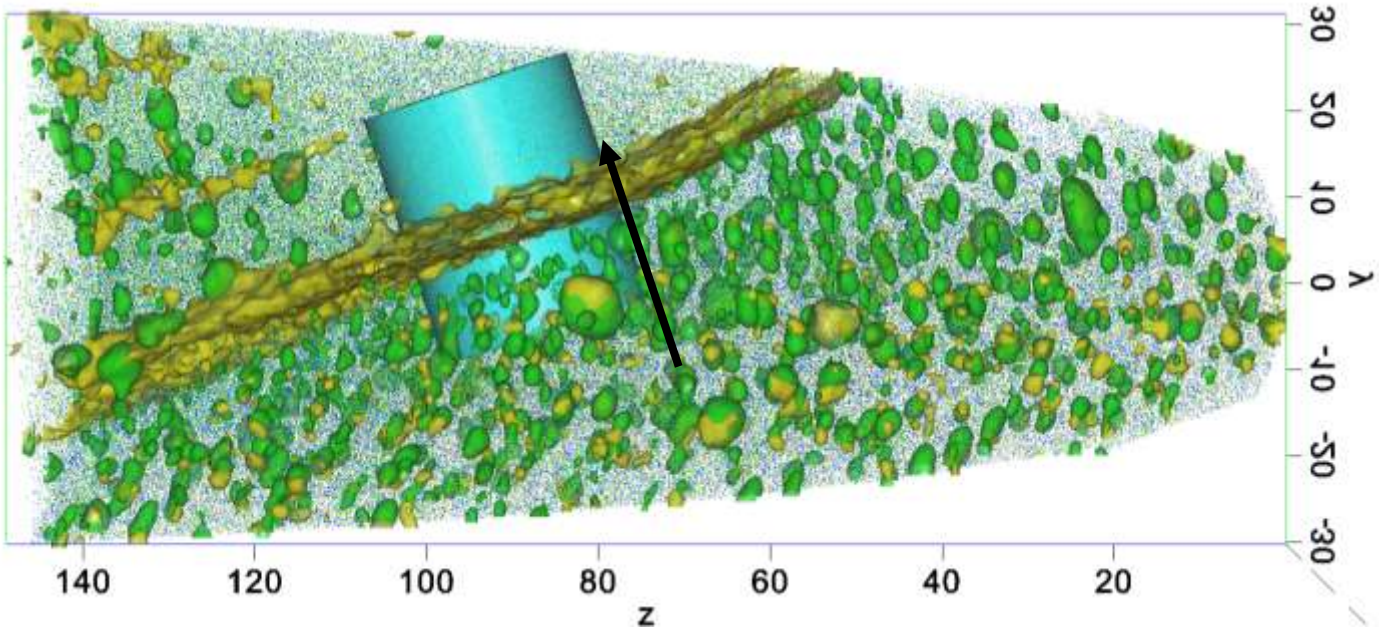
Scale: nm

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

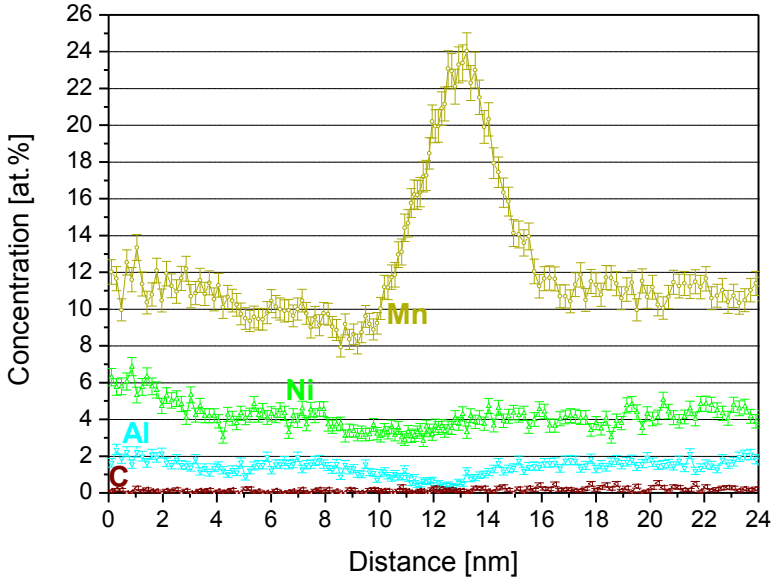
70 million ions
Laser mode
(0.4nJ, 54K)

Dmitrieva et al. Acta Mater 59 (2011)

Mn segregation at grain boundary, (450°C/65h)



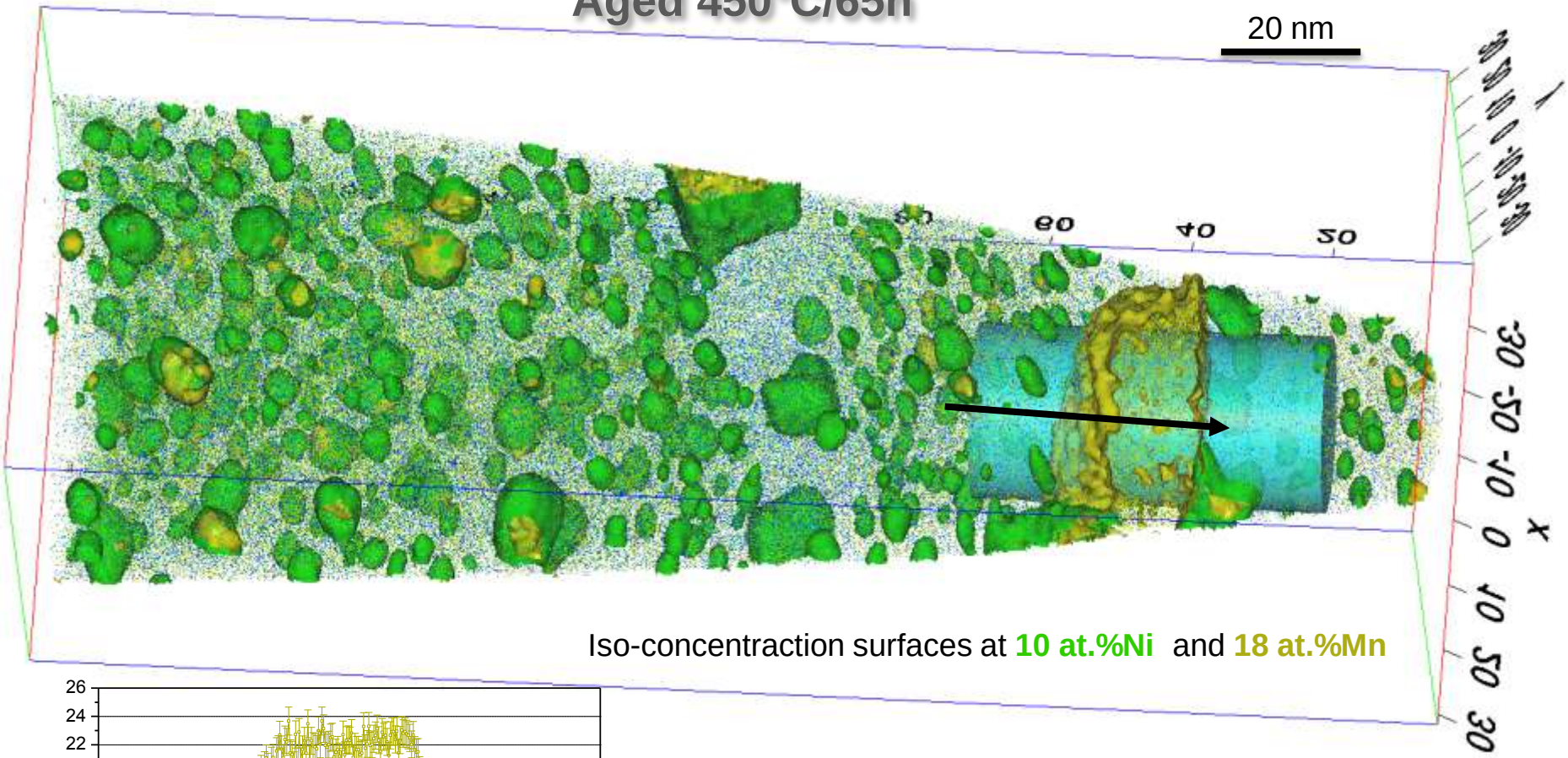
20 nm

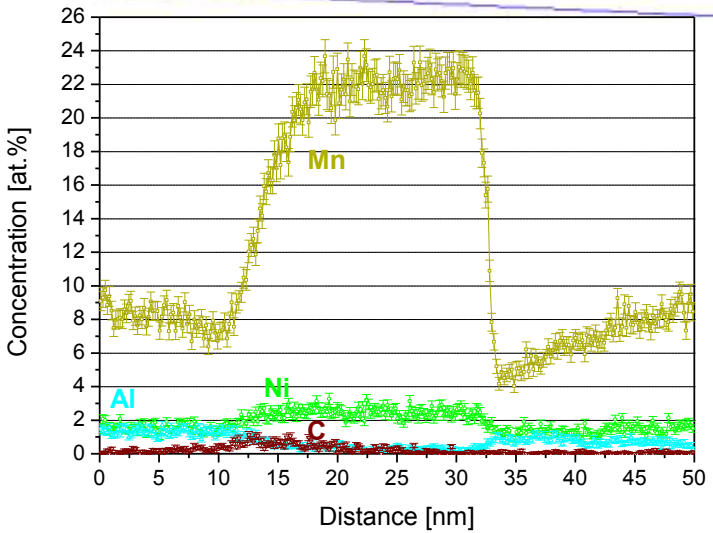


9Mn-2Ni-0.15Al-1Ti-1Mo (wt.%)

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

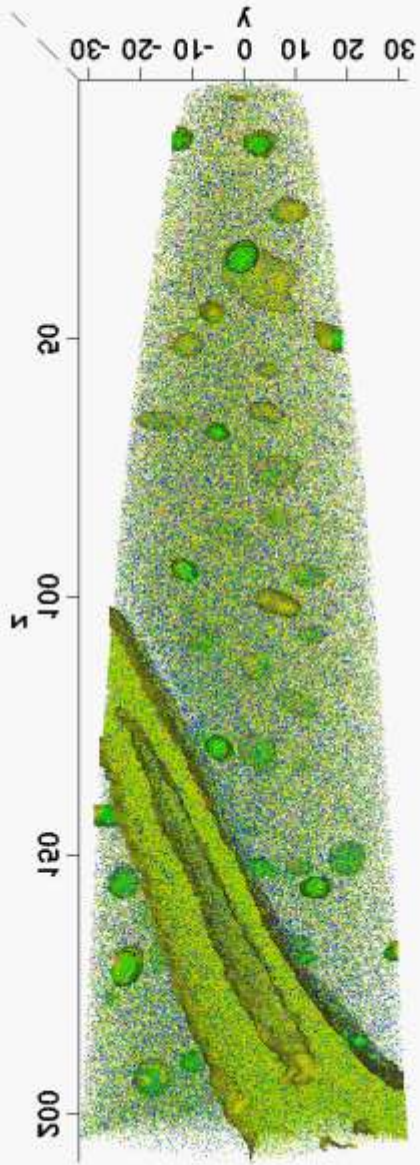
Aged 450°C/65h

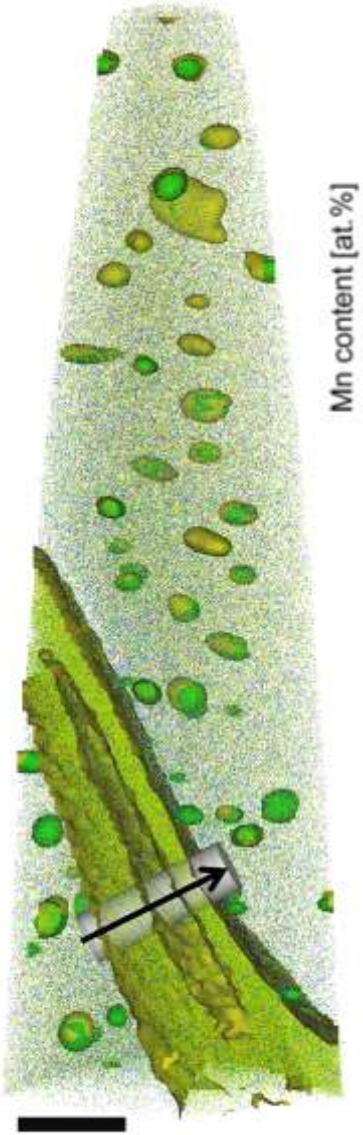




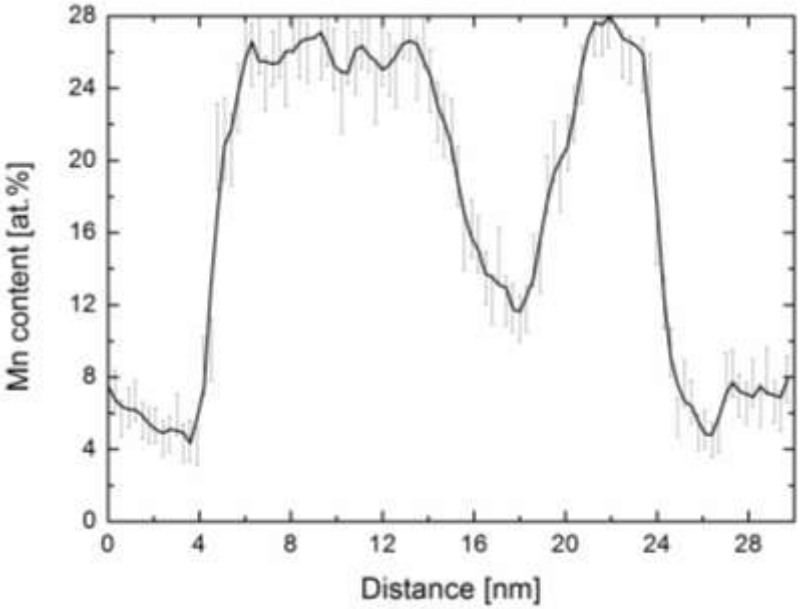
9Mn-2Ni-0.15Al-1Ti-1Mo (wt.%)

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



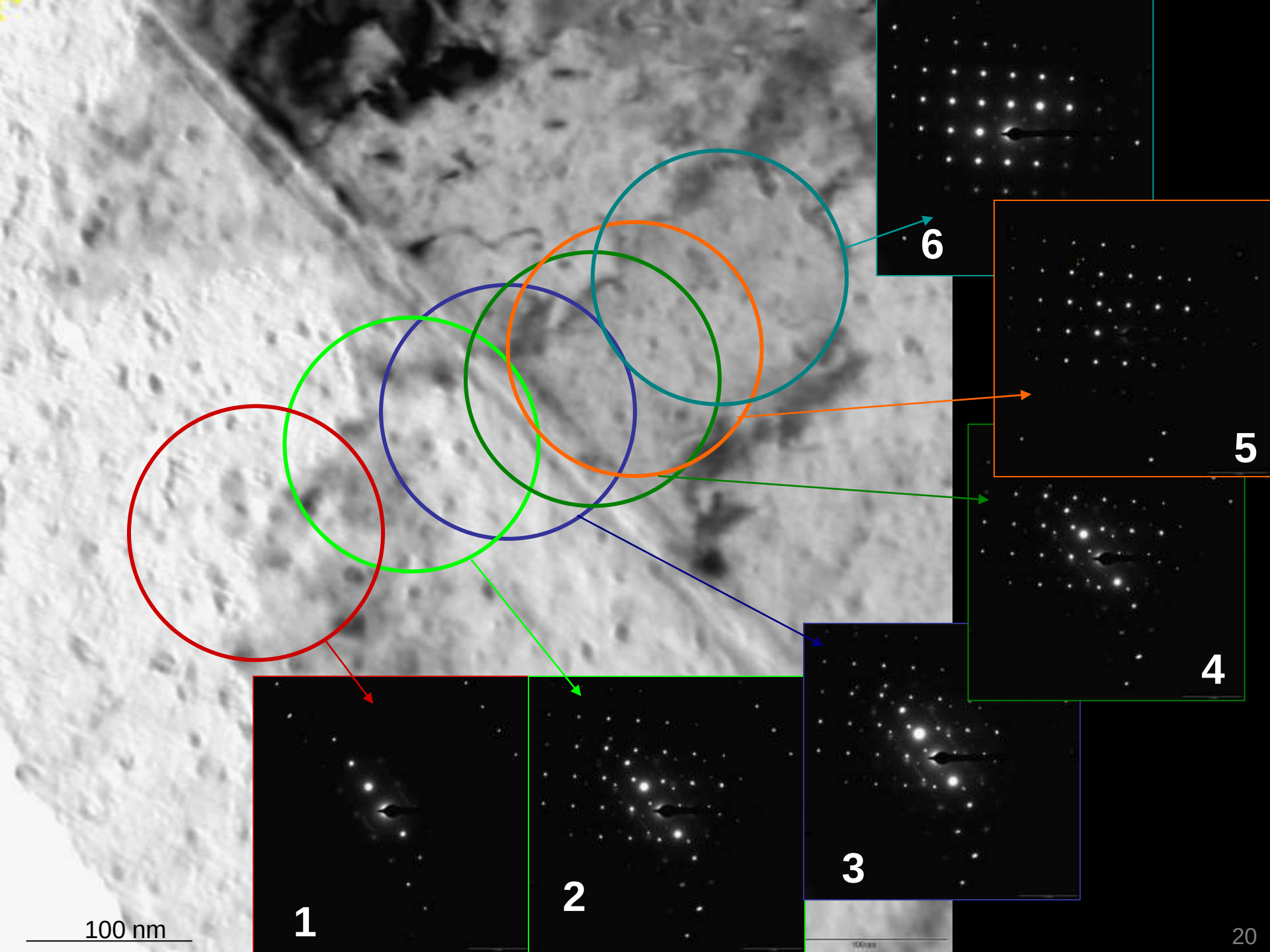


Mn profile

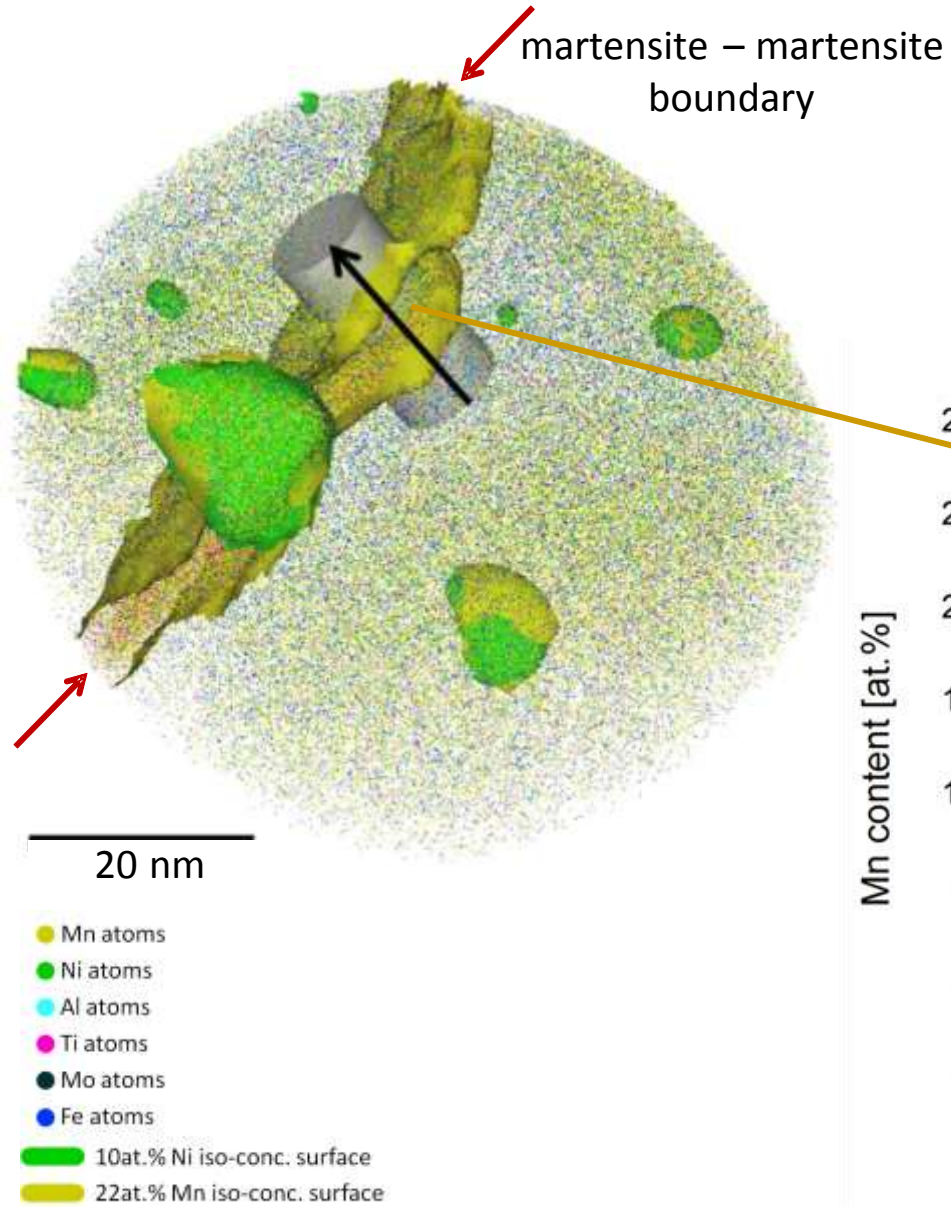


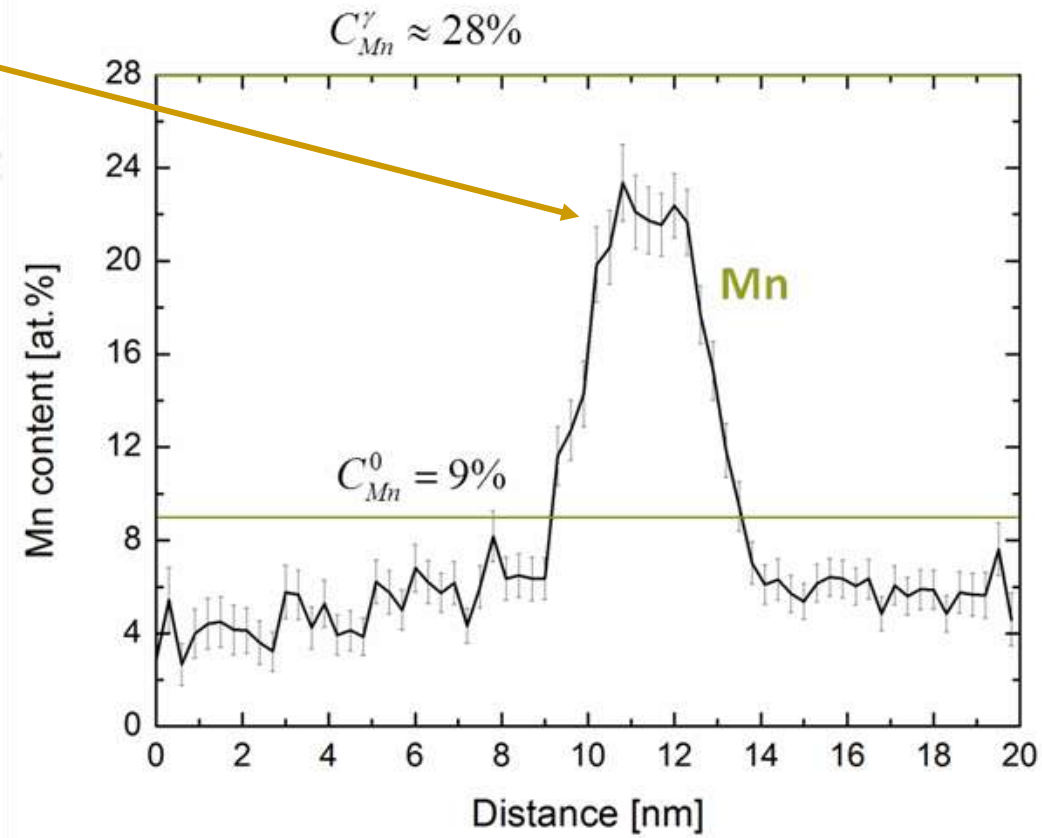
- Mn atoms
- Ni atoms
- Al atoms
- Ti atoms
- Mo atoms
- Fe atoms
- 10at.% Ni iso-conc. surface
- 22at.% Mn iso-conc. surface

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

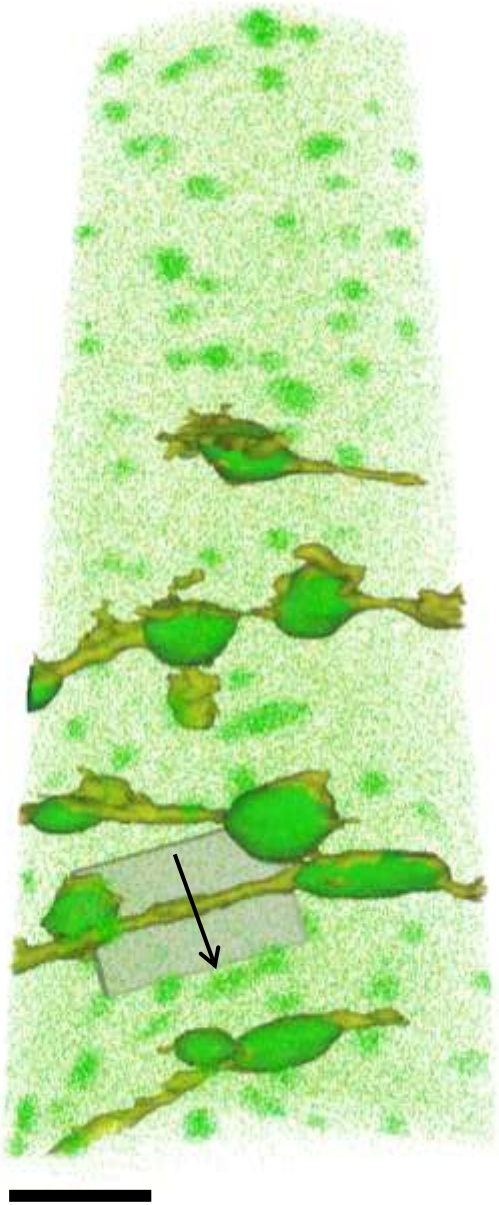

1
2
3
4
5
6
100 nm

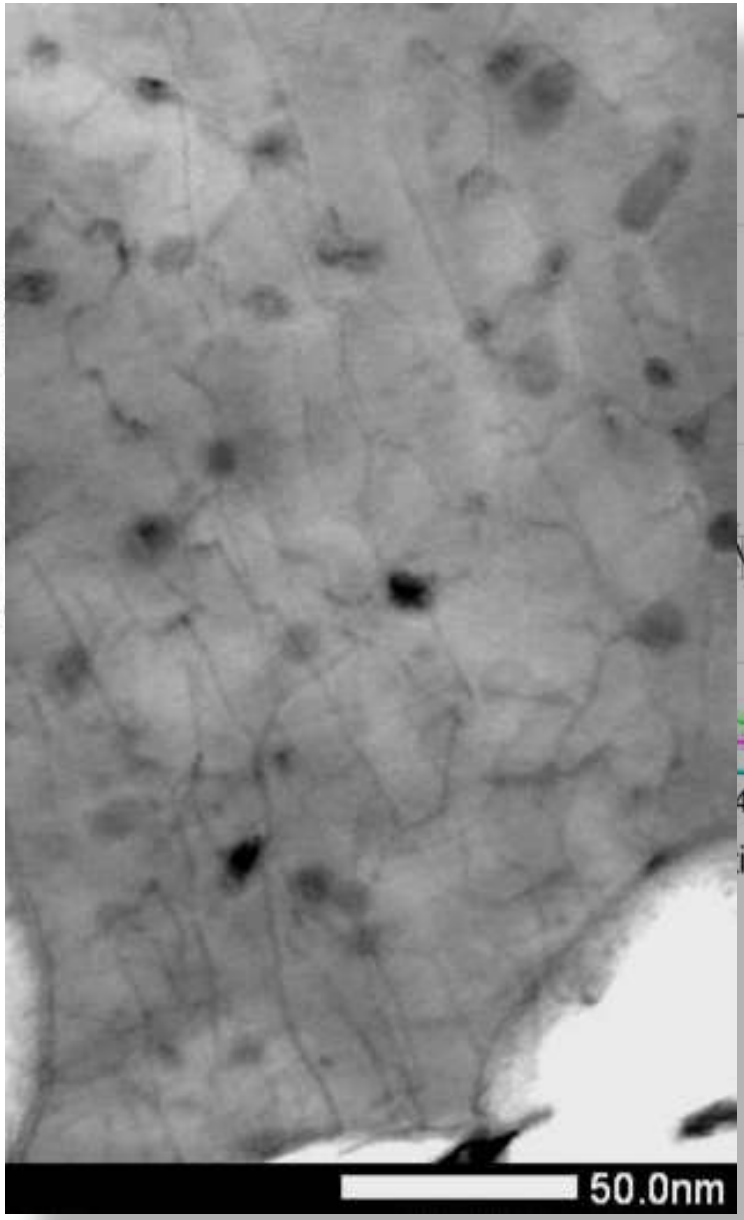
Thin intergranular FCC layer among two martensite crystals, APT

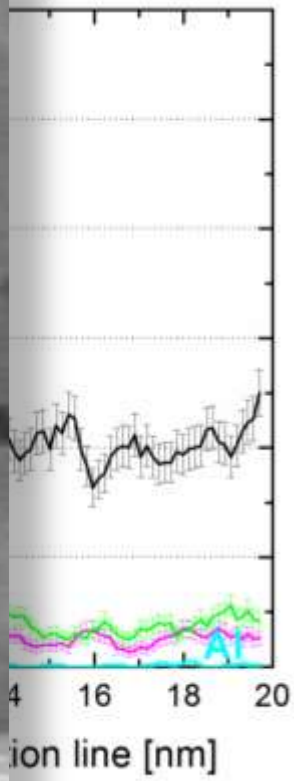




Mn segregation at dislocations, (450°C/48h)







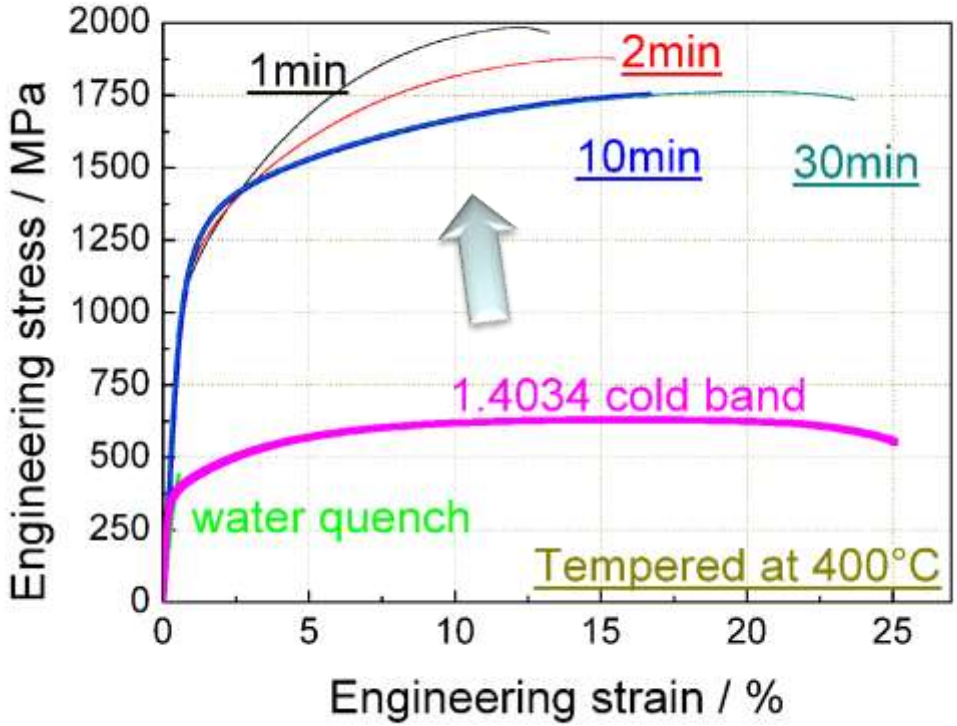
12Mn-2Ni-0.15Al-1Ti-1Mo (wt.%)

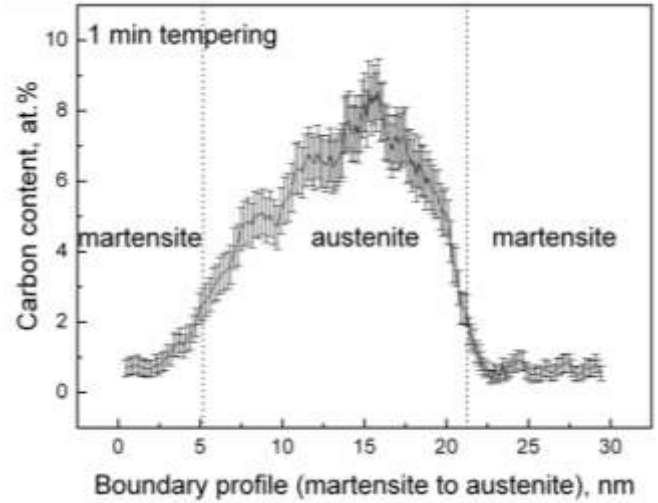
iso-conc surfaces at **14at.%Mn** and **8at.%Ni**

Raabe, Ponge, Dmitrieva, Sander: Adv. Eng. Mat. 11 (2009) 547

Martensite relaxation & aging & nanoscale austenite reversion

650 MPa to 2 GPa



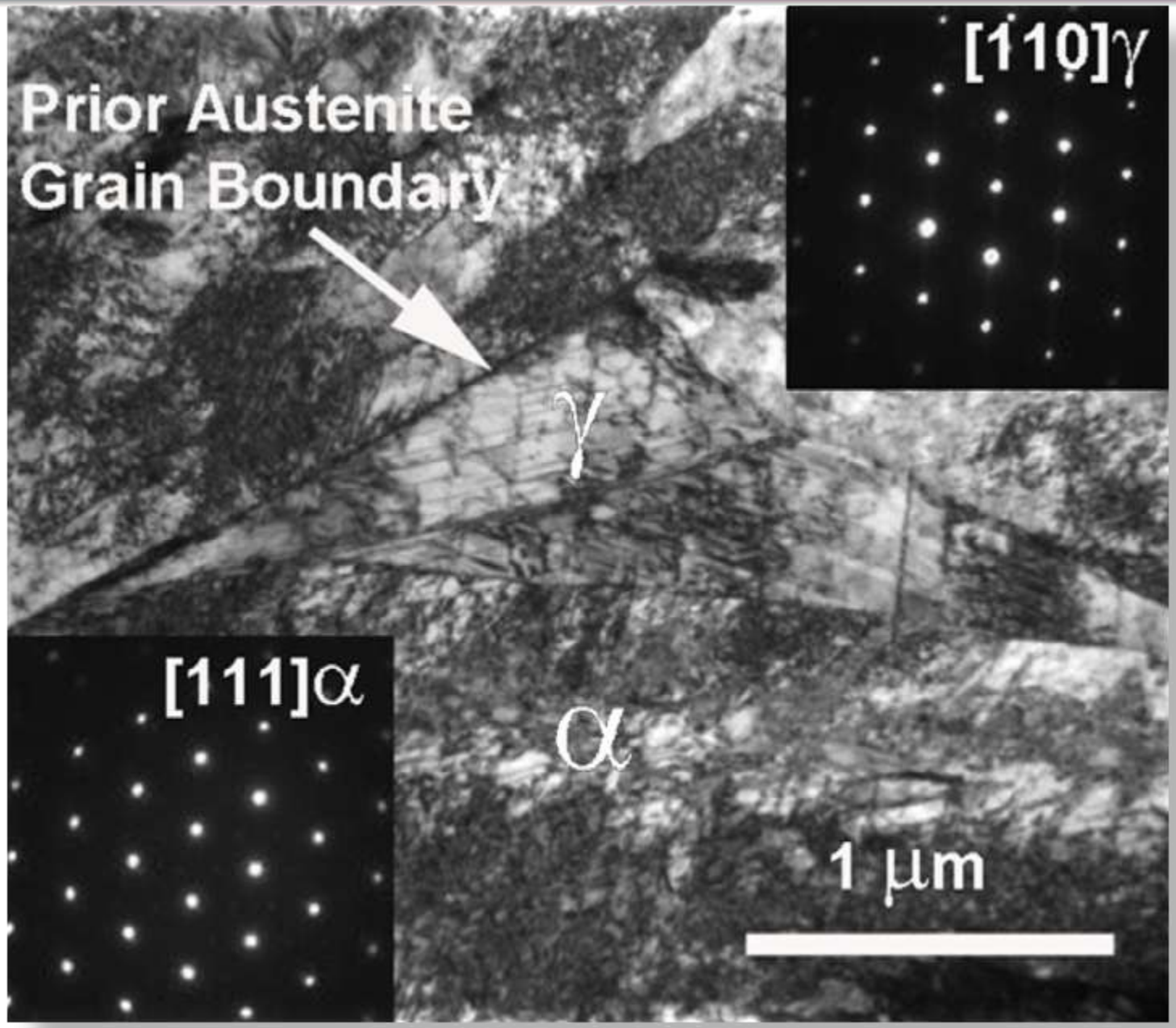


400°C aging:
Ms-relaxation + precipitation + <u>austenite reversion</u>

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

L. Yuan et al. Acta Mater (2012)

Martensite relaxation & aging & nanoscale austenite reversion



L. Yuan et al. Acta Mater (2012)

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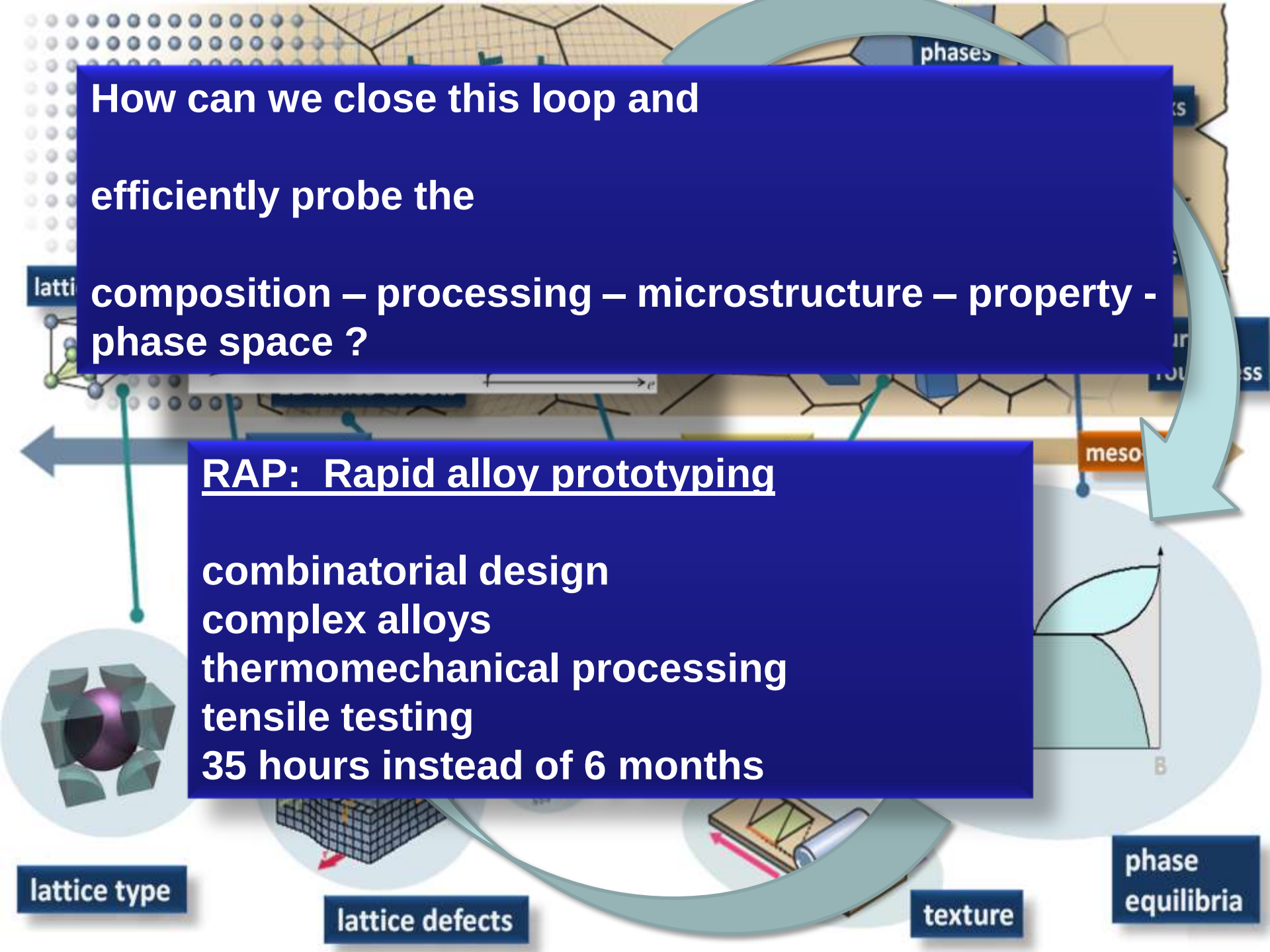


How can we close this loop and

efficiently probe the

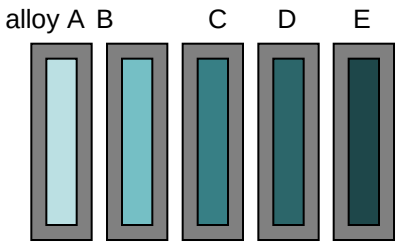
composition – processing – microstructure – property - phase space ?

RAP: Rapid alloy prototyping

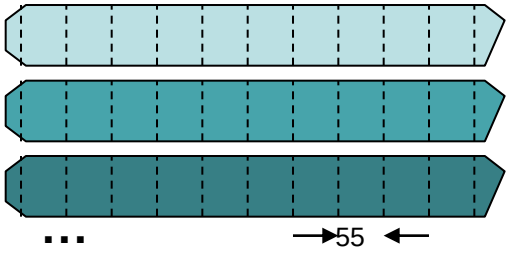
combinatorial design
complex alloys
thermomechanical processing
tensile testing
35 hours instead of 6 months

Rapid alloy prototyping: combinatorial design of complex alloys

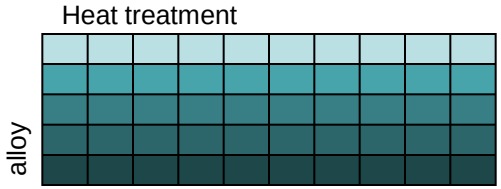
1. **Multi-ingot vacuum or inert gas inductive melting and casting**



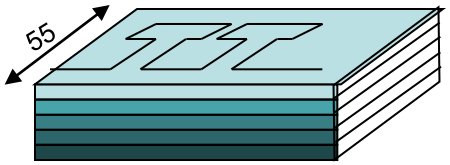
2. **Homogenization and hot rolling**



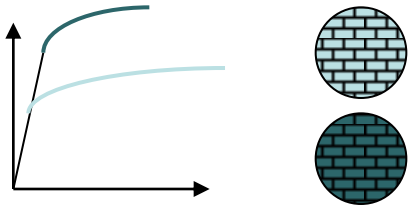
3. **Heat treatment and / or thermomechanical processing**



2. **Discharge sample preparation**

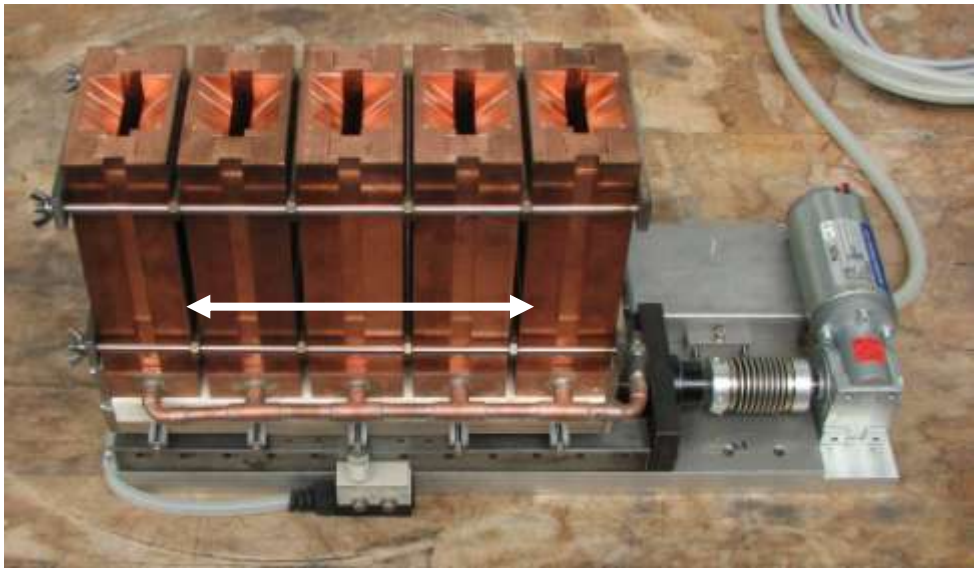


3. **Tensile testing (3 test per state)**



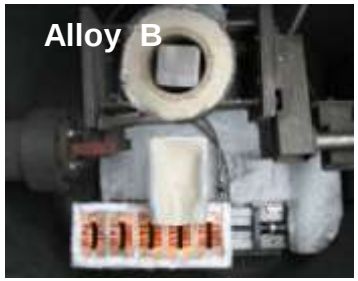
Springer, Raabe, Acta Mater (2012) in press

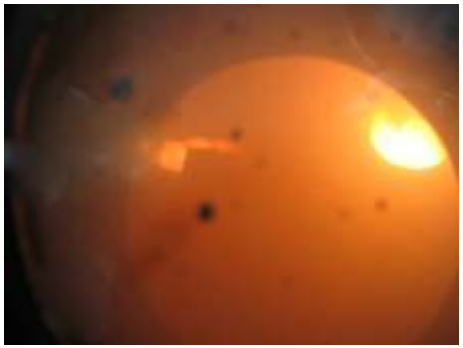
Rapid alloy prototyping: multiple ingot casting



5 Cu-moulds, 60 kW vacuum induction furnace (vacuum, Ar, air)

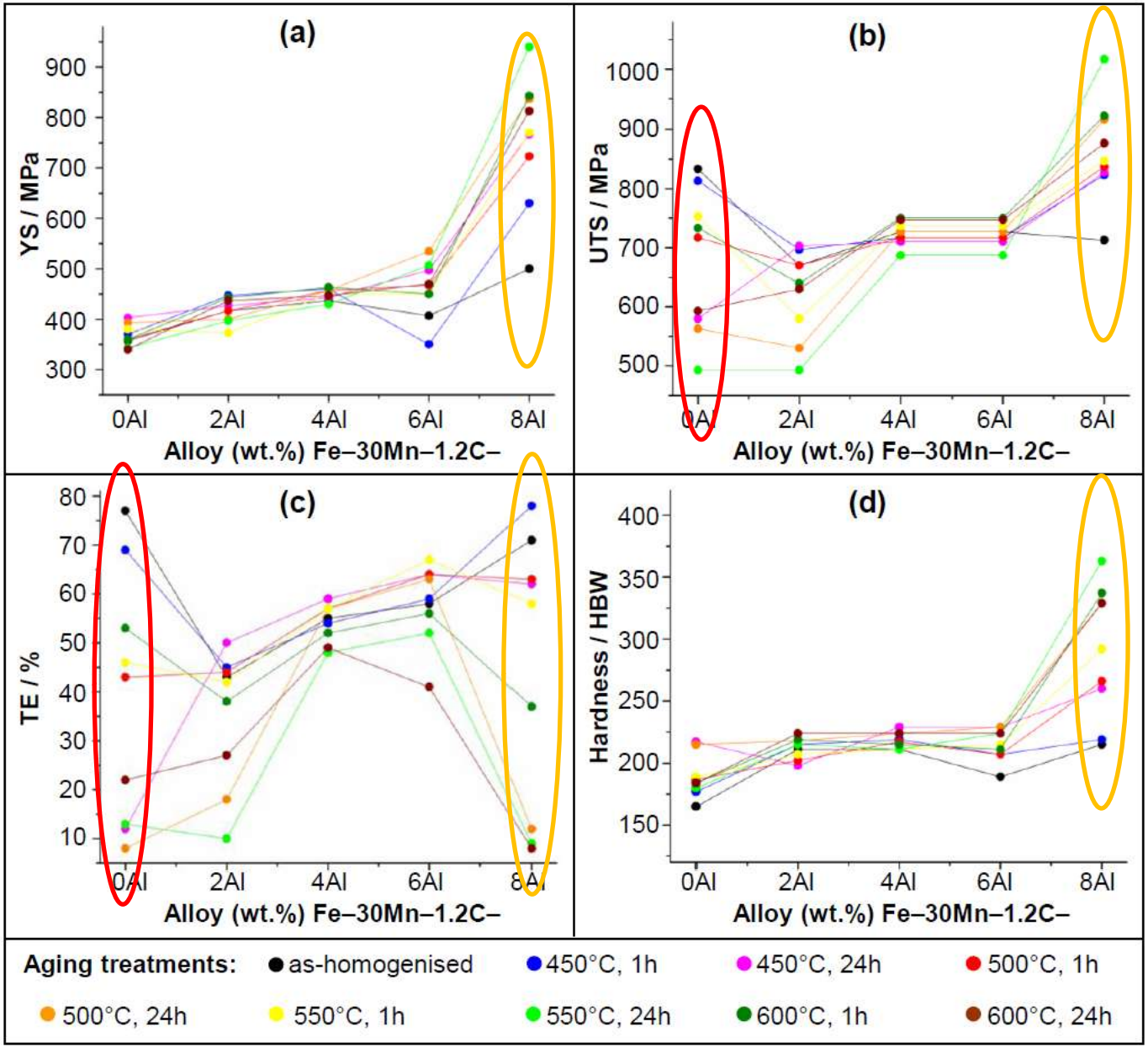
10 x 50 x 150 mm^3



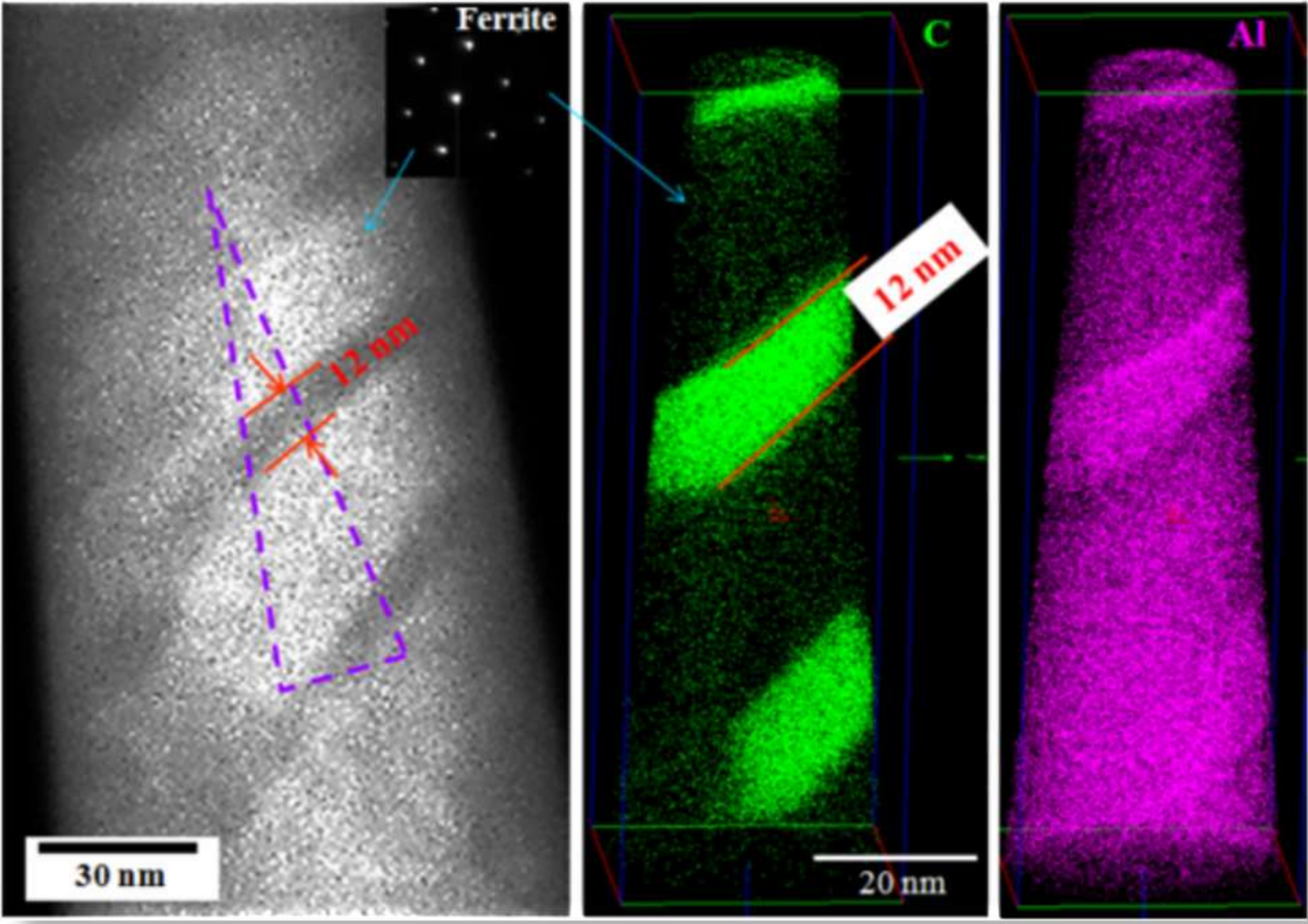


Springer, Raabe, Acta Mater (2012) in press

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

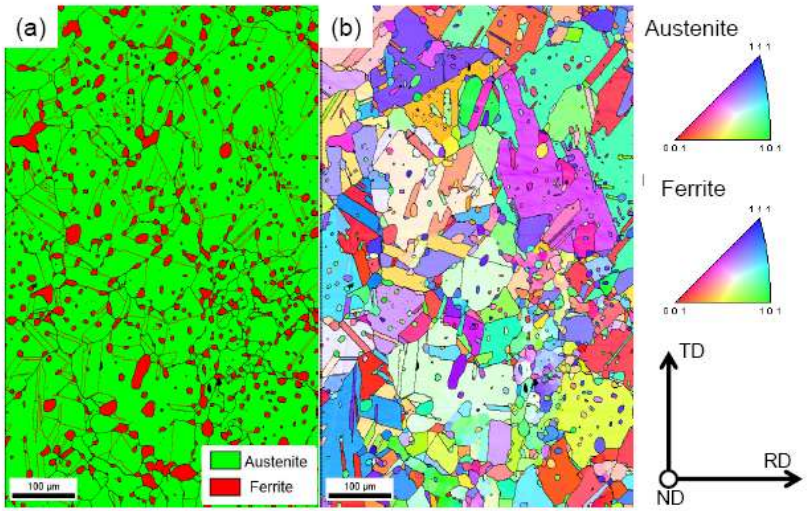


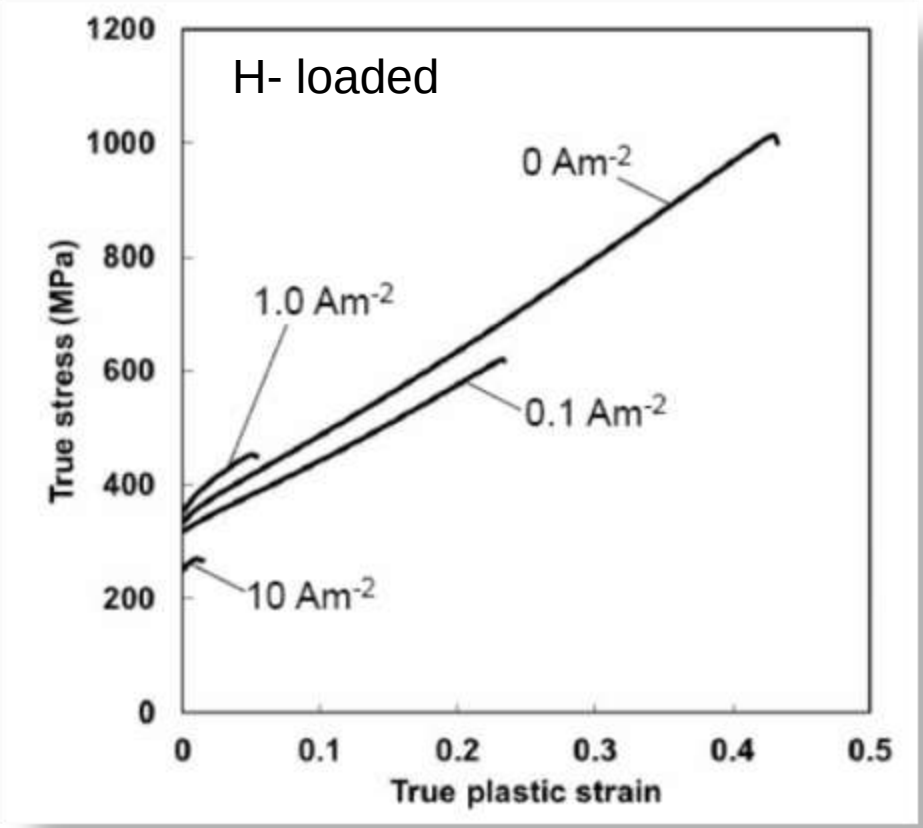
Springer, Raabe, Acta Mater (2012) in press


Ferrite
12 nm
30 nm
C
12 nm
20 nm
Al

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

Fe-24Mn–0.5C–8.6Al (wt%)





Courtesy of Dr. Koyama (NIMS, MPI)

Overview

- First principles guided design of structural alloys
  - Mg-Li
  - Mg-Y
  - TWIP steel
  - Phase transformation at lattice defects
- RAP (Rapid Alloy Prototyping)
  - Combinatorial design of bulk alloys
  - Density-reduced TRIPLEX steels
- Conclusions