Integrated micromechanical experimentation and simulation for complex alloys

C.C. Tasan

Max-Planck-Institut
für Eisenforschung GmbH

12.06.15
Aachen / Germany

STRUCTURAL
ADAPTIVE
MATERIALS

DFG

CHINA SCHOLARSHIP COUNCIL

JFE

M2i Materials innovation institute

TATA STEEL

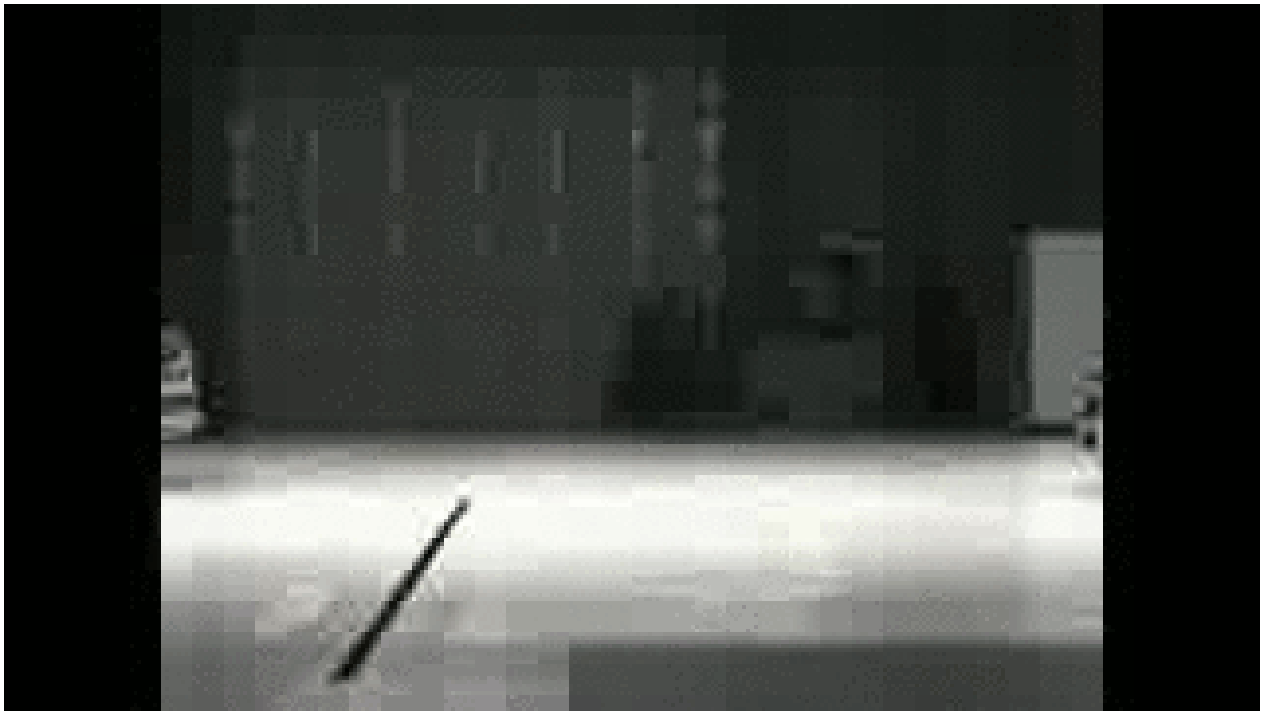
ArcelorMittal

imprs surmat

erc European Research Council

S. Kalidindi
(GT, USA)
D. Raabe
(MPIE, Germany)
J. Neugebauer
(MPIE, Germany)
M. Geers
(TU/e, Netherlands)
K. Tsuzaki
(NIMS, Japan)

Motivation

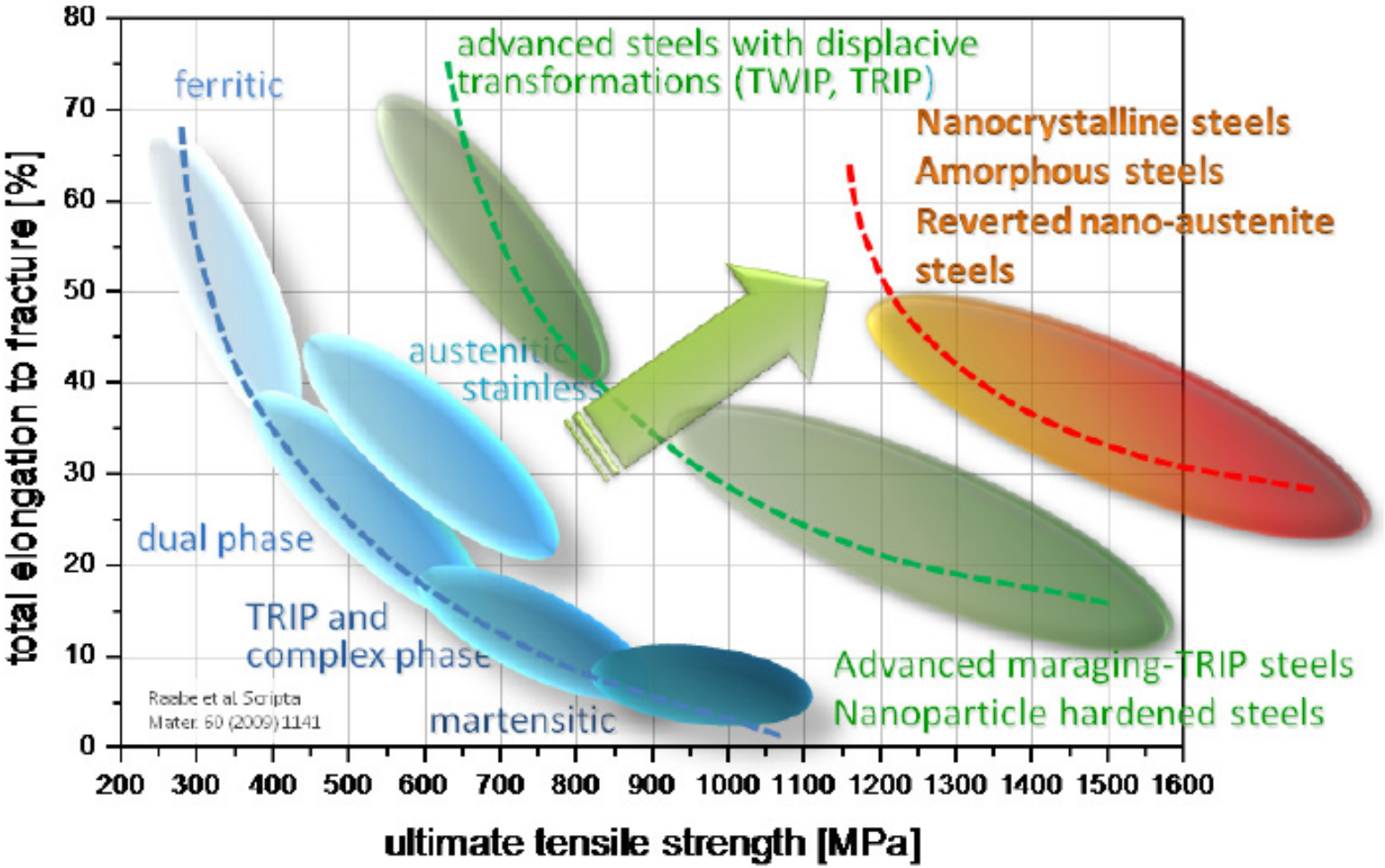


*Insurance Institute for Highway Safety, http://youtu.be/joMK1WZjP7g

Integrated computational materials engineering (ICME)

- Materials innovations are the core of (all!) technological advances ☺
- Technological advances are <u>dependent</u> on materials innovations ☹

- Problem: Product design rate >>> materials development rate

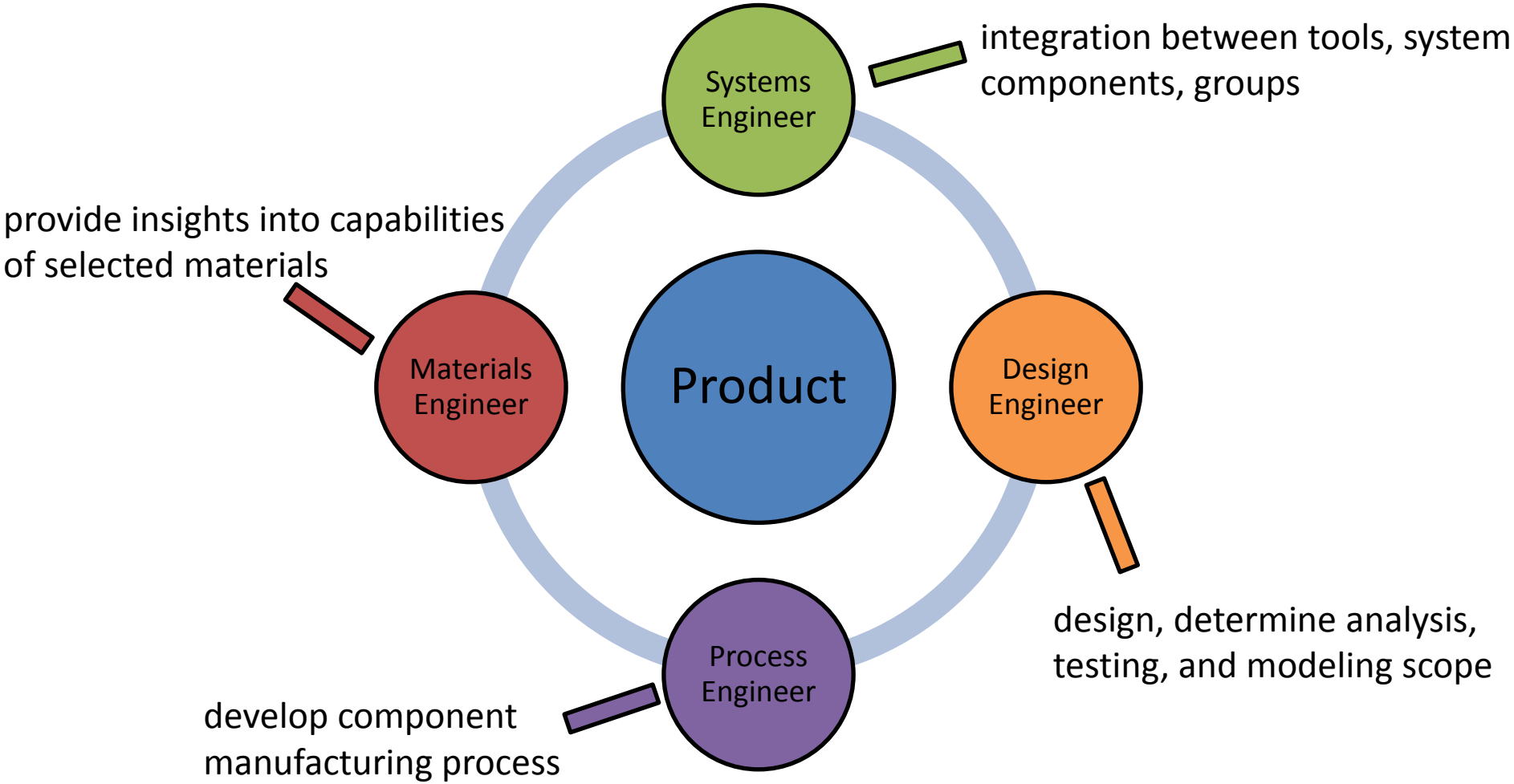


ICME Strategy

- Problem: Product design rate >>> materials development rate
- Solution: integrated optimization of design-manufacturing-materials

ICME Strategy

- Problem: Product design rate >>> materials development rate
- Solution: integrated optimization of design-manufacturing-materials

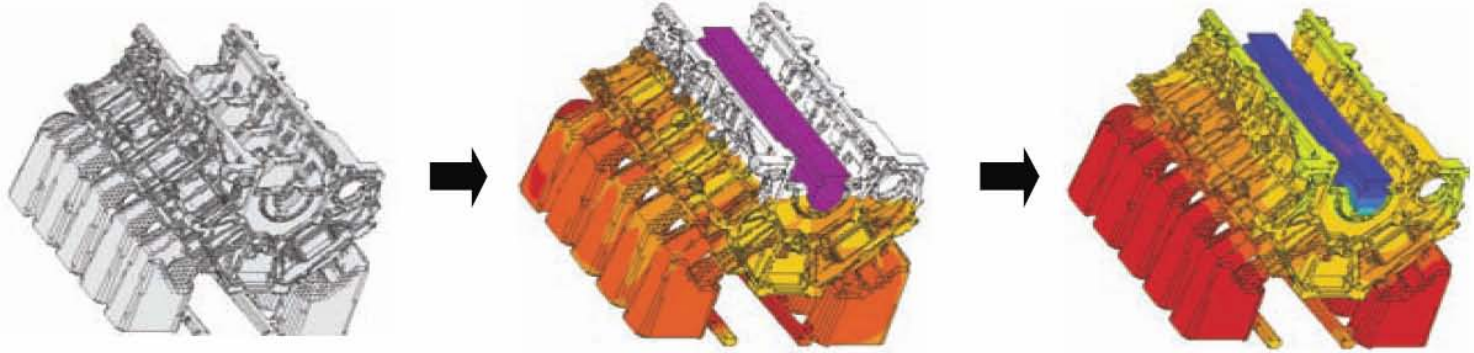


ICME Example: Virtual Aluminum Castings

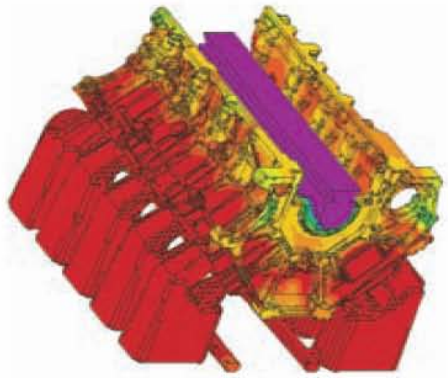
Initial Geometry
- CAD Geometry and Mesh

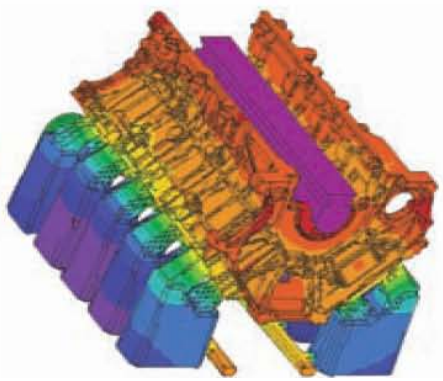
Filling
- Accurate filling Profile (ProCast, OPTCAST)

Thermal Analysis
- Boundary Conditions (OPTCAST)
- Fraction solid Curves (ThermoCALC)



Microstructure (Al_2Cu)
- Micromodel (MicroMod, PanDat)
- Solution treatment (Dictra)
- Aging Model (NanoPPT, PanDat)





Yield Strength
- Local YS

- Integration & validation (very) challenging!

Integrated in-situ experiments & full-field crystal plasticity simulations to analyze stress –strain partitioning in multi-phase alloys

C. Tasan, D. Yan, M. Diehl, C. Zambaldi, P. Shanthraj, P. Eisenlohr, F. Roters, D. Raabe

Max-Planck-Institut
für Eisenforschung GmbH

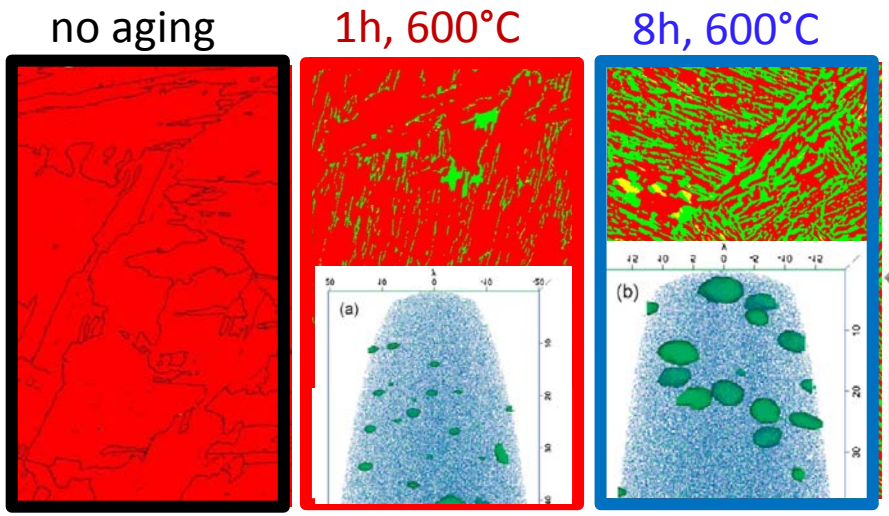
Tasan, Yan, Diehl, et al., Acta Materialia, 2014

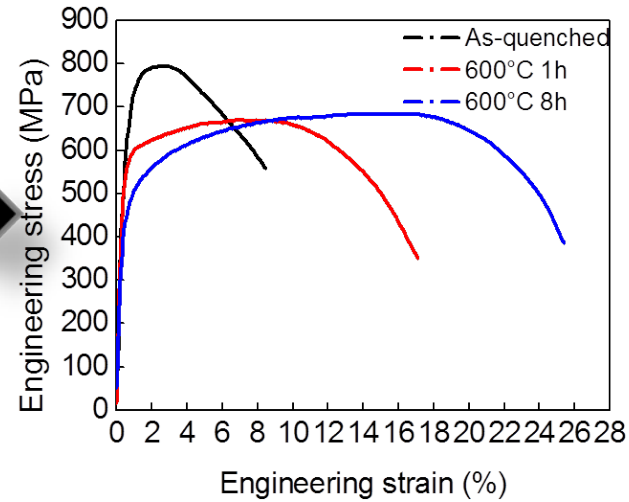
Tasan, Hoefnagels, et al., Int. J. of Plasticity, 2014

Yan, Tasan, Raabe, Acta Materialia, 2015

Goal & challenges

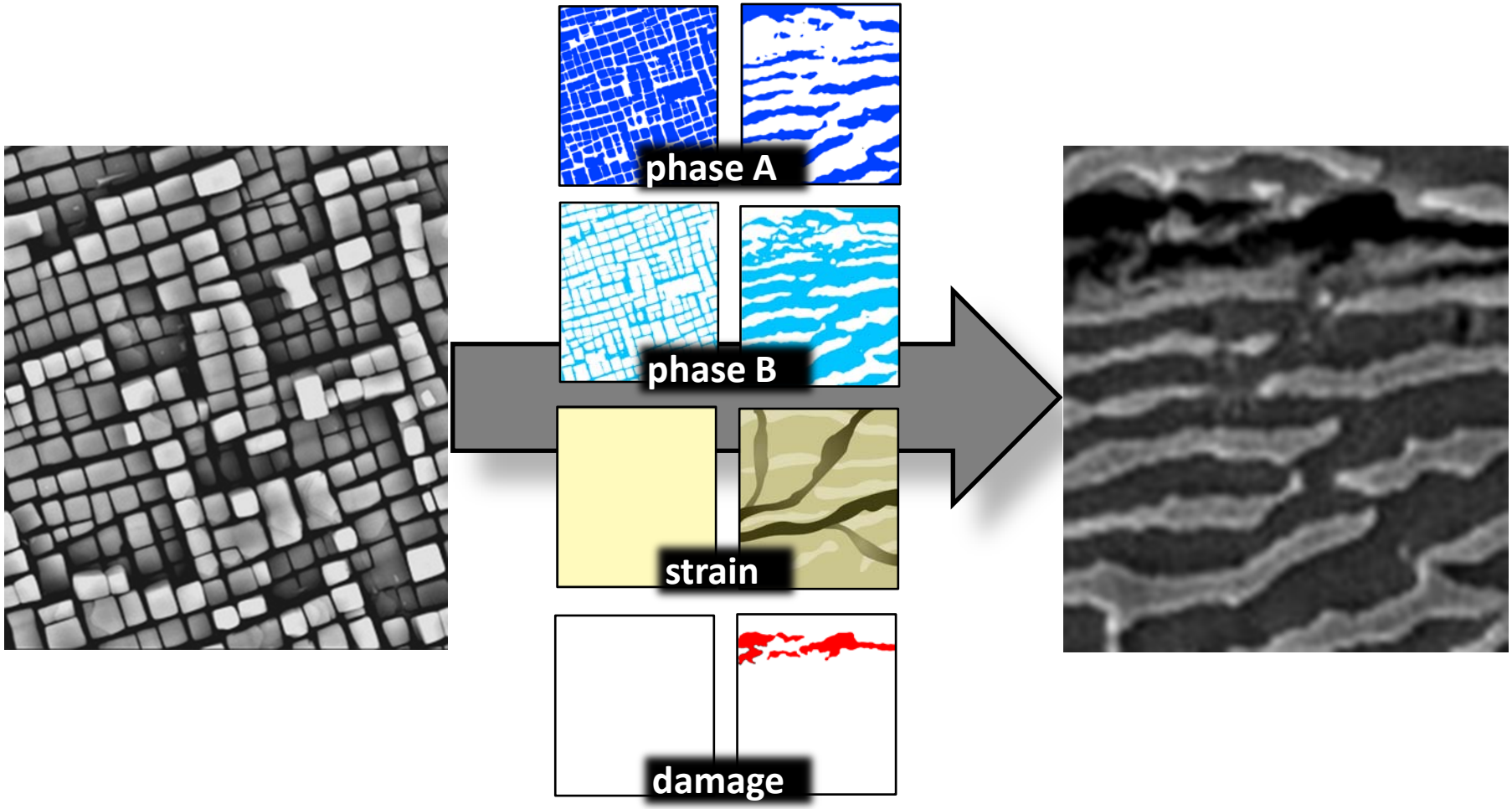
- Goal (i): direct link between microstructure-properties
  (ii):micro-mechanics based alloy design (guidelines)





Needed

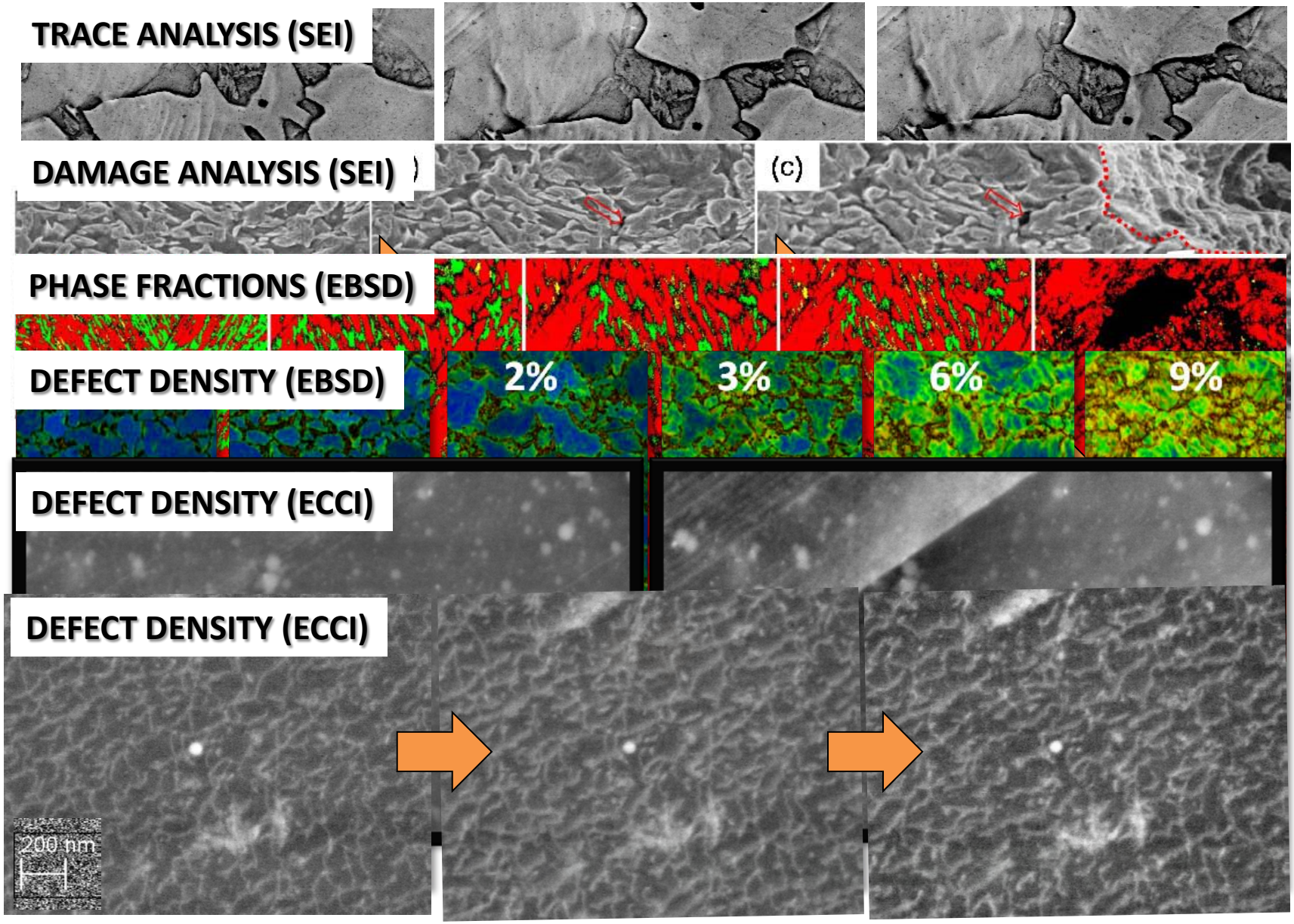
- Needed: evolution of (i) micro-structure (ii) micro-strain (iii) micro-stress



Overview

Need	Got	OK?	Challenges	Solutions
Microstructure				
Strain				
Stress				

In-situ SEM – Imaging modes



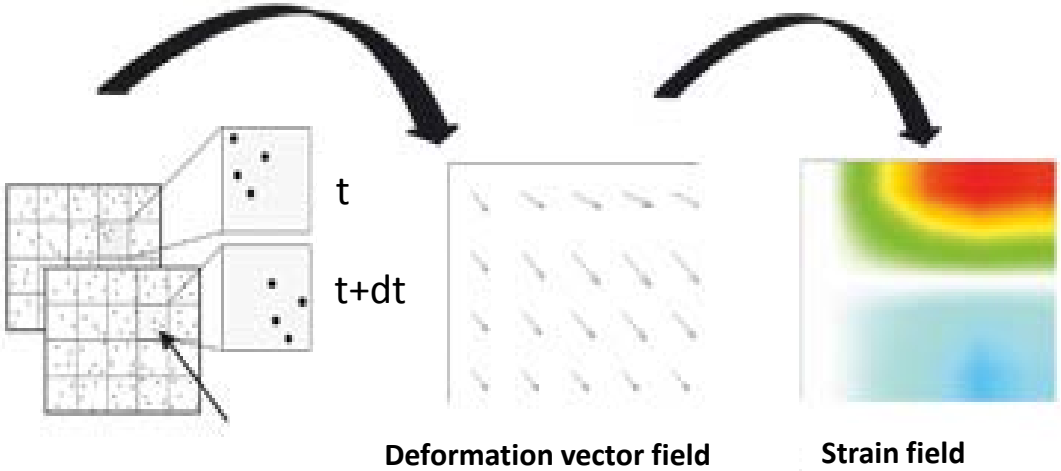
Overview

Need	Got	OK?	Challenges	Solutions
Microstructure	• SEI • ECCI • EBSD		• Surface • Strain level • Pattern-free	
Strain				
Stress				

Overview

Need	Got	OK?	Challenges	Solutions
Microstructure	• SEI • ECCI • EBSD		• Surface • Strain level • Pattern-free	
Strain				
Stress				

Introduction

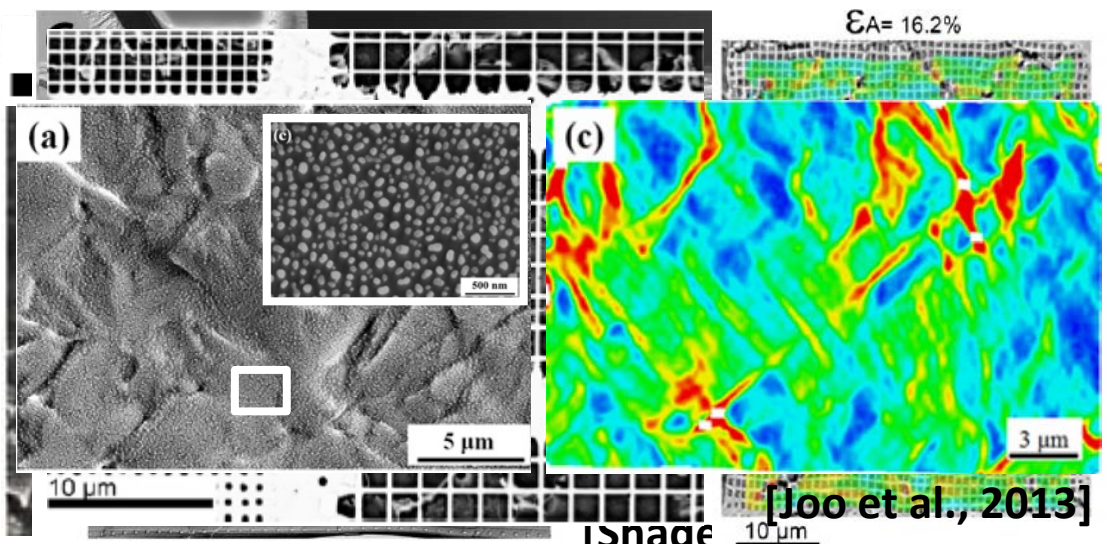


Microstructure

FIB holes

Grid

Annealed Ag



[Joo et al., 2013]

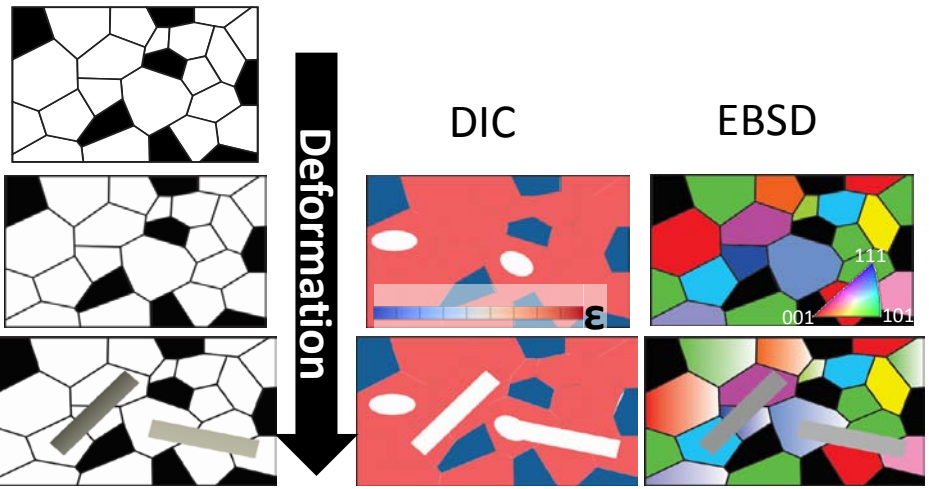
[Shade

[Tam et al., 2010]

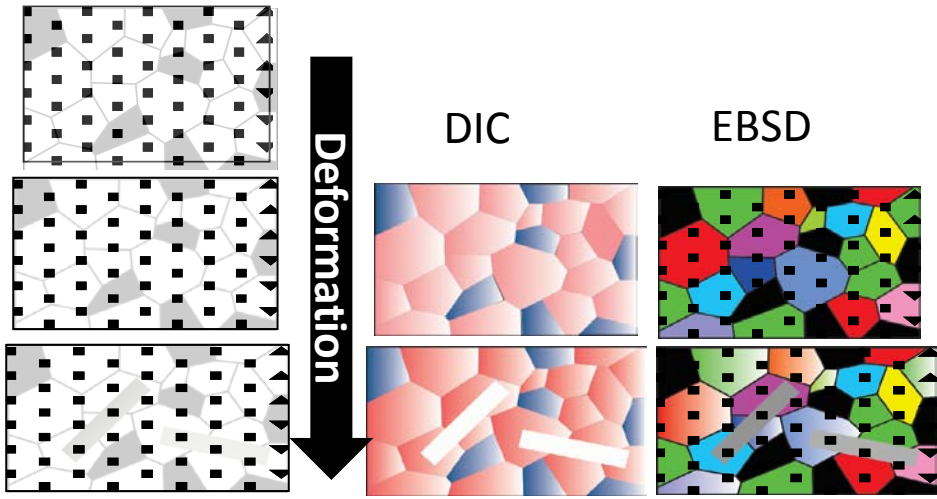
[Marteau et al., 2013]

Challenge

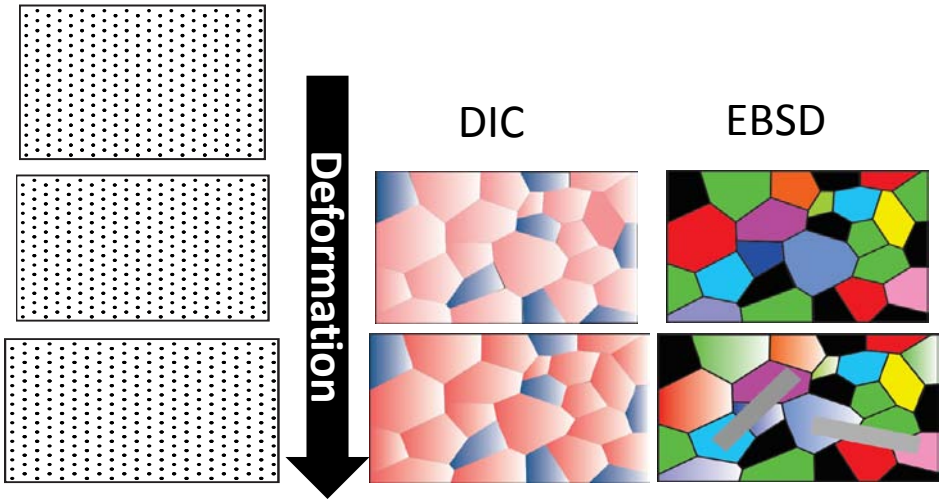
Microstructure-based pattern



Artificial pattern



IDEAL CASE: Selective Imaging



Overview

Need	Got	OK?	Challenges	Solutions
Microstructure	• SEI • ECCI • EBSD		• Surface • Strain level • Pattern-free	
Strain	**• μ-DIC**		**• Selective imaging** **• Strain level** **• Resolution**	
Stress				

Overview

Need	Got	OK?	Challenges	Solutions
Microstructure	• SEI • ECCI • EBSD		• Surface • Strain level • Pattern-free	
Strain	• µ-DIC		• Selective imaging • Strain level • Resolution	
Stress				

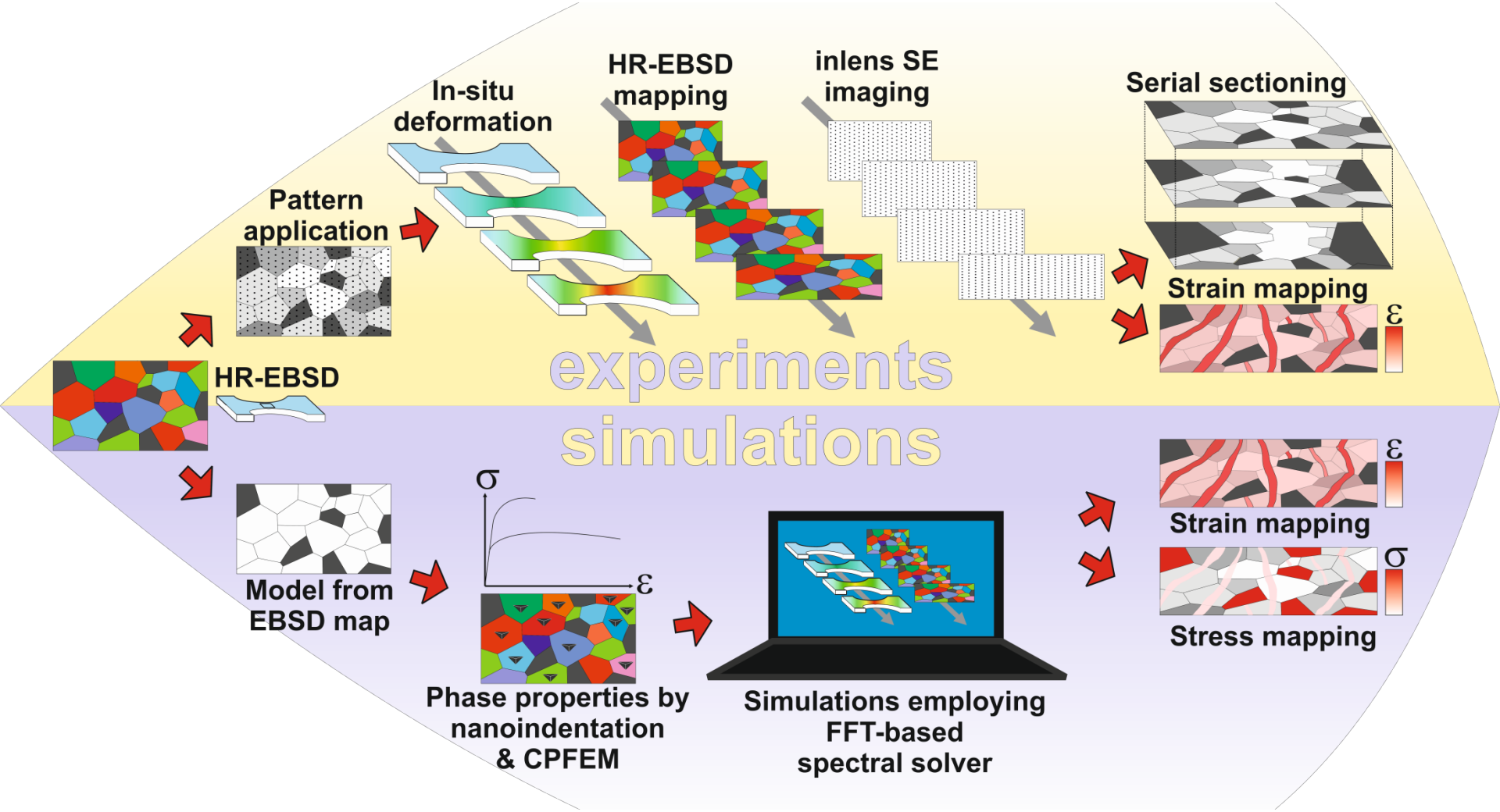
Overview

Need	Got	OK?	Challenges	Solutions
Microstructure	• SEI • ECCI • EBSD		• Surface • Strain level • Pattern-free	
Strain	• μ-DIC		• Selective imaging • Strain level • Resolution	
Stress	**• CP**		**• Microstructure • Phase properties • Efficiency**	

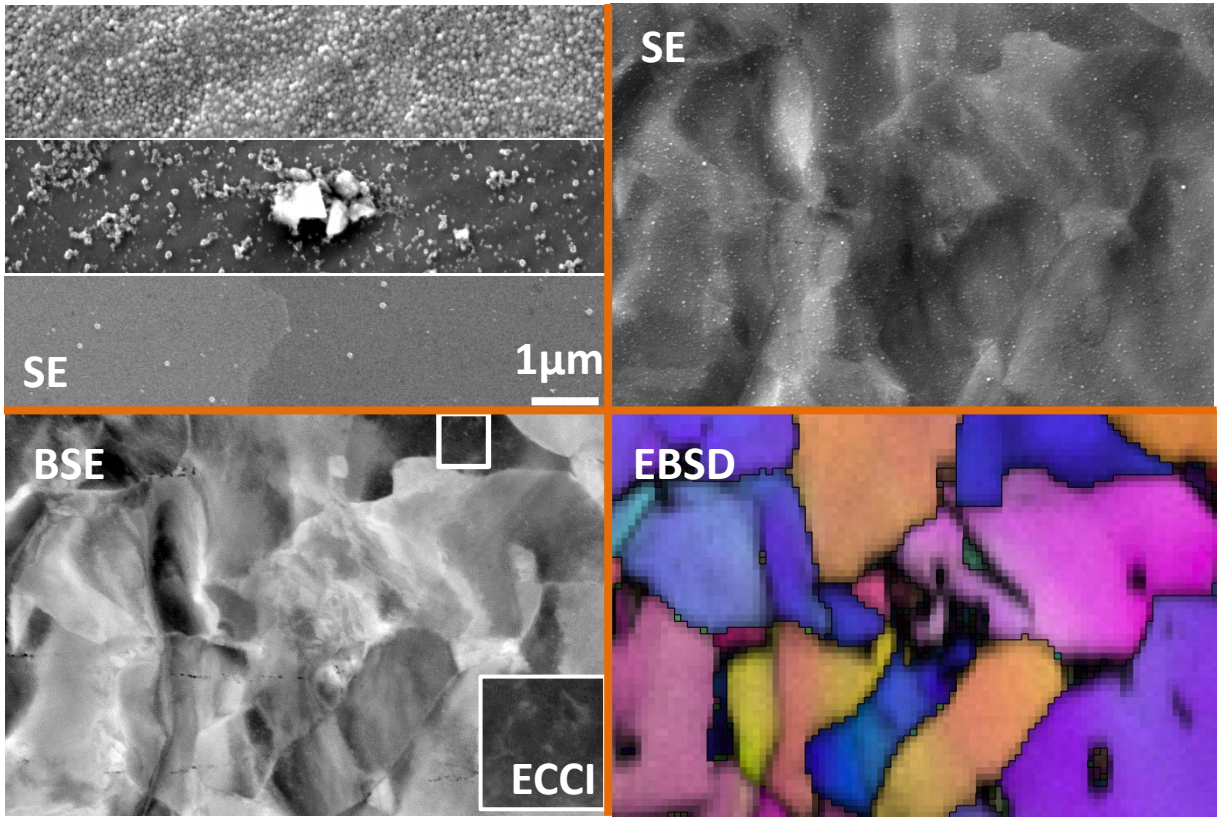
Overview

Need	Got	OK?	Challenges	Solutions
Microstructure	• SEI • ECCI • EBSD		• Surface • Strain level • Pattern-free	
Strain	• µ-DIC		• Selective imaging • Strain level • Resolution	
Stress	• CP		• Microstructure • Phase properties • Efficiency	

Methodology – Example of DP Steel



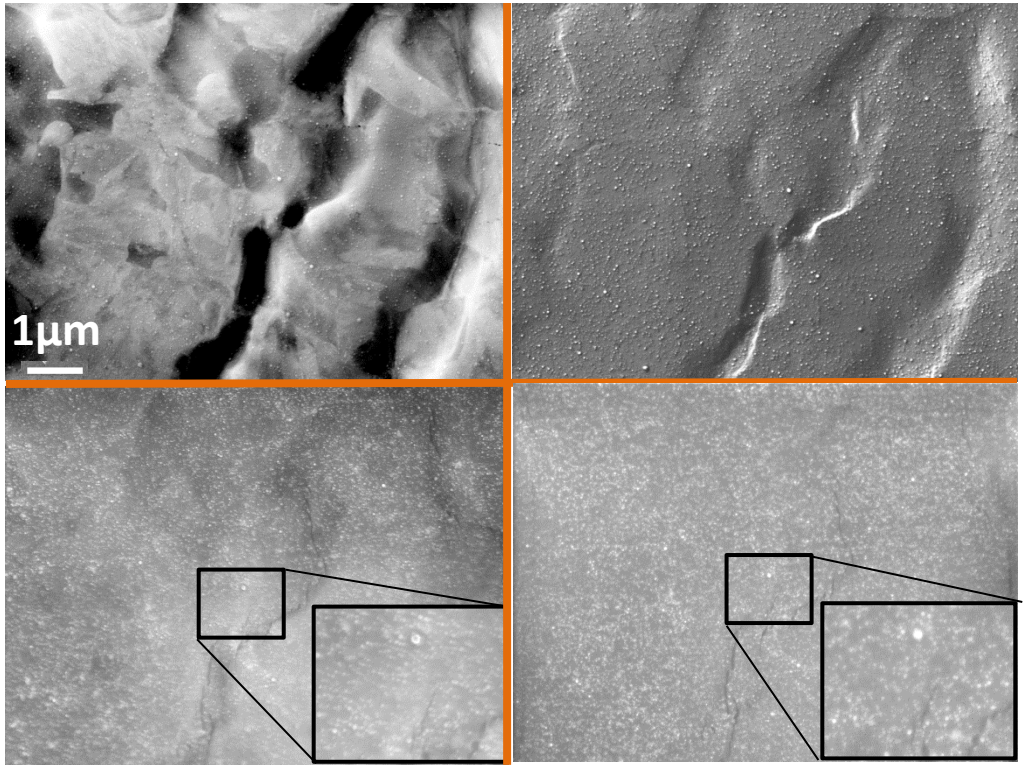
SiO_2 Pattern



Overview

Need	Got	OK?	Challenges	Solutions
Microstructure	• SEI • ECCI • EBSD		• Surface • Strain level • Pattern-free →	• SiO_2
Strain	• µ-DIC		• Selective imaging • Strain level • Resolution	
Stress	• CP?		• Microstructure • Phase properties • Efficiency	

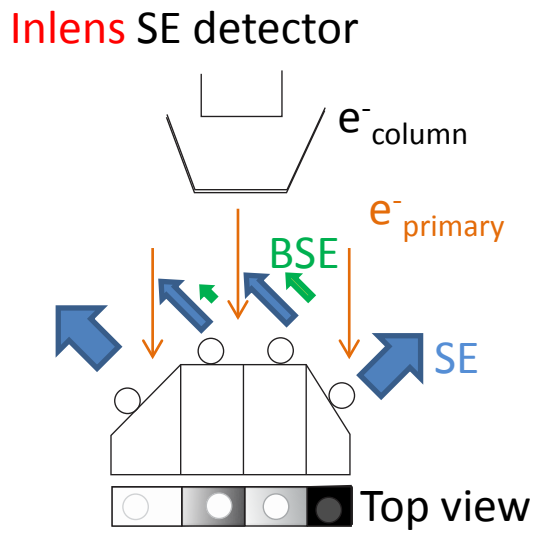
Inlens Imaging (i)



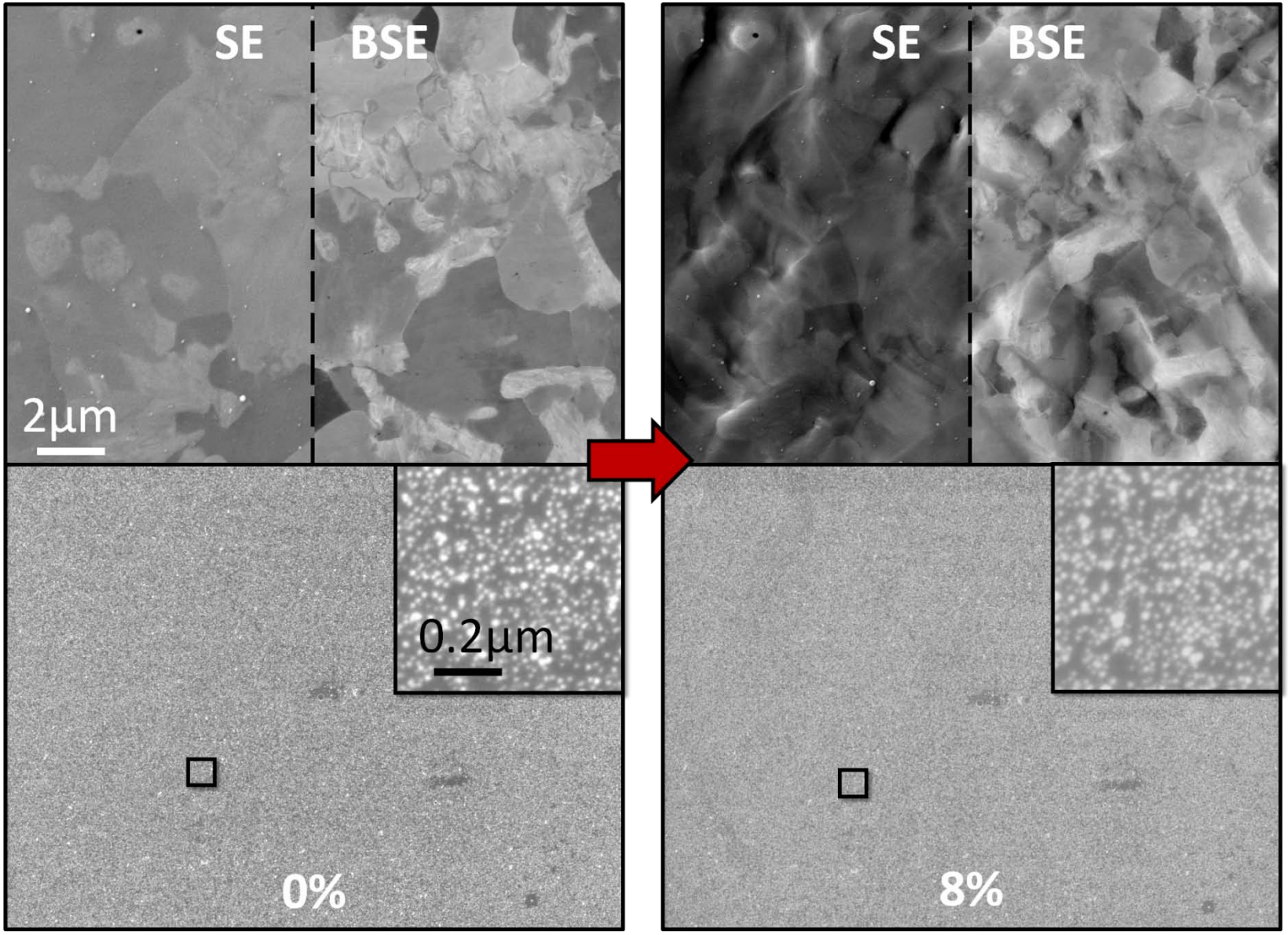
SE detector

Inlens SE detector

Aperture, Voltage, Current



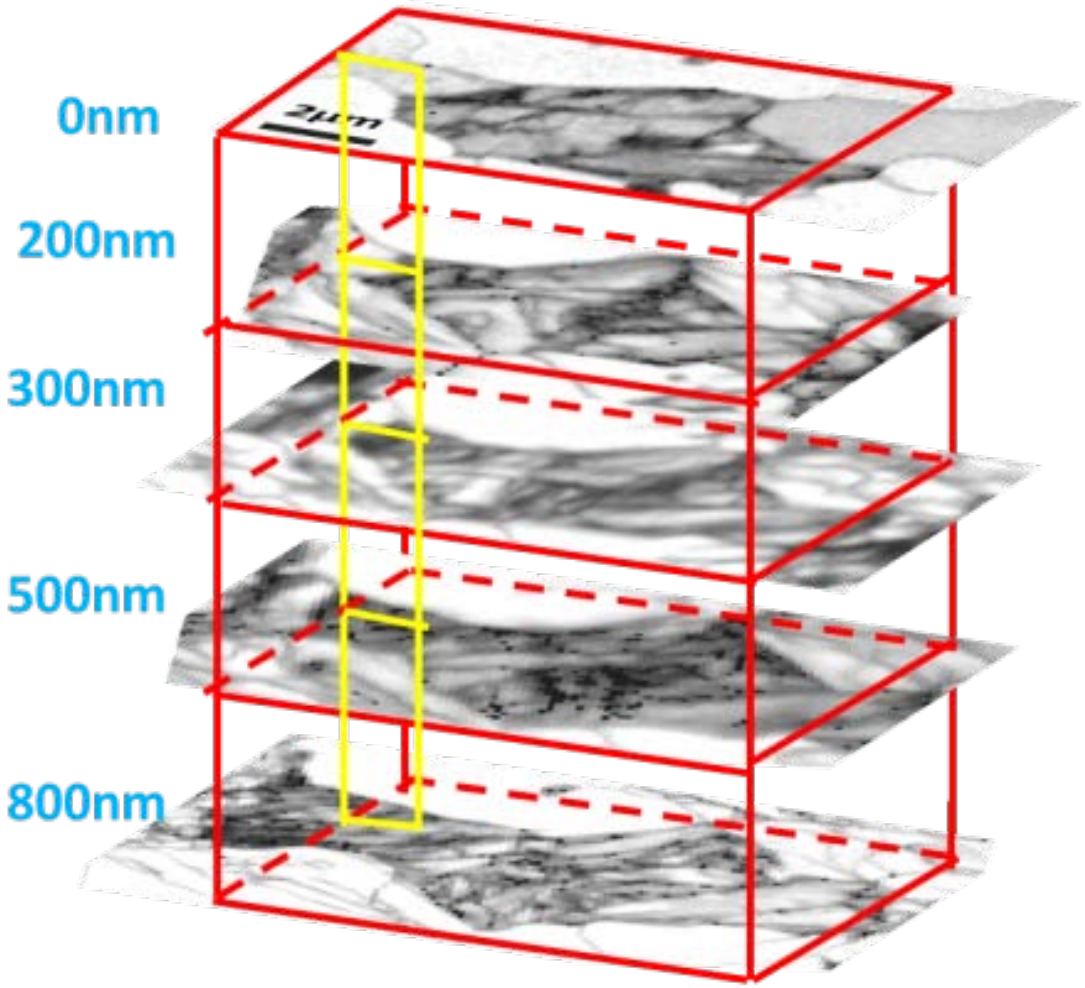
Inlens Imaging (ii)



Overview

Need	Got	OK?	Challenges	Solutions
Microstructure	• SEI • ECCI • EBSD		• Surface • Strain level • Pattern-free	• SiO_2
Strain	• µ-DIC		• Selective imaging • Strain level • Resolution	→ Inless detector → SiO_2 → SiO_2
Stress	• CP?		• Microstructure • Phase properties • Efficiency	

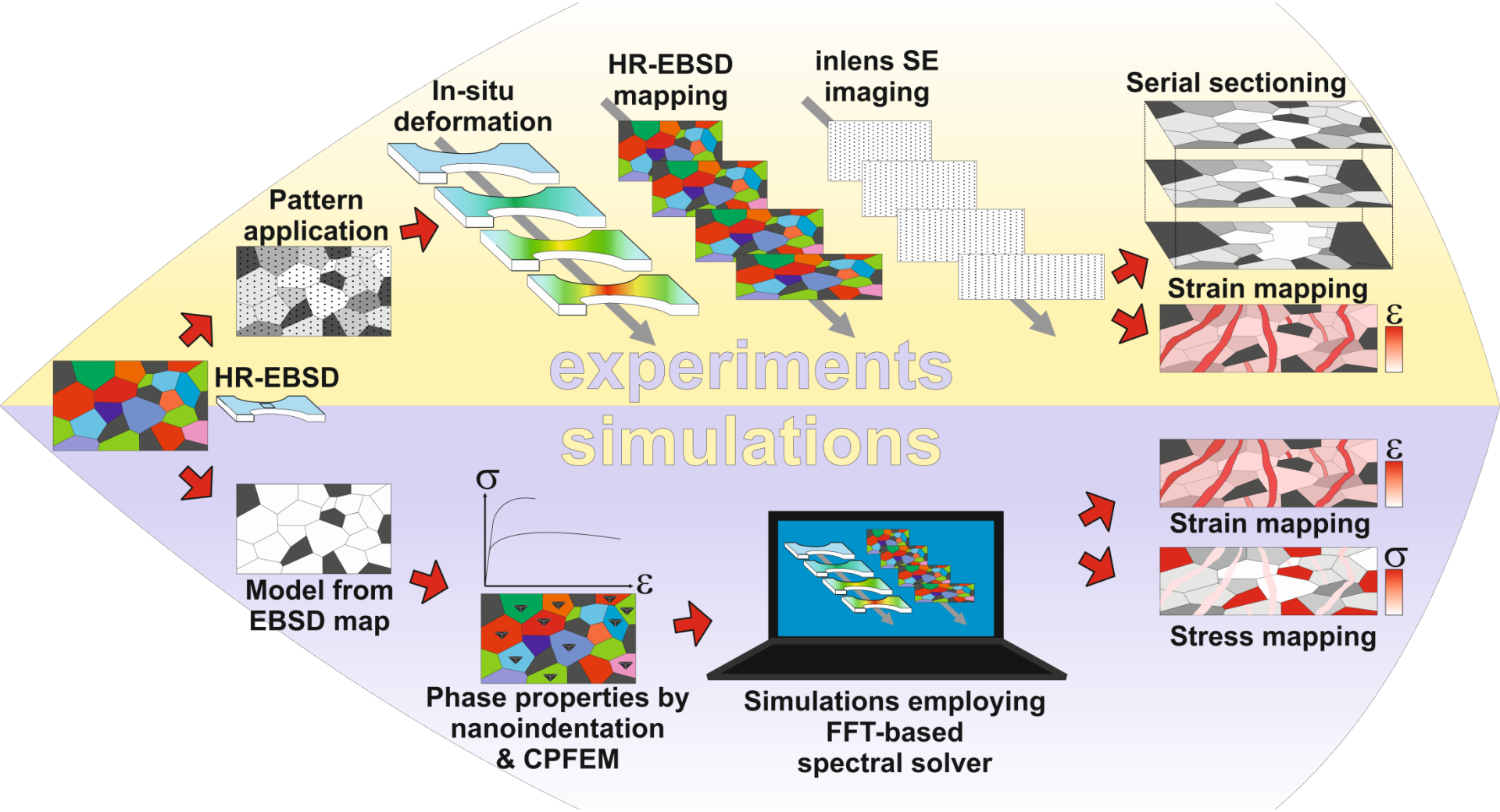
Serial sectioning



Overview

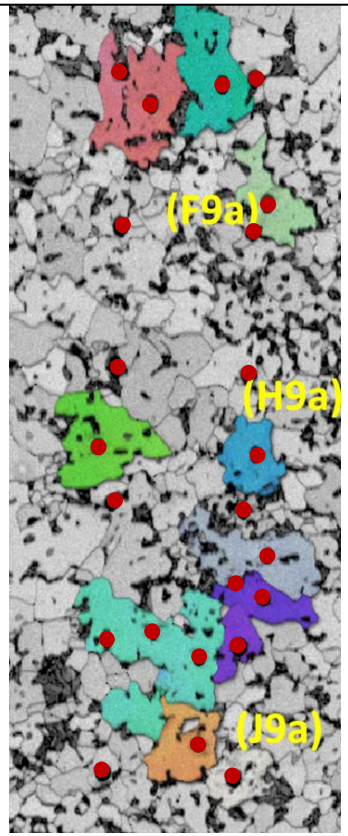
Need	Got	OK?	Challenges	Solutions
Microstructure	• SEI • ECCI • EBSD		• Surface • Strain level • Pattern-free	→ 3D sectioning • No solution • SiO_2
Strain	• µ-DIC		• Selective imaging • Strain level • Resolution	• Inless detector • SiO_2 • SiO_2
Stress	• CP?		• Microstructure • Phase properties • Efficiency	

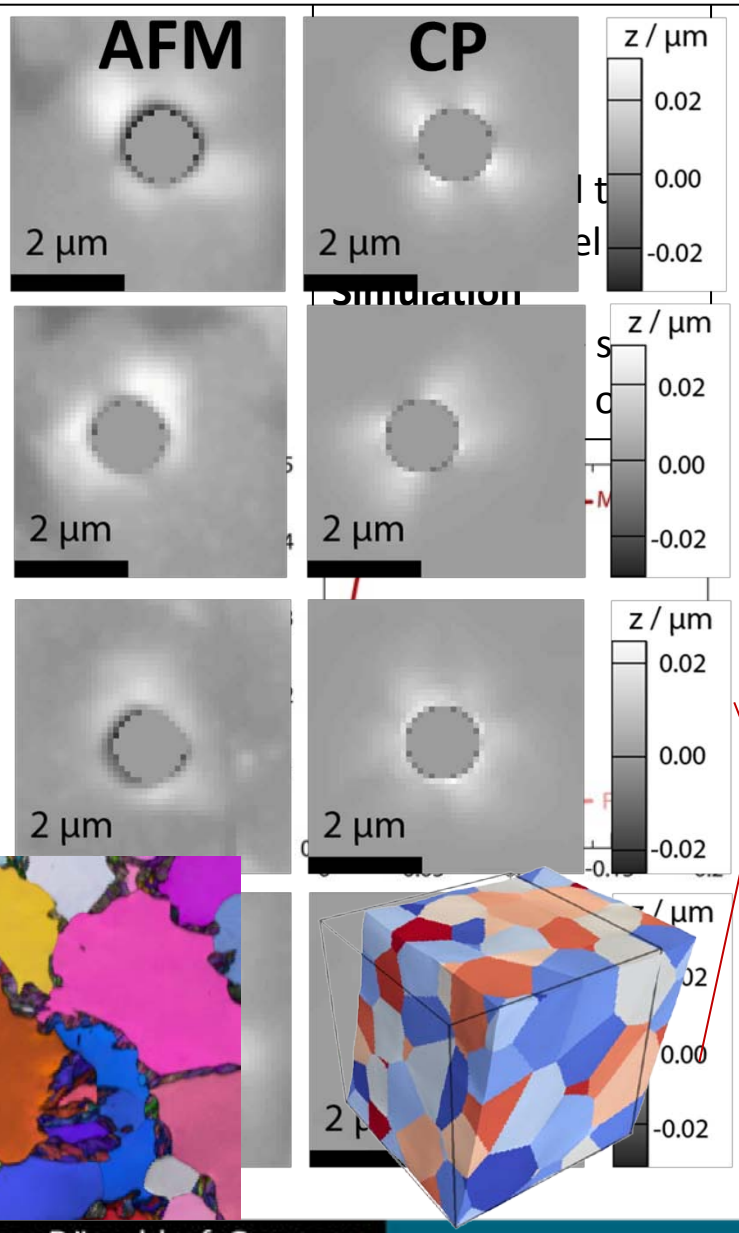
Methodology – Example of DP Steel

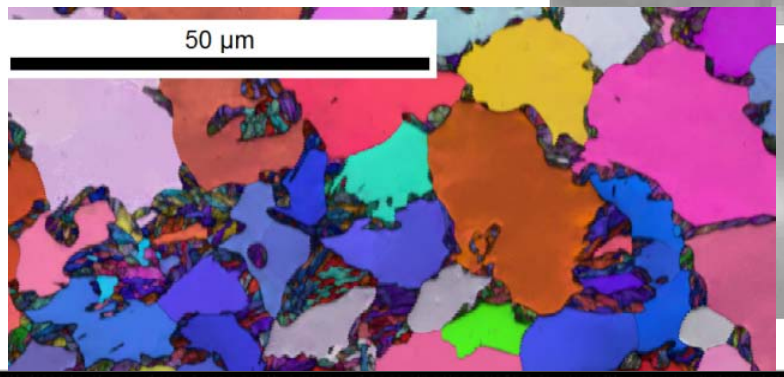


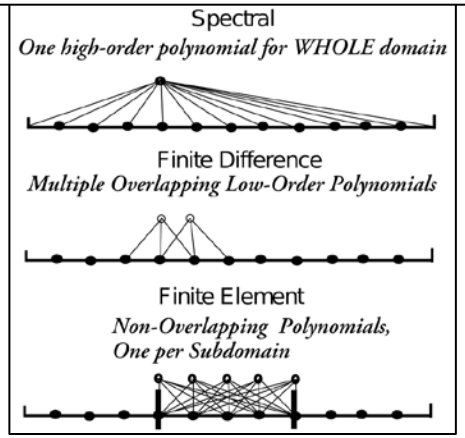
Methodology – Crystal plasticity simulations

-Phenomenological bcc model (Peirce et al., 1982) implemented in DAMASK (Roters et al.,2010)









Computational efficiency ✓

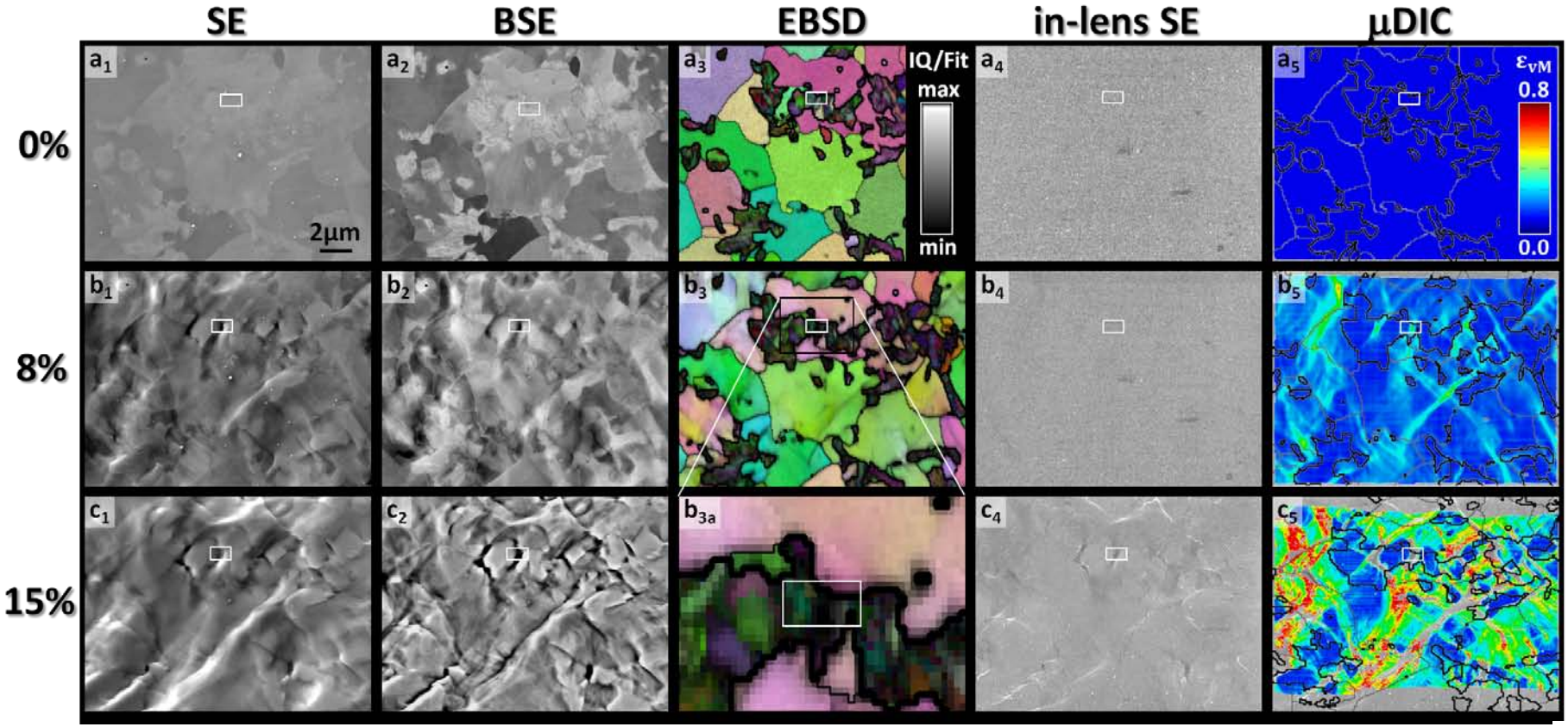
Realistic Microstructures ✓

[Eisenlohr et al.,IJP, 2013]
[Zambaldi et al.,JMR, 2013]

Overview

Need	Got	OK?	Challenges	Solutions
Microstructure	• SEI • ECCI • EBSD		• Surface • Strain level • Pattern-free	• 3D sectioning • No solution • SiO_2
Strain	• µ-DIC		• Selective imaging • Strain level • Resolution	• Inless detector • SiO_2 • SiO_2
Stress	• CP?		• Microstructure → • Phase properties → • Efficiency →	• EBSD to model • Indentation & CP • Spectral

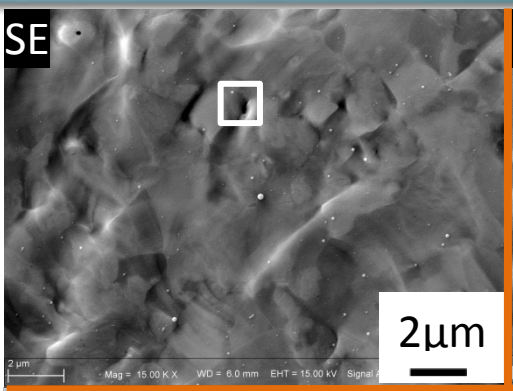
Typical results

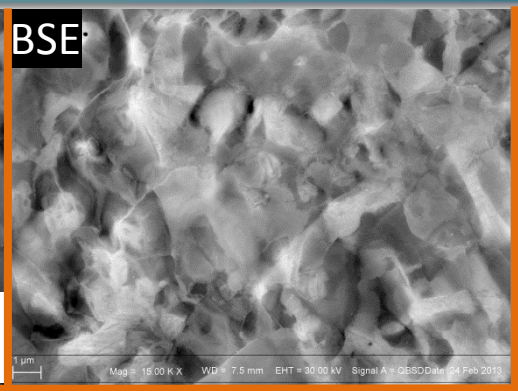


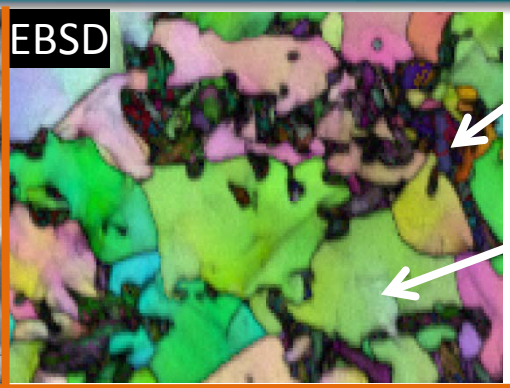
Crystal Plasticity

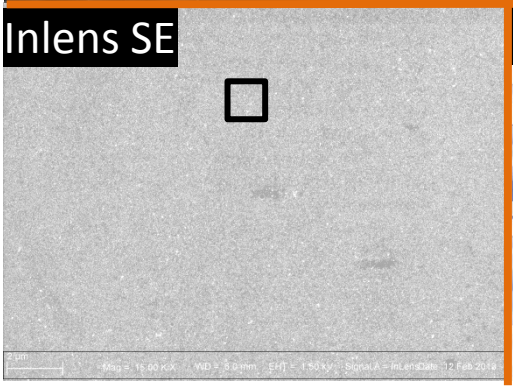
Micro- and nano-scale access to the evolution of:
strain, **stress**, **texture**, **phase morphology**, **phase stability**, **defect density**, **damage**, **surface topography**, etc!

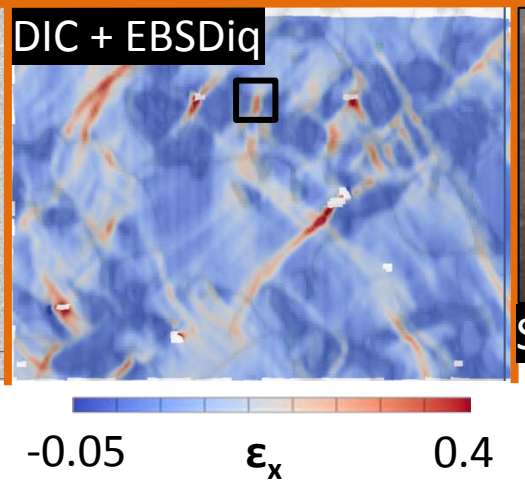
Results – resolution & strain level

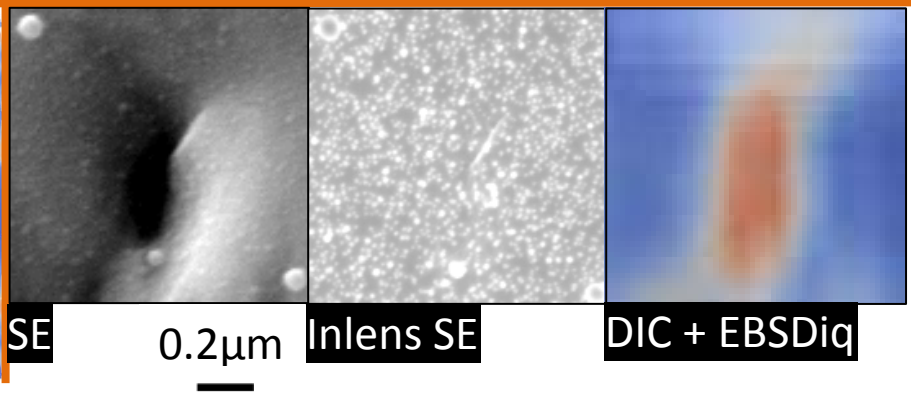








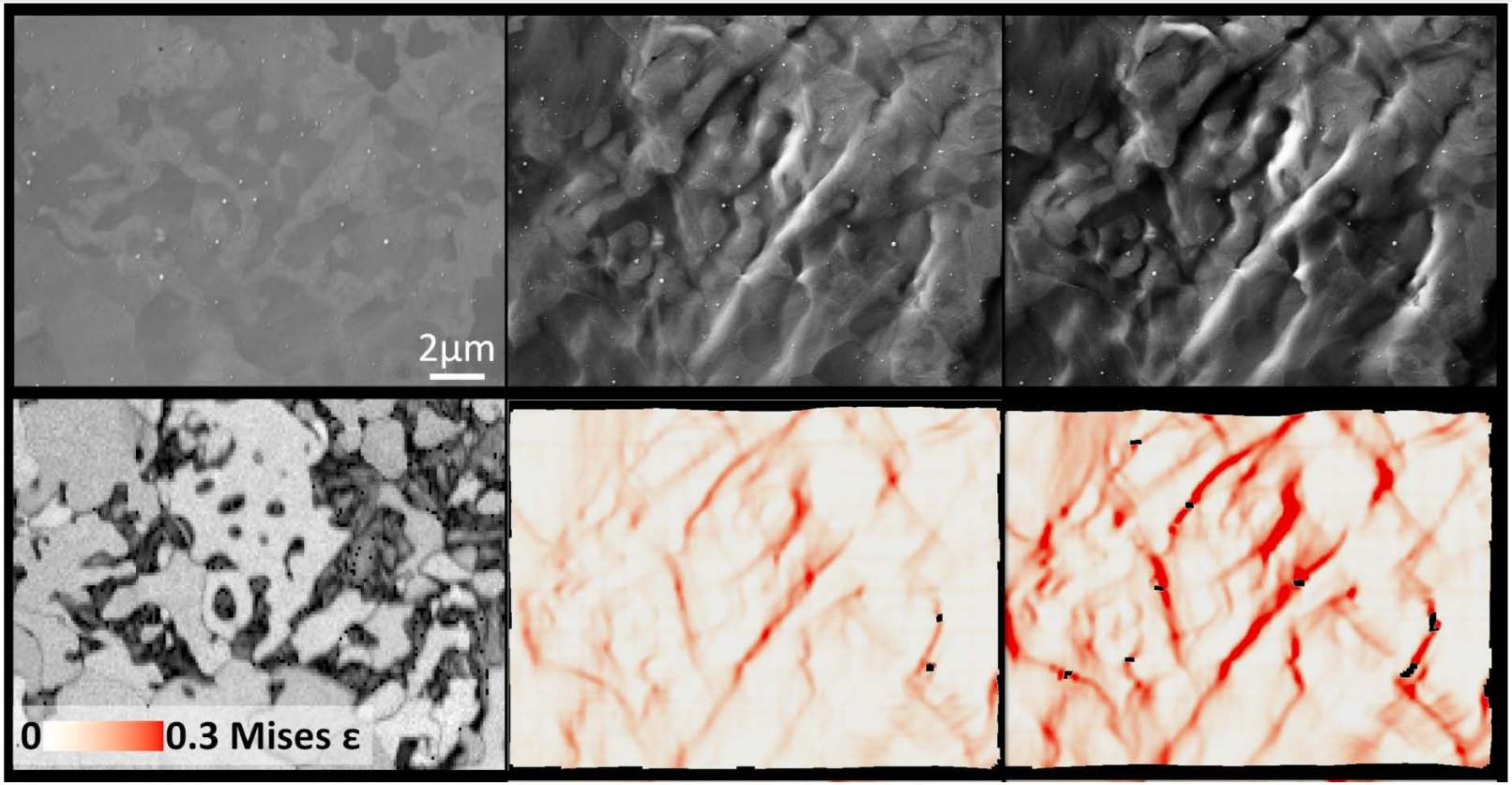




Results – Experiments vs simulation results (i)

SE→

DIC→

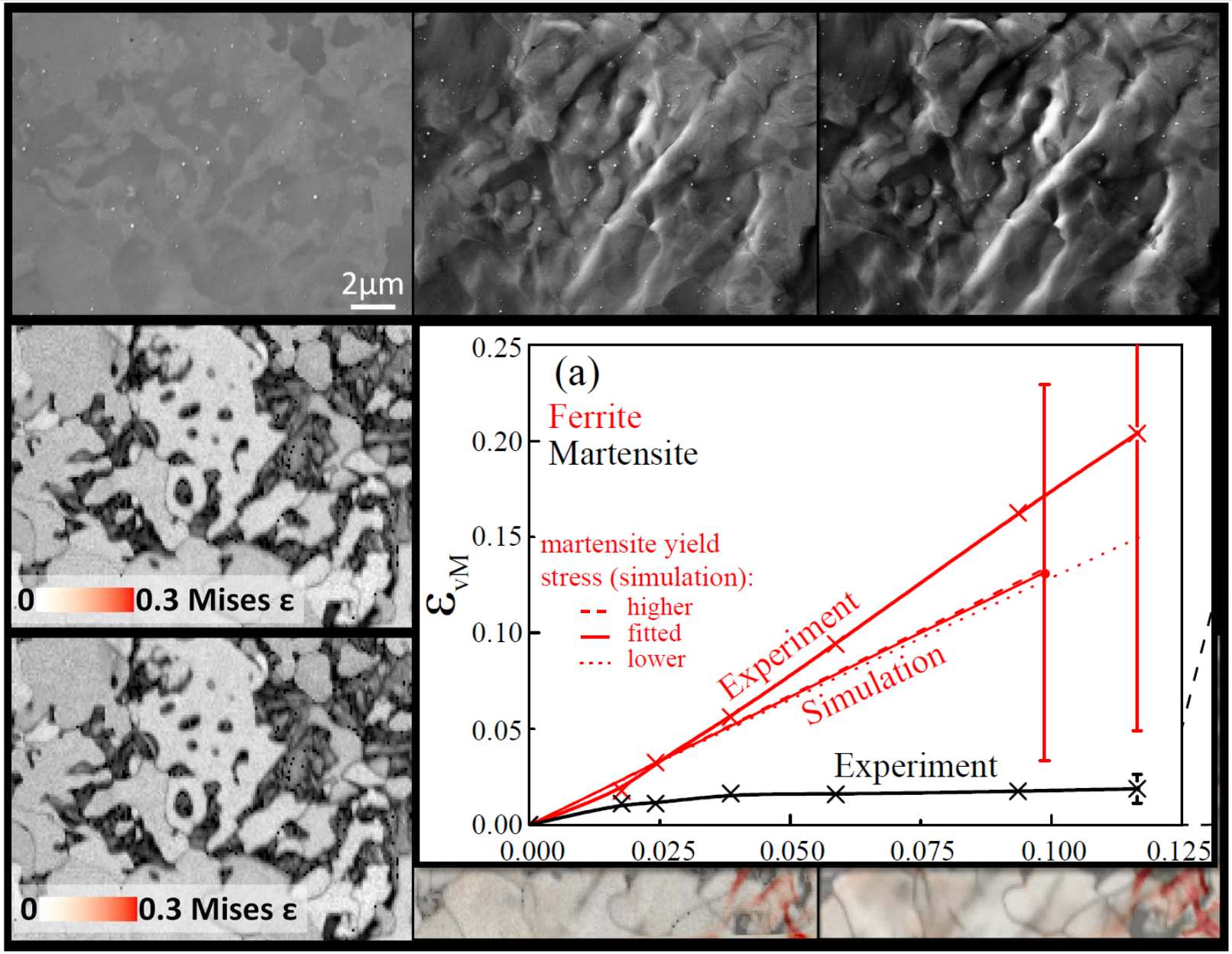


Results – Experiments vs simulation results (ii)

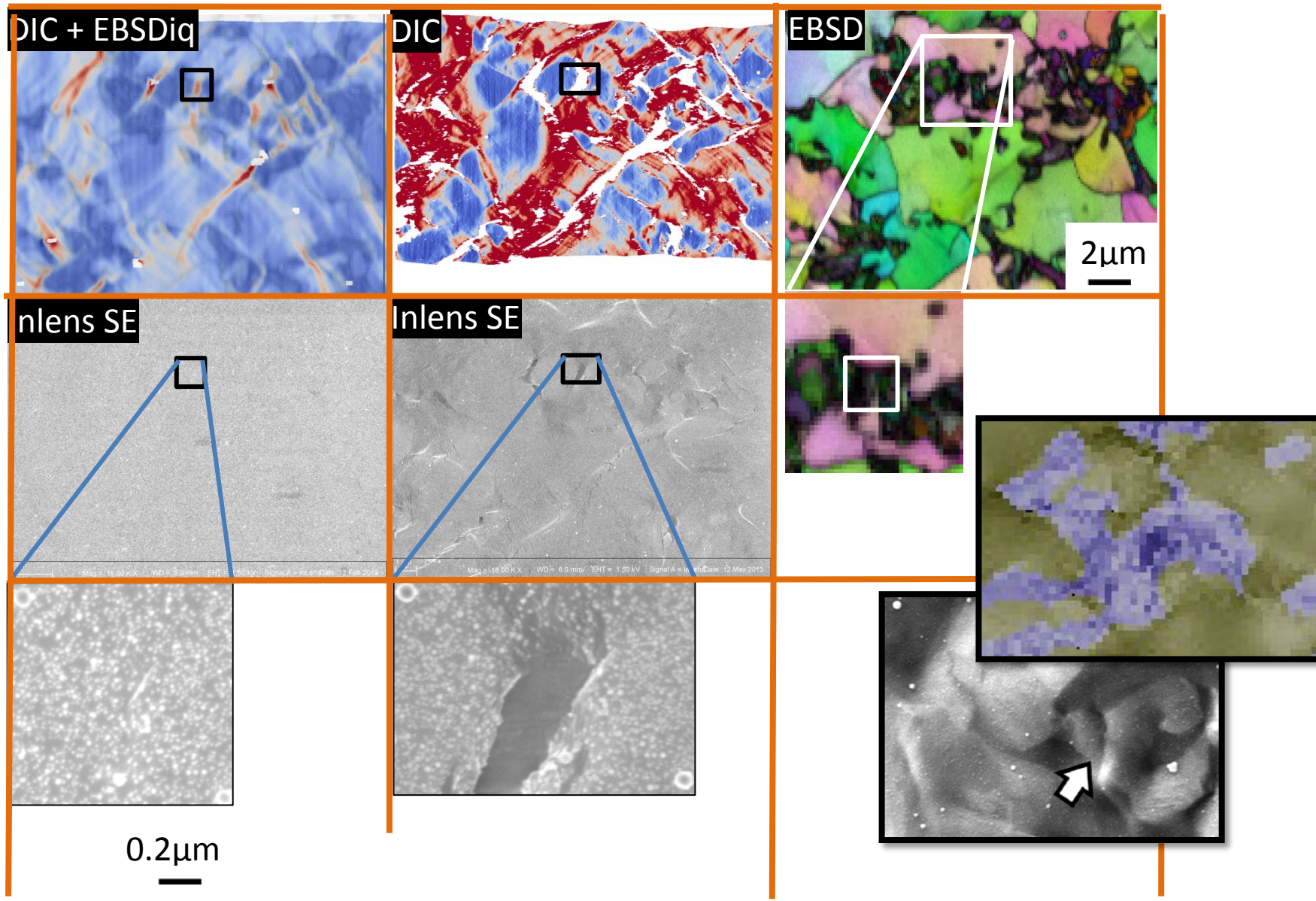
SE→

DIC→

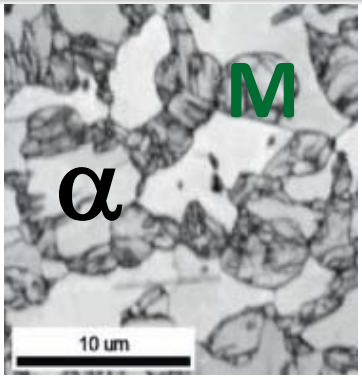
CP→

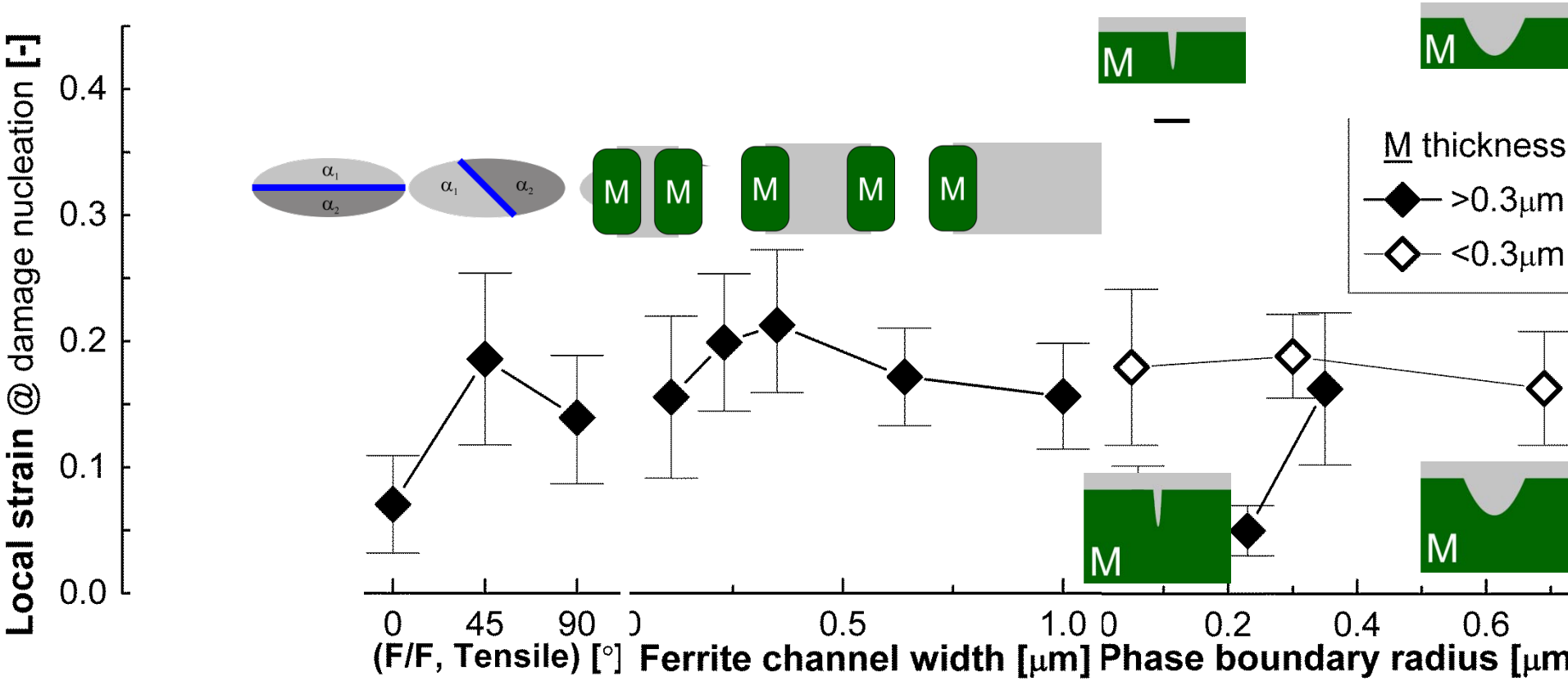


Results – Damage sites



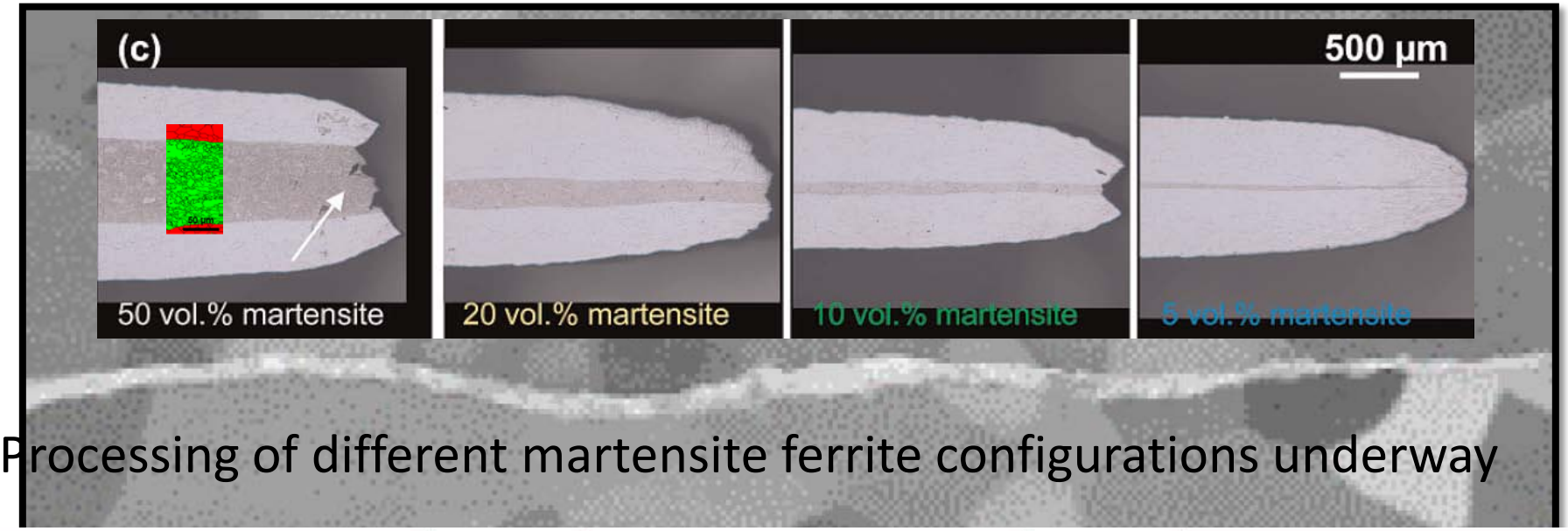
Damage-resistant microstructural constituents



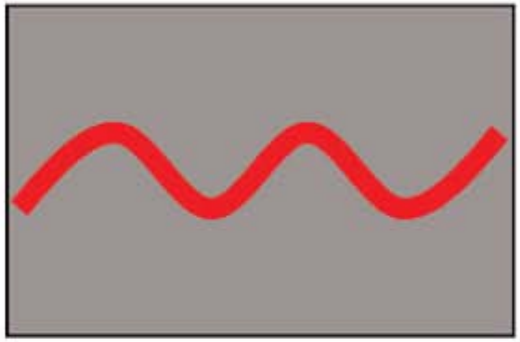


Approach 1: Accummulative roll bonding

- Accummulative roll bonding

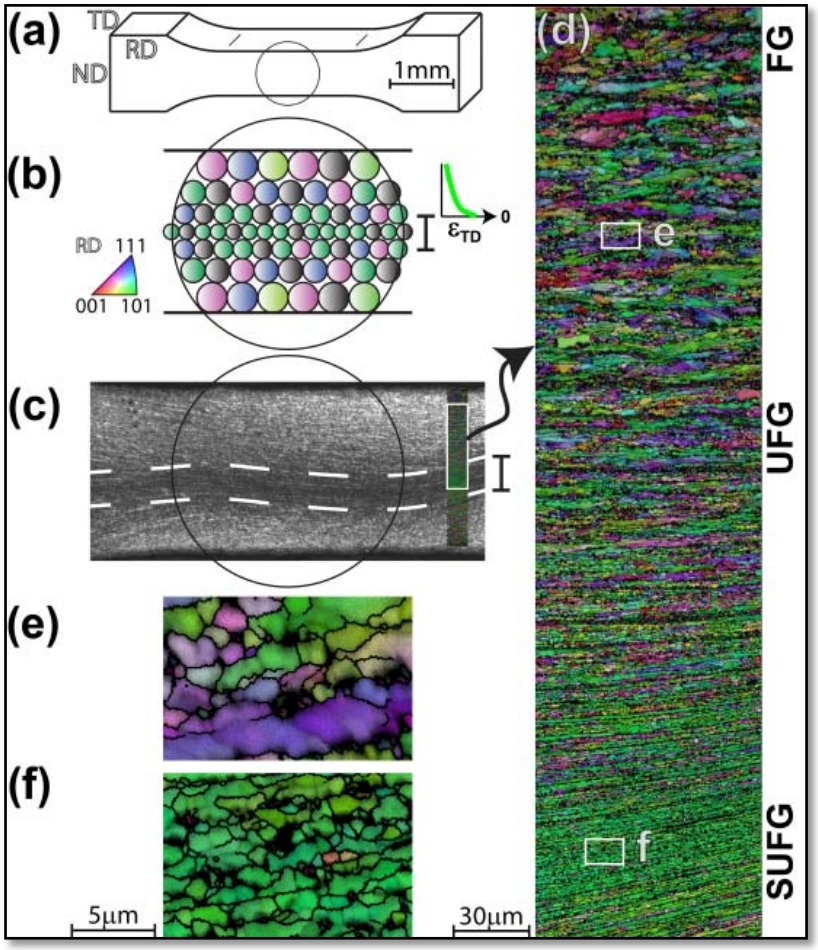


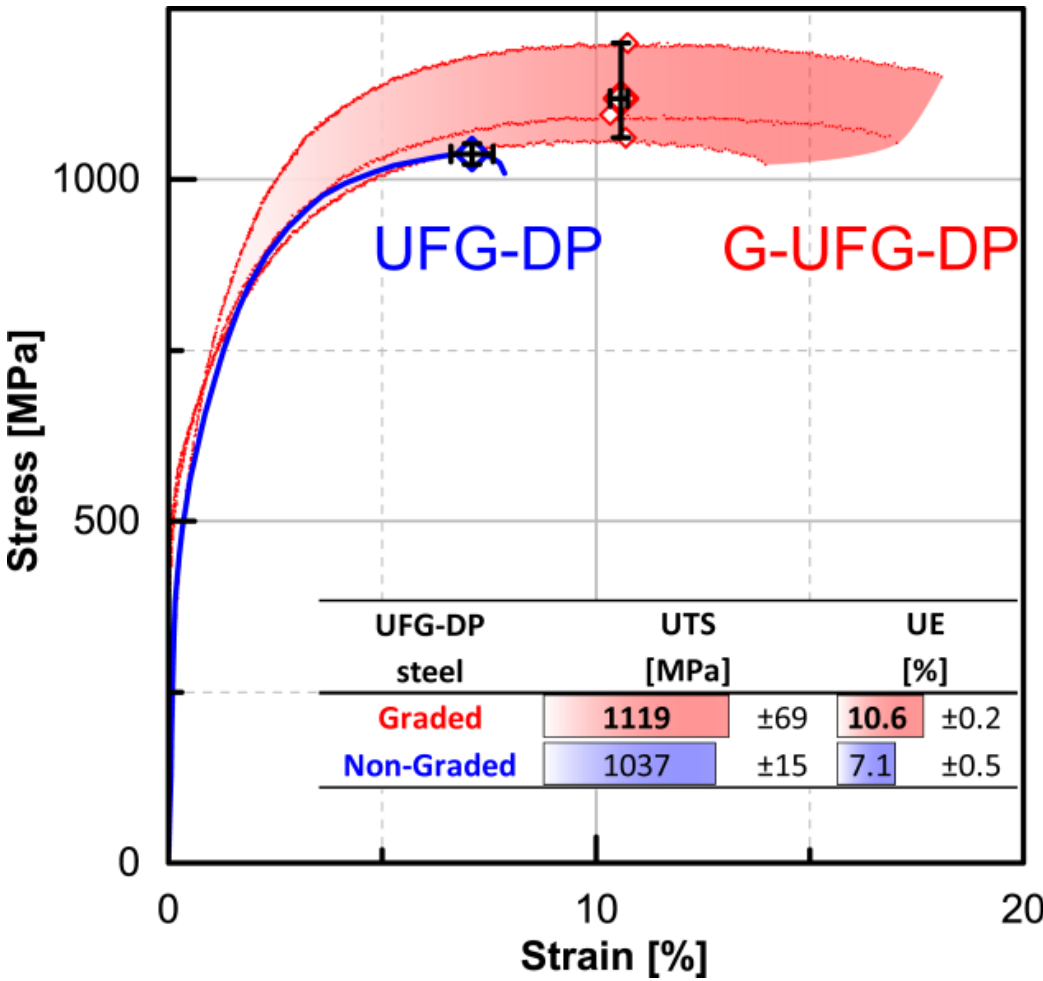
- Processing of different martensite ferrite configurations underway



Springer, Tasan et al., JMR, 2014

Approach 2 – Non-axial forging





UFG-DP steel	UTS [MPa]		UE [%]	
Graded	1119	±69	10.6	±0.2
Non-Graded	1037	±15	7.1	±0.5

Summary & Conclusions

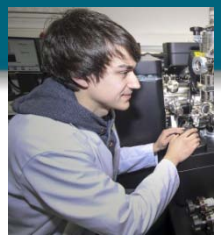
- New method to investigate bulk nanostructured alloys
- Provides microstructural design guidelines for damage-resistance

Need	Got	Challenges	Solutions
Microstructure	• SEI • ECCI • EBSD	• Surface • Strain level • Pattern-free	• 3D sectioning • No solution • SiO_2
Strain	• µ-DIC	• Selective imaging • Strain level • Resolution	• Inless detector • SiO_2 • SiO_2
Stress	• CP?	Microstructure • Phase properties • Efficiency	• EBSD to model • Indentation & CP • Spectral

[Tasan et al.,ActaMat, 2014]
[Tasan et al.,IJP, 2014]
[Eisenlohr et al.,IJP, 2013]
[Zambaldi et al.,JMR, 2013]

Understanding Martensitic Steels and Design of TRIP-Maraging Steels

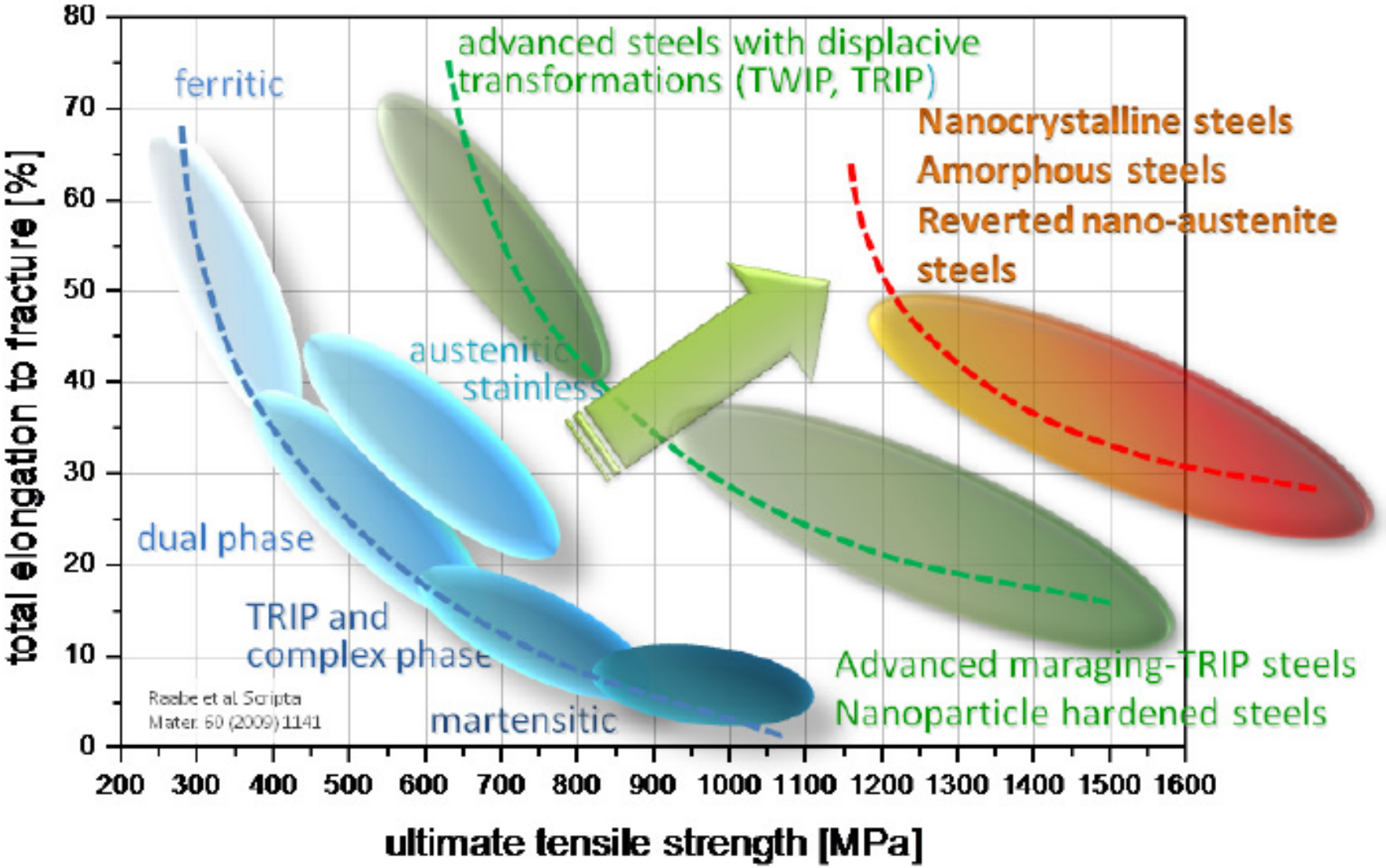
C.C. Tasan, M. Wang, L. Morsdorf, D.Ponge, D. Raabe



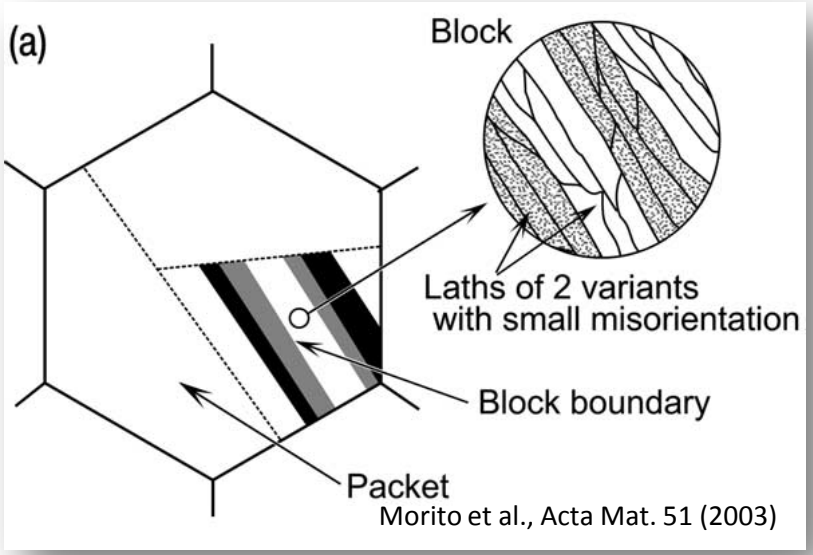
Max-Planck-Institut für Eisenforschung GmbH

Wang, Tasan, et al.,	Acta Materialia,	2014
Wang, Tasan, et al.	Acta Materialia,	2015
Morsdorf, Tasan, et al.	Acta Materialia,	2015

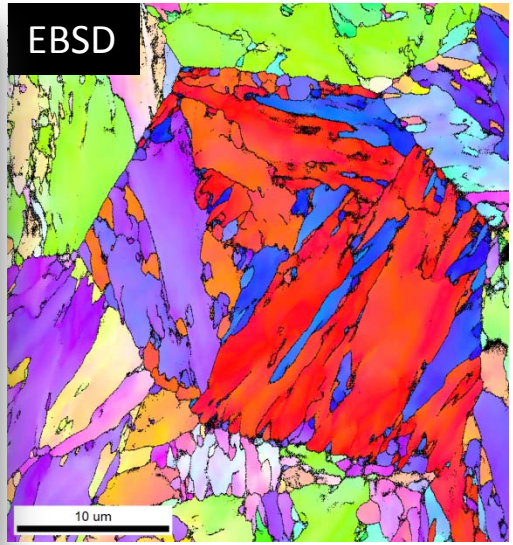
Why martensite?

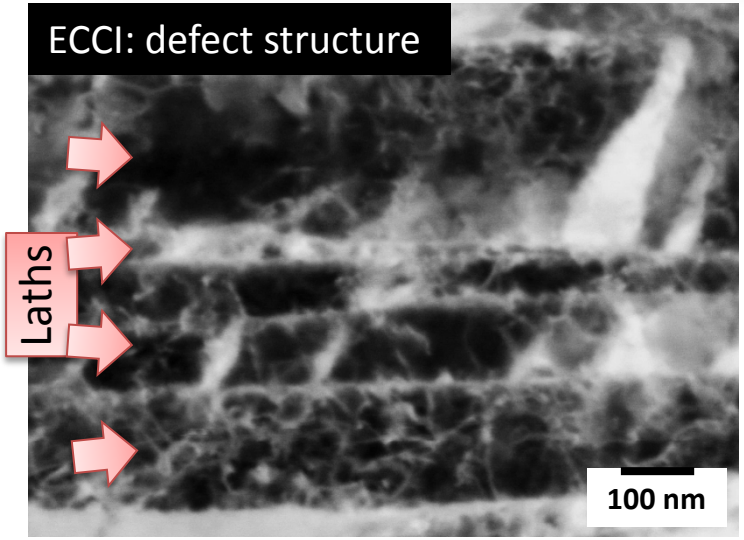


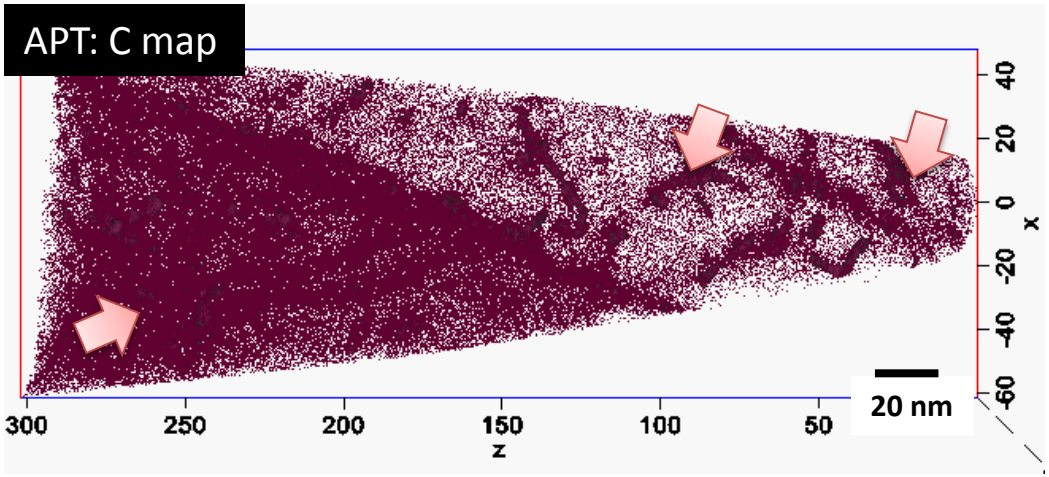
Why challenging?



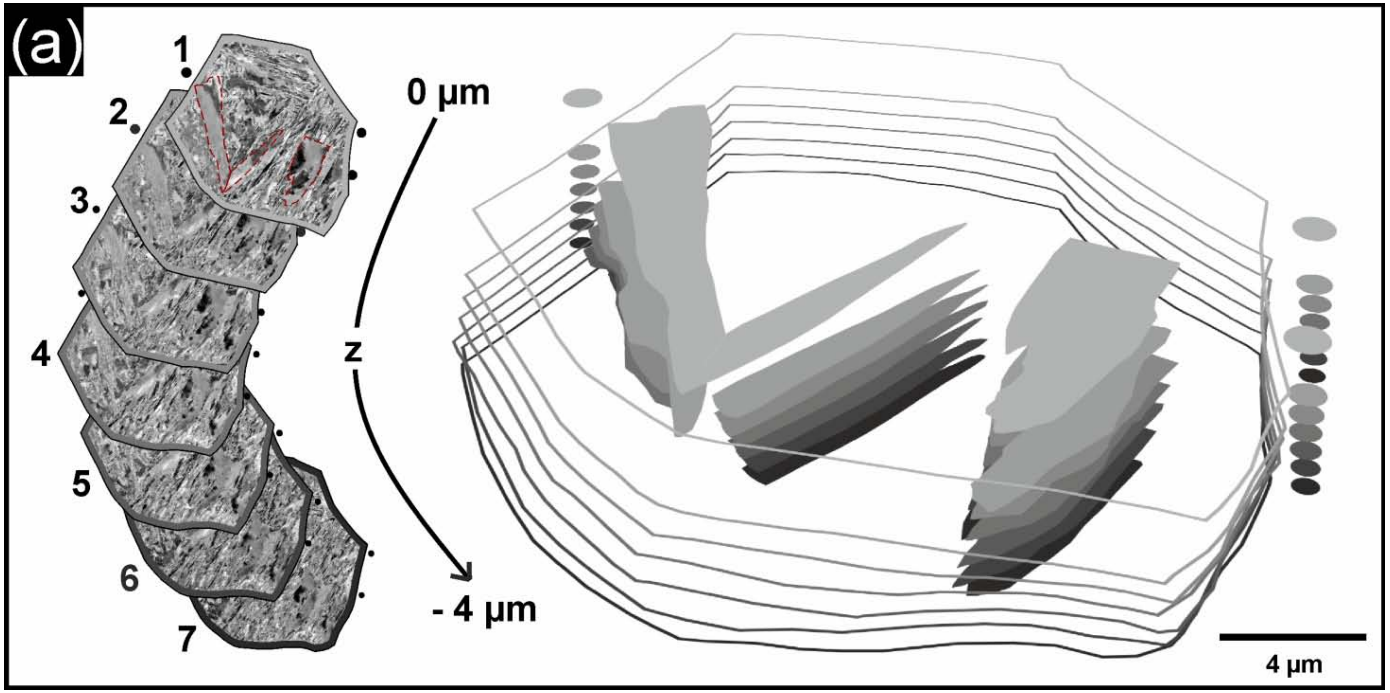
Morito et al., Acta Mat. 51 (2003)

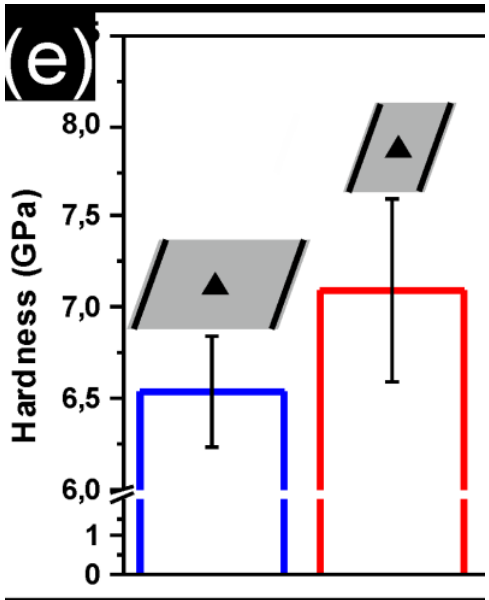






Why challenging? (ii)

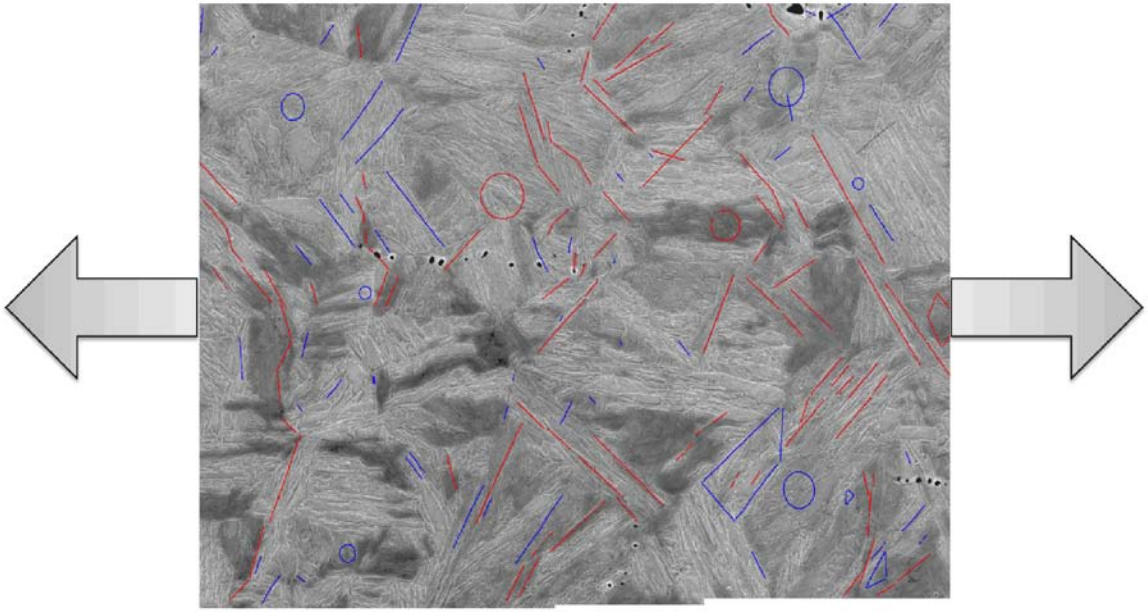


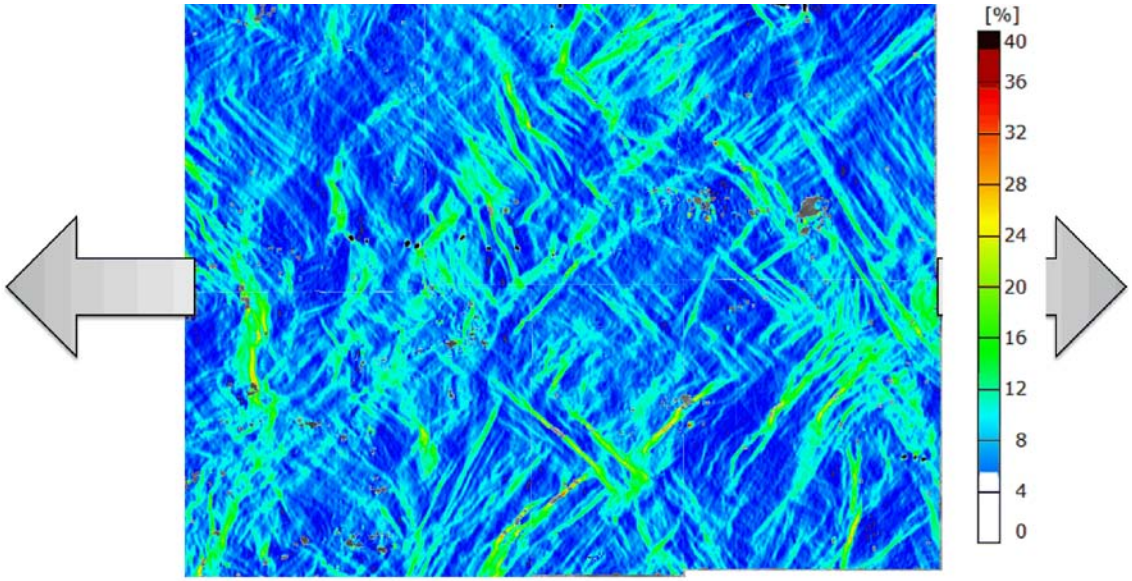


Results

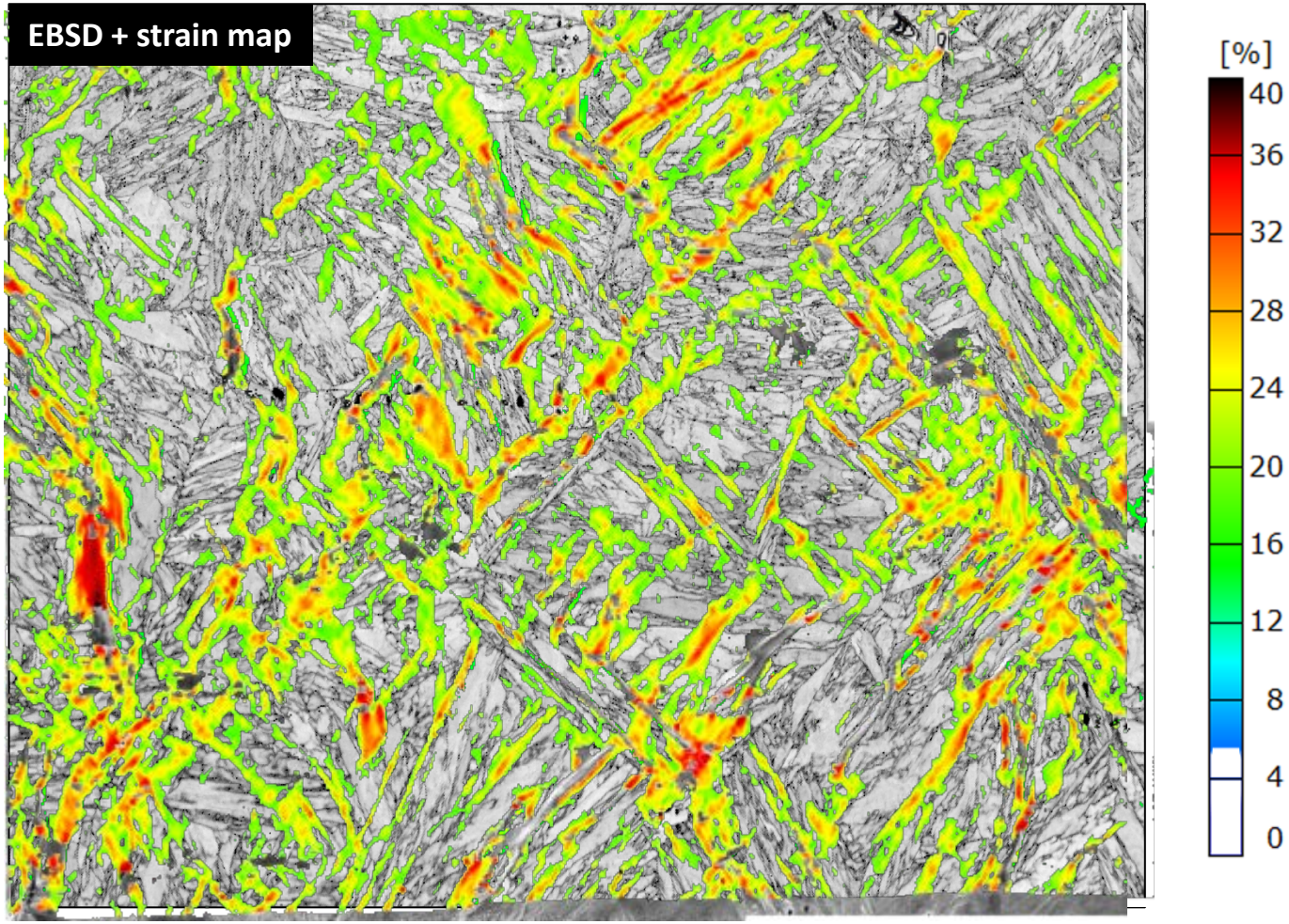
Fe-0.15%C-5%Ni (wt%)
5min @ 900°C + WQ
GS$_\gamma$ ~ 25 µm
35 um

Stress (MPa)
Strain (%)

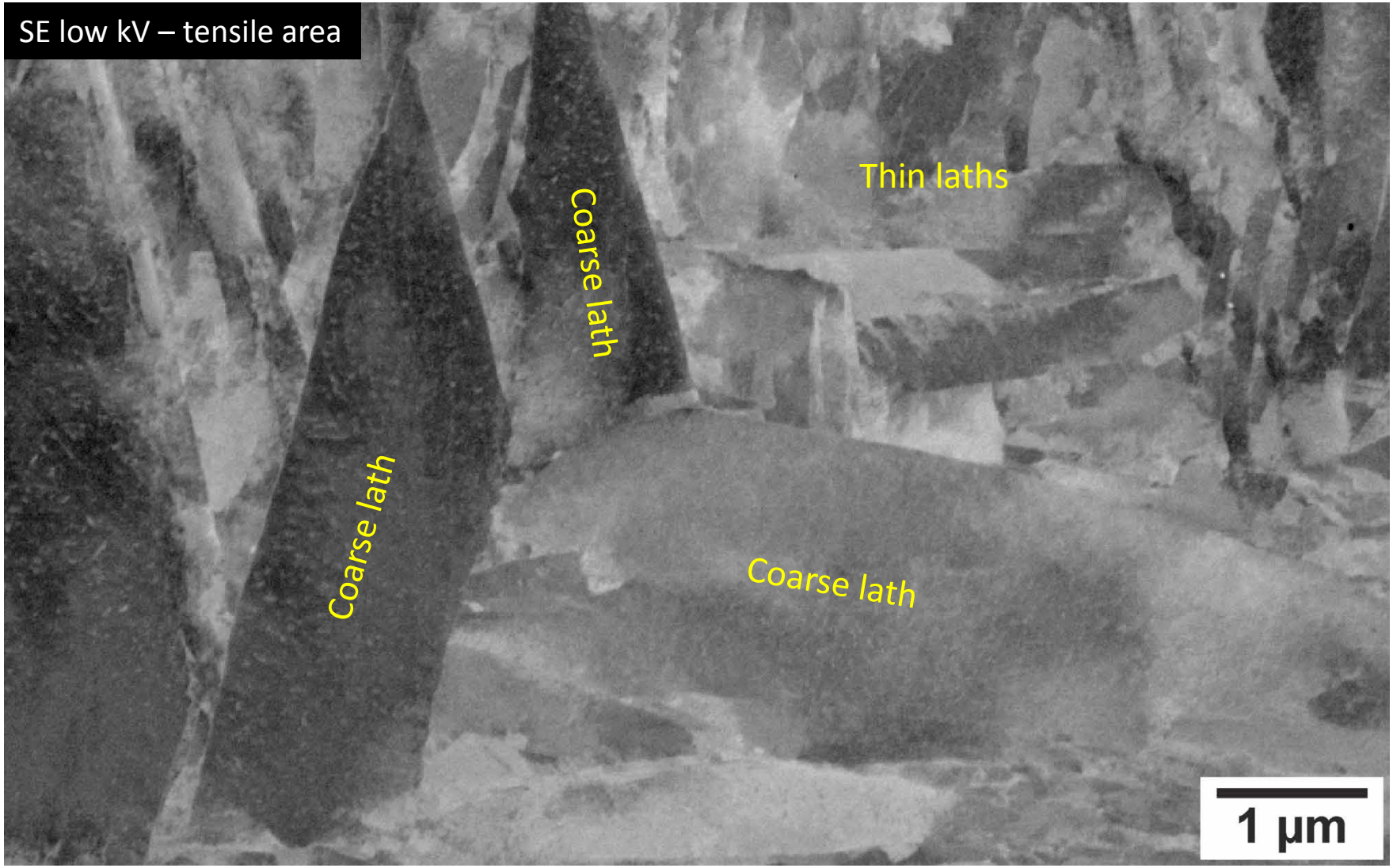



[%]
40
36
32
28
24
20
16
12
8
4
0

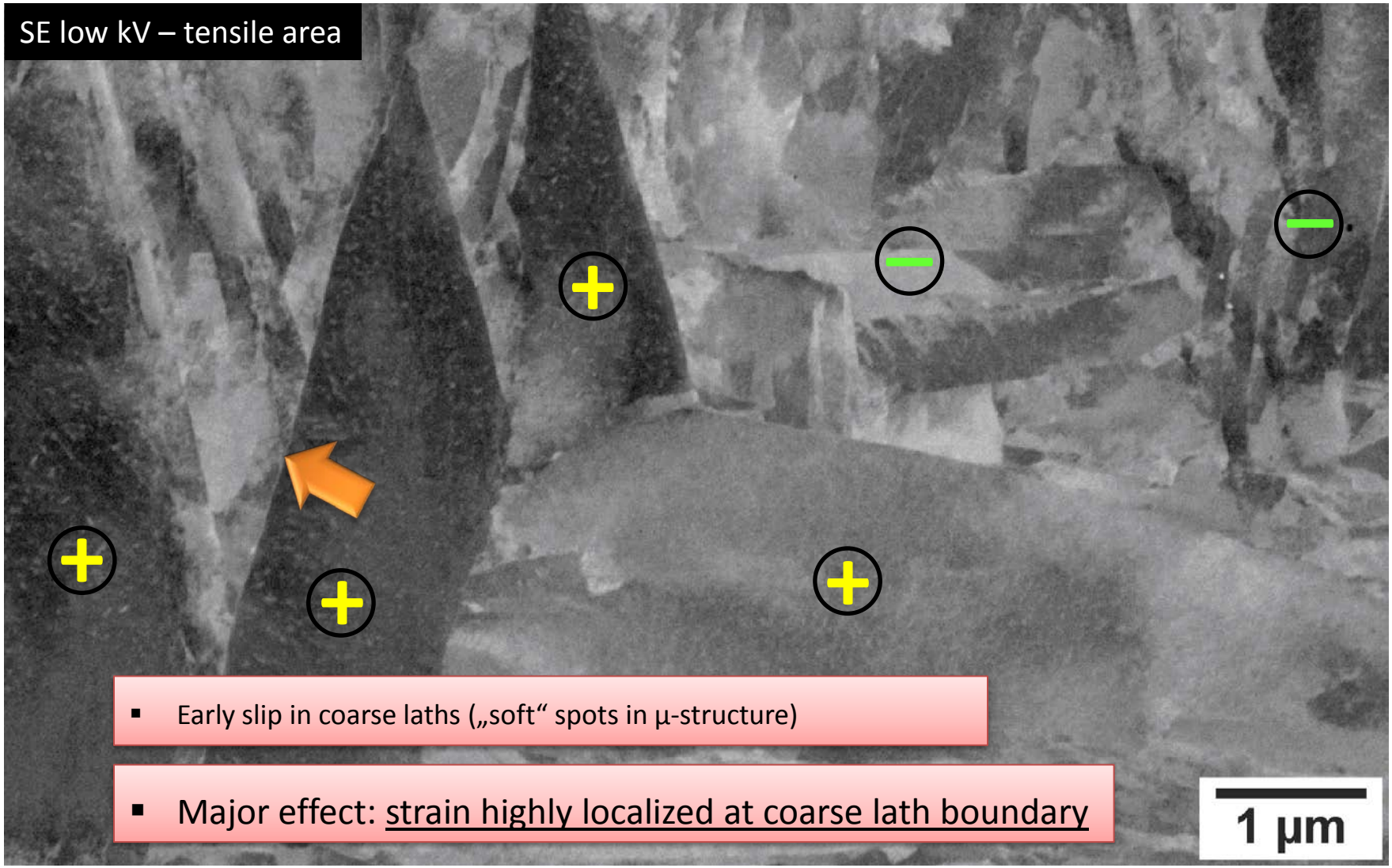
Results (ii)



In-situ bending – coarse laths

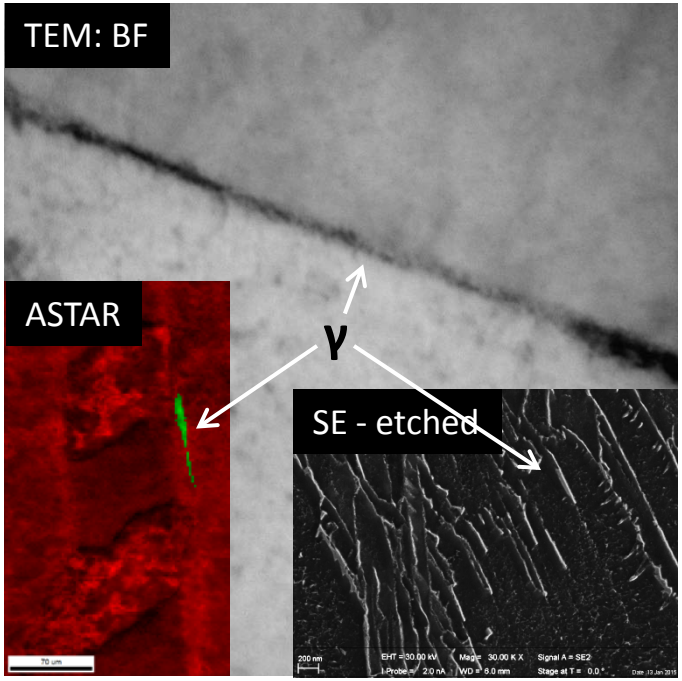


In-situ bending – coarse laths

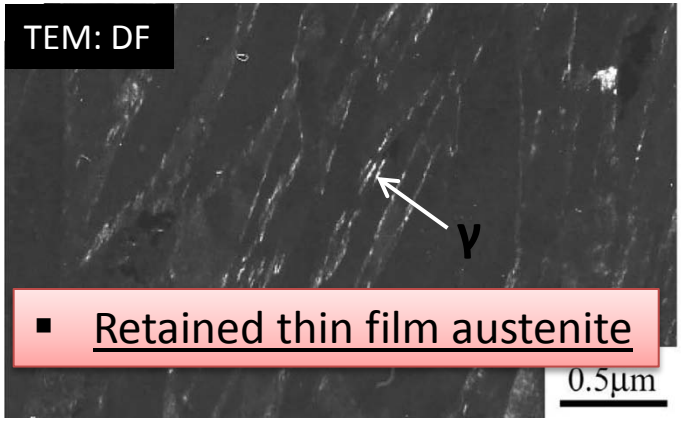


- Early slip in coarse laths („soft“ spots in µ-structure)
- Major effect: <u>strain highly localized at coarse lath boundary</u>

Ductile boundaries?

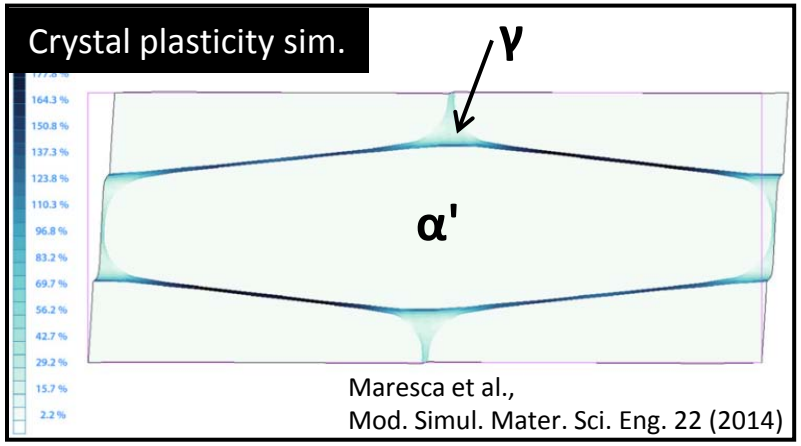


Own data

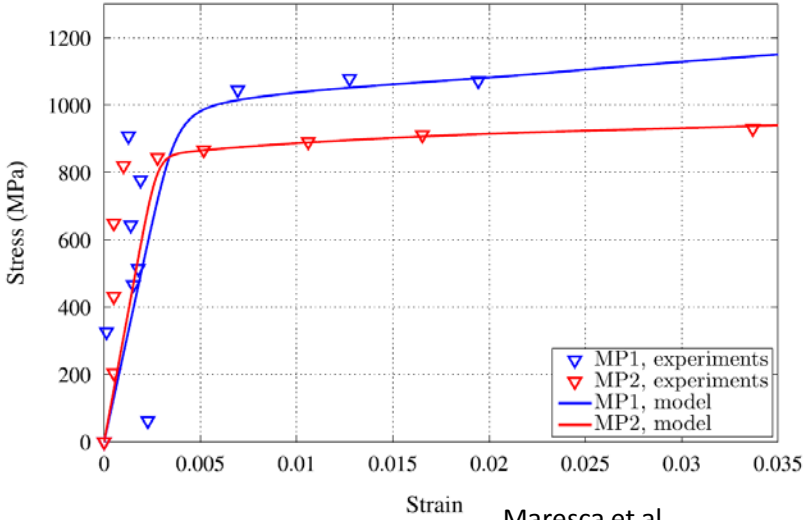


- Retained thin film austenite

Morito et al., ISIJ Int., 51 (2011)



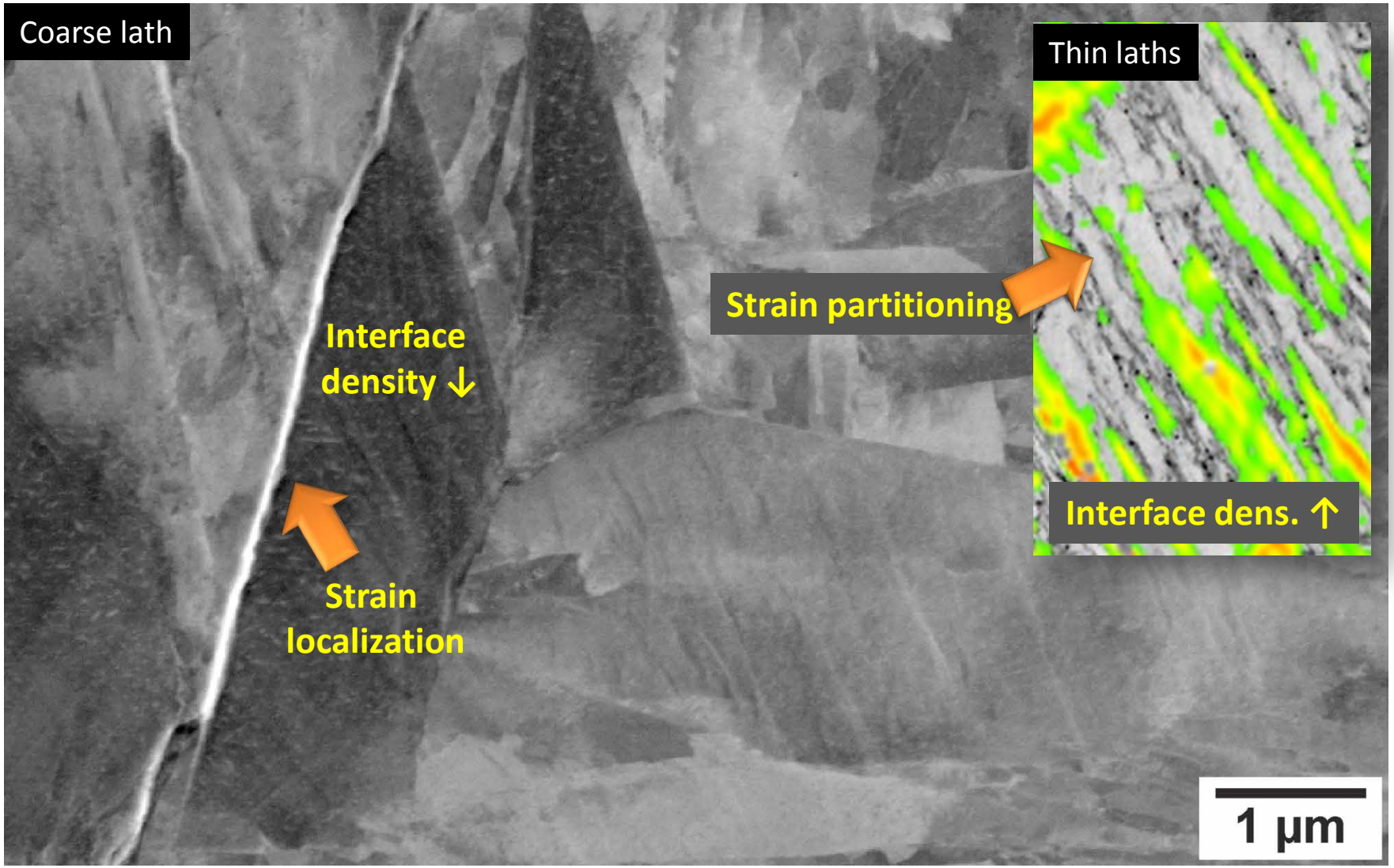
Maresca et al.,
Mod. Simul. Mater. Sci. Eng. 22 (2014)



Maresca et al.,
J. Mech. Phys. Solids 73 (2014)

- *Thin austenite as greasy film*

Coarse lath effect?



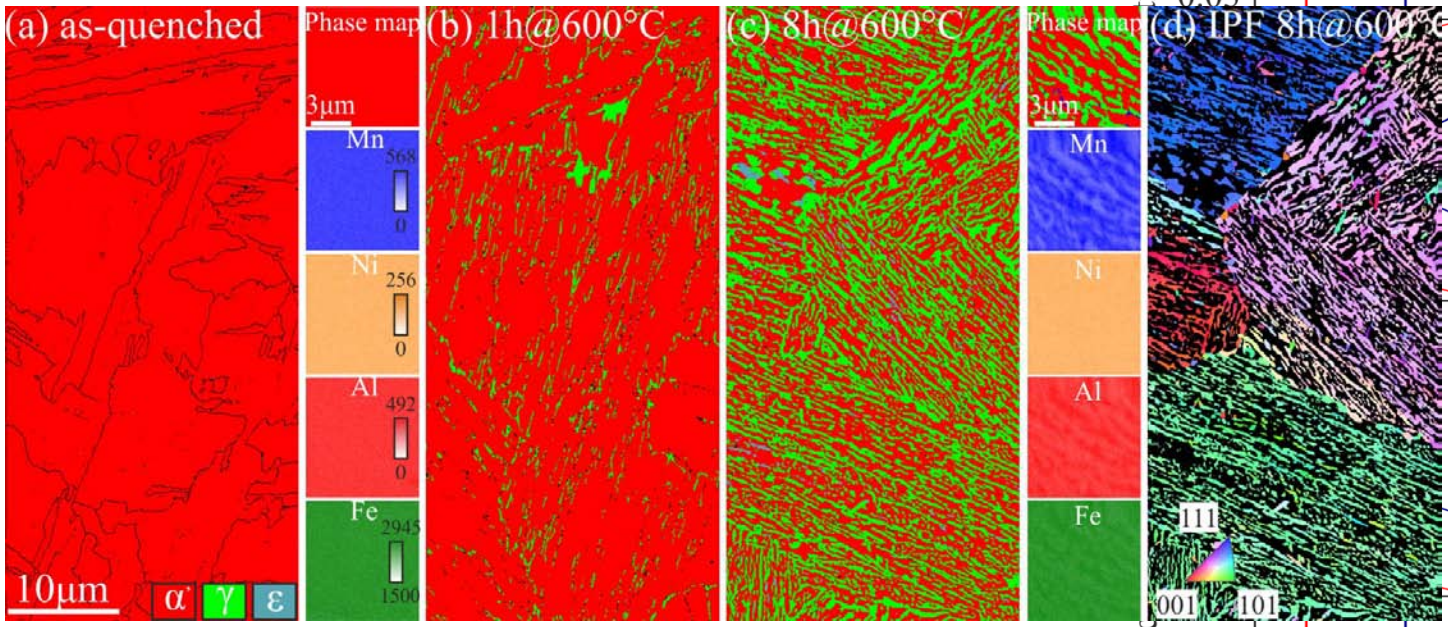
Methodology (B) – Microstructure design

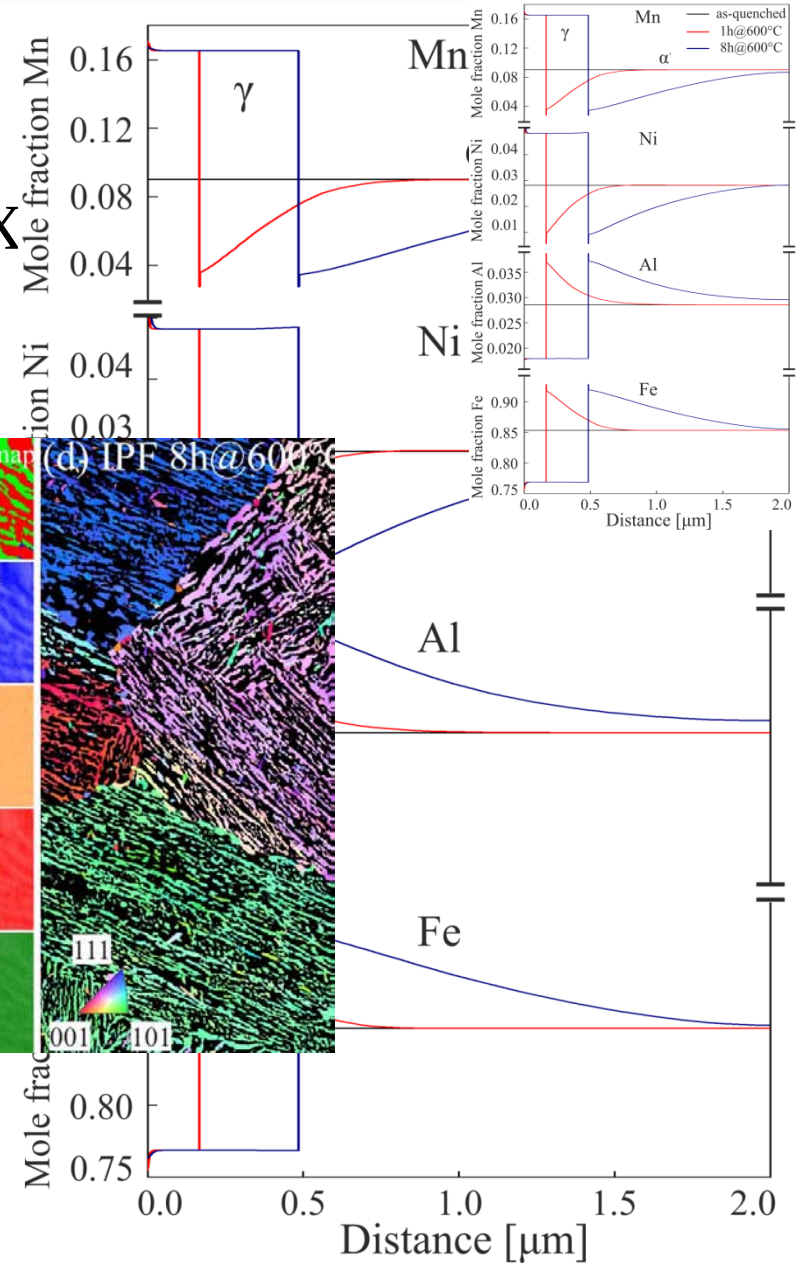
- γ reversion is calculated by Dictra

-Composition:Fe9Mn3Ni1.4Al (wt. %)

-Start microstructure: Martensite

- γ reversion is confirmed by EBSD & EDX

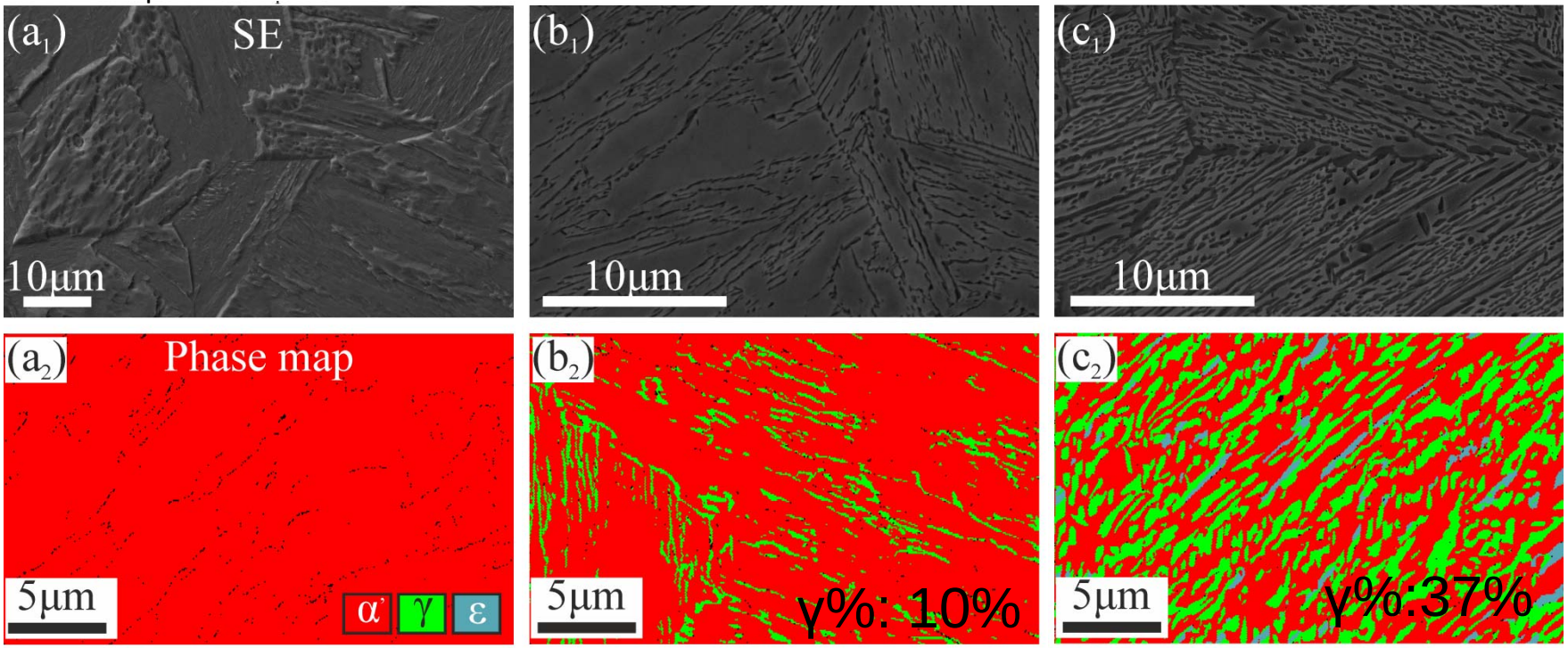




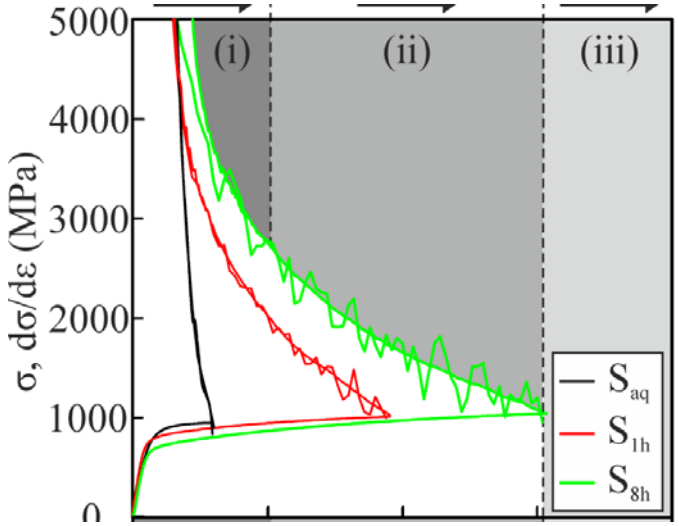
Design of ductile martensitic steels

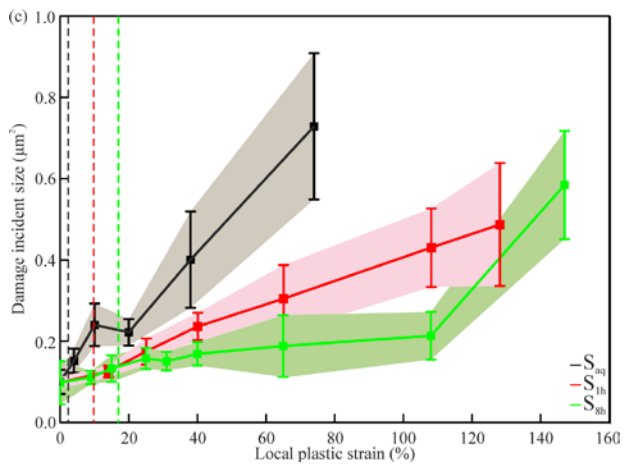
- Chemical composition: Fe9Mn3Ni1.4Al0.01C (wt.%)
- Cast in vacuum, hot rolled (1100°C) & homogenized (1100°C, 1h)
- Aging (for austenite reversion and maraging)

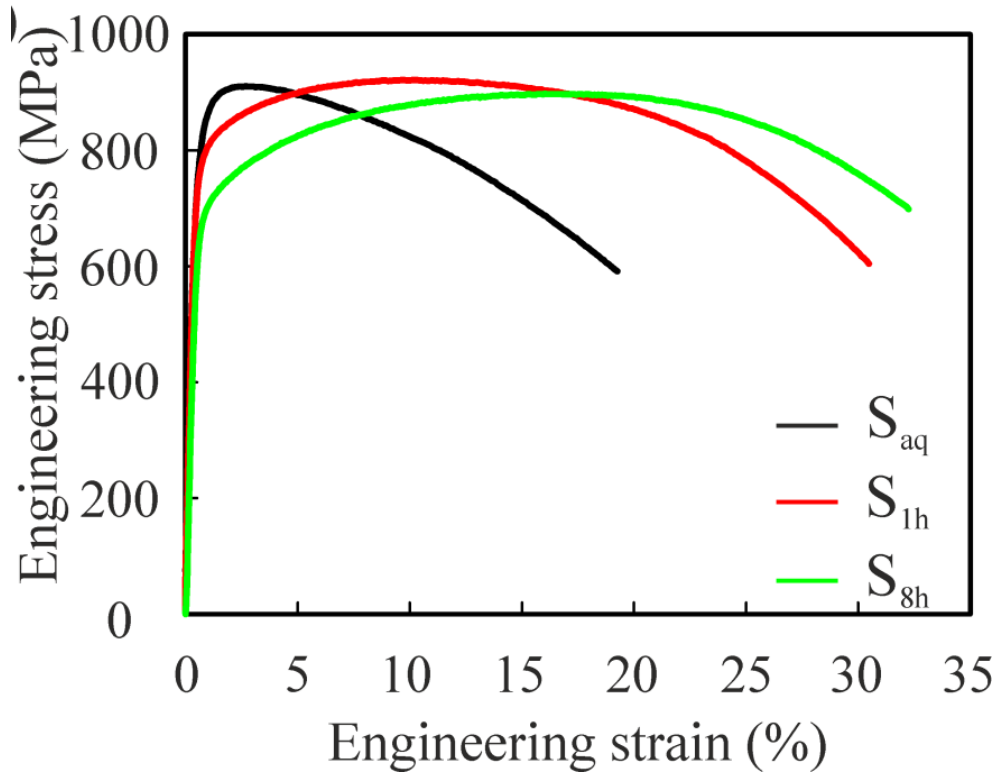
S_{aq}: As-quenched | S_{1h}: 600°C 1h | S_{8h}: 600°C 8h



Mechanical properties



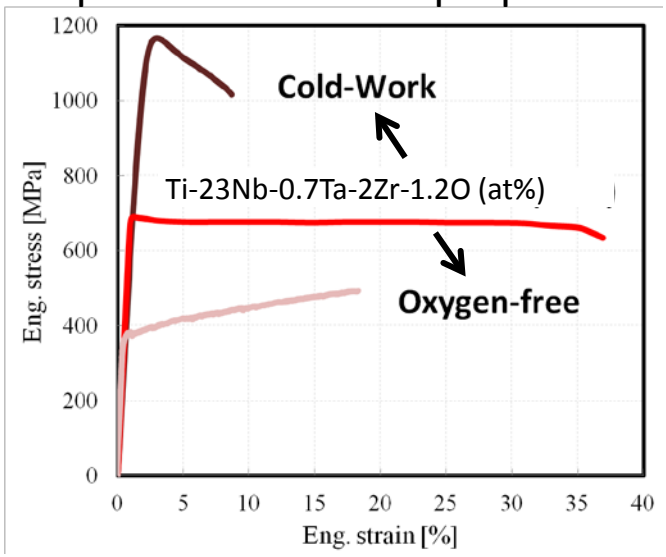




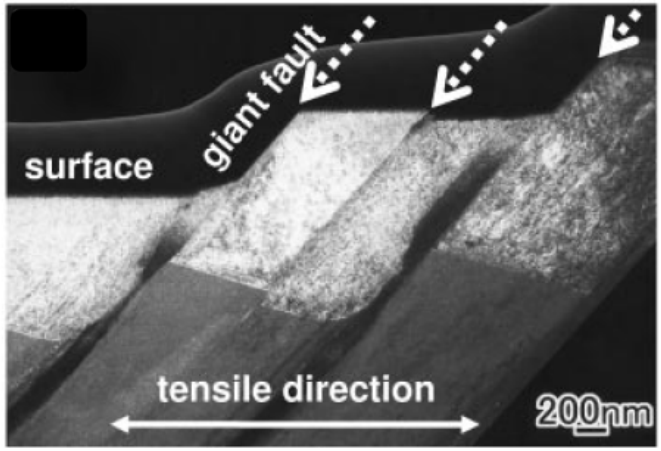
Wang, Tasan et al., Acta Mat (2014)
Wang, Tasan et al., Acta Mat (2015)

Gum metal

special mechanical properties



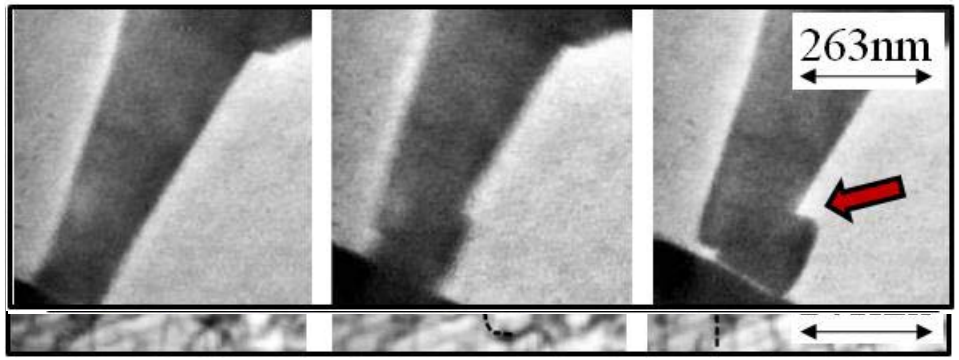
dislocation-free bulk shear mechanism



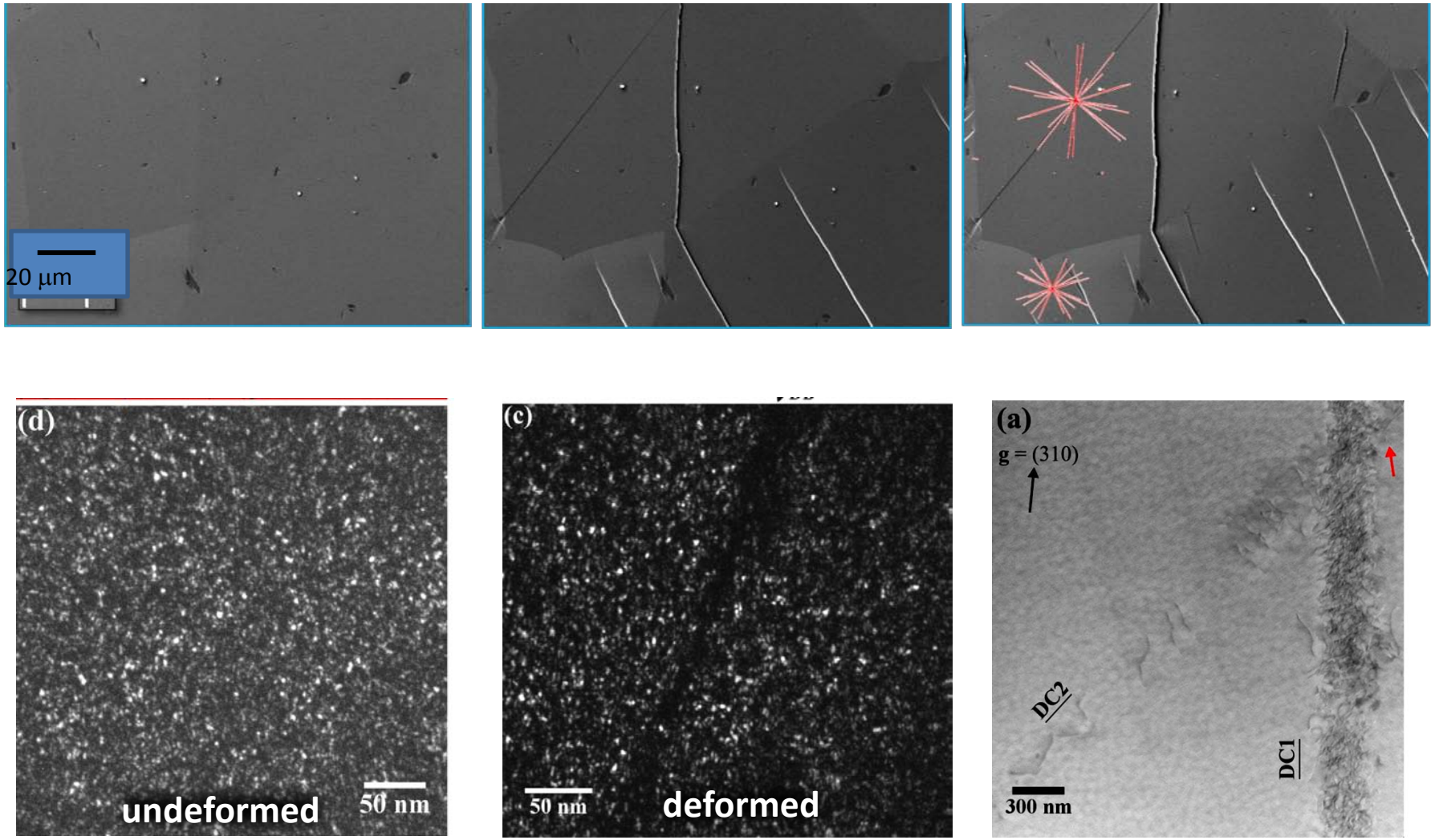
[Saito *et al.*, Science, 2003]

conflicting results in literature

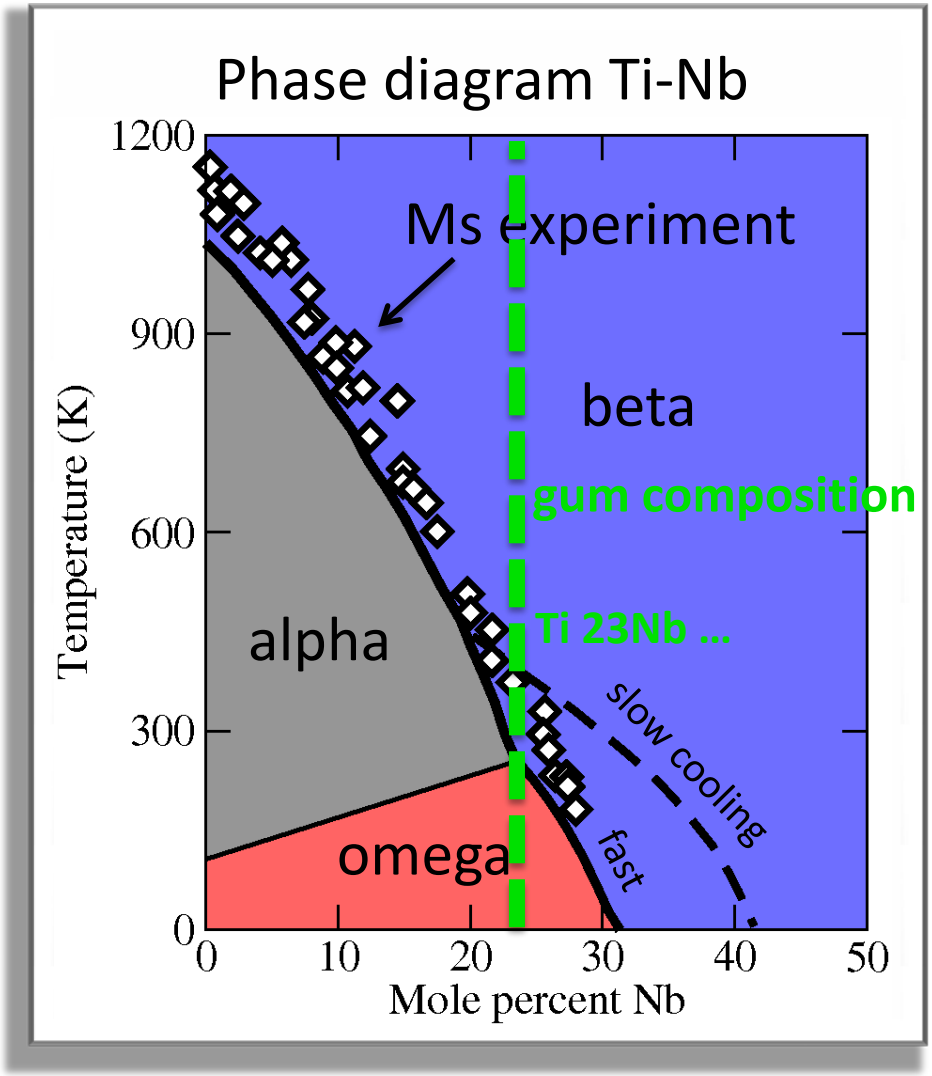
Bulk Shear [Withey *et al.*, ActaMat, 2010]



Real deformation mechanism



Triple point effect

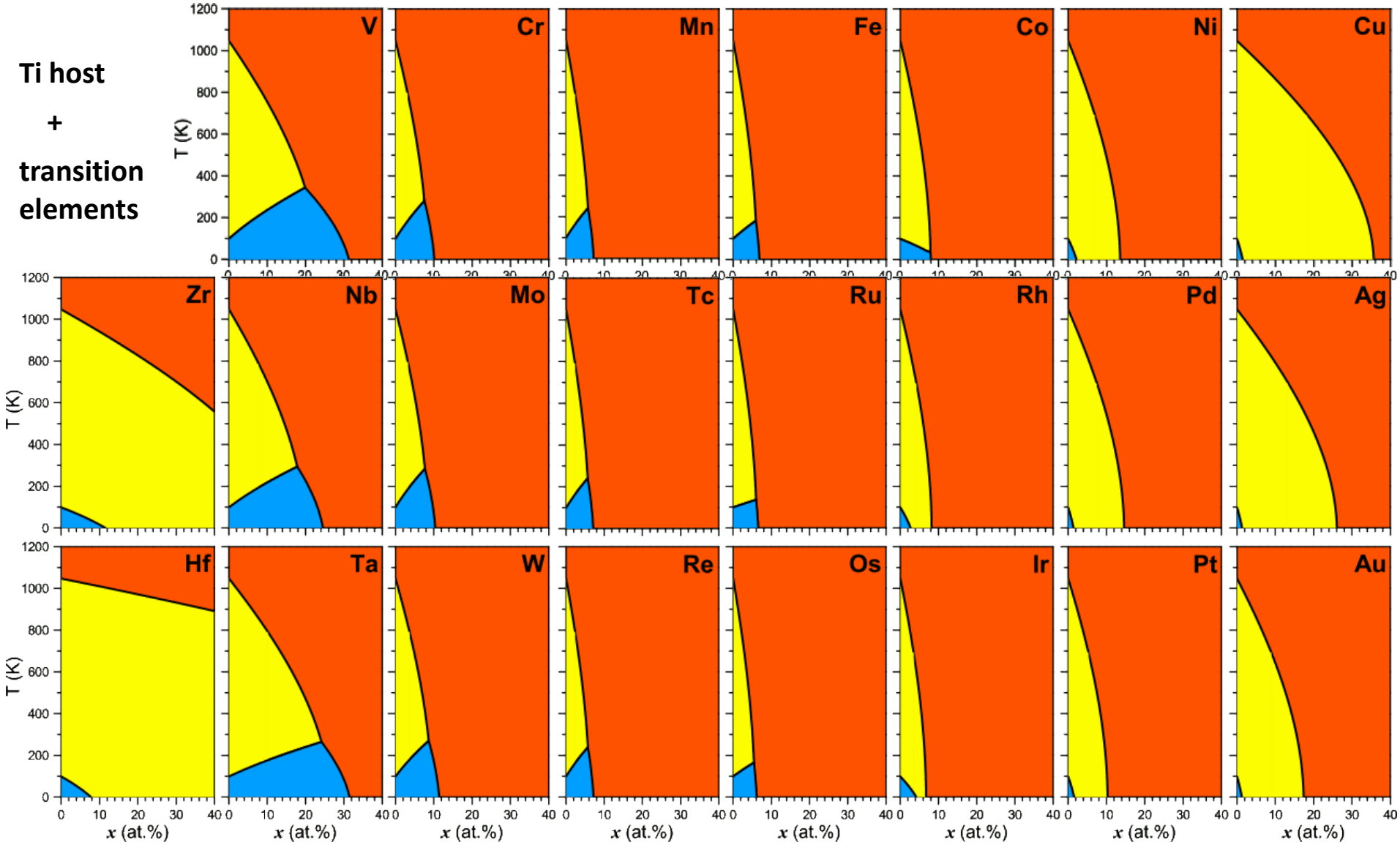


New gum metals? Phase diagram calculations from *ab initio*

Ti host

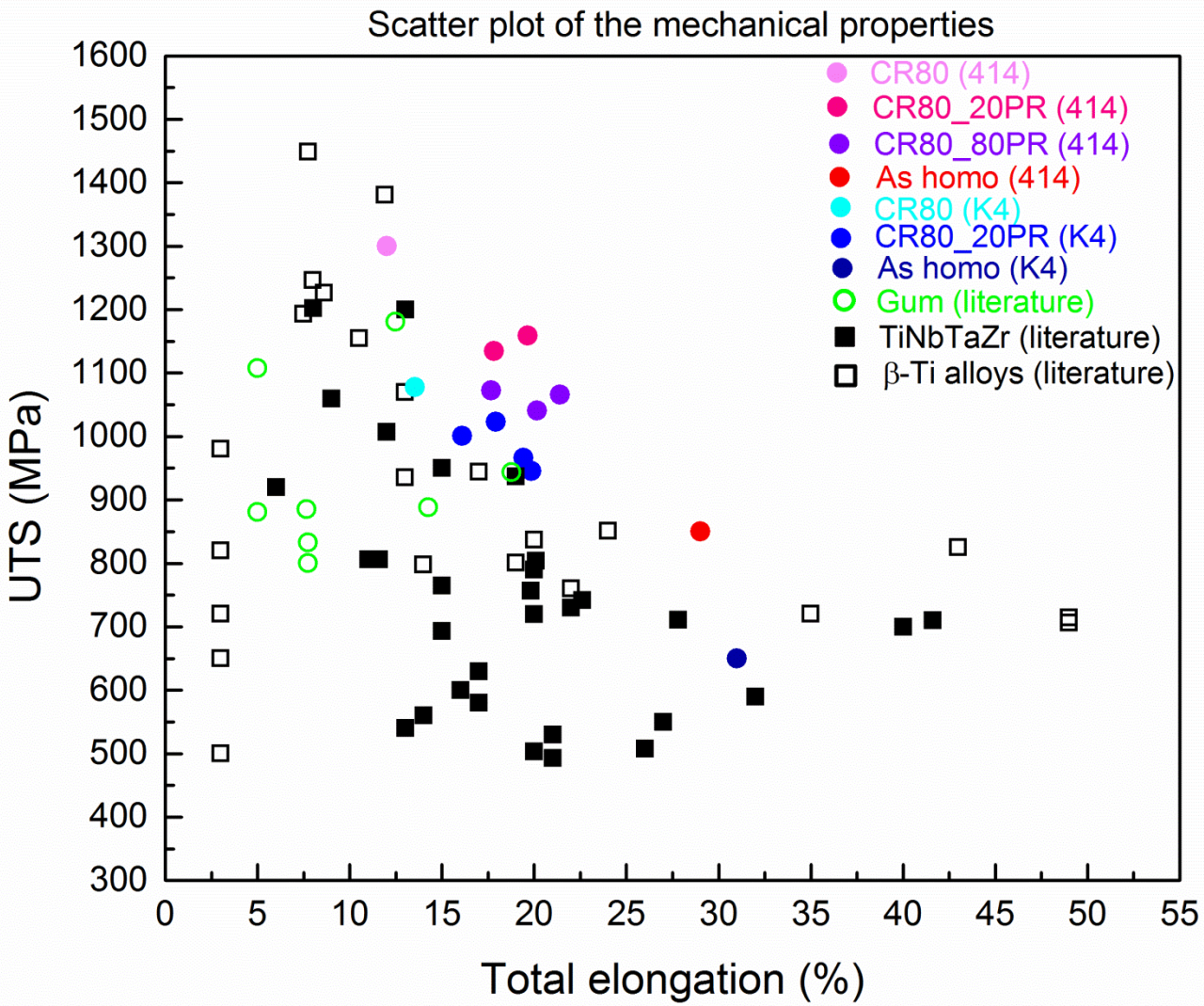
+

transition elements



Huang, Grabowski, Tasan, et al., submitted (2015)

Optimization of w and texture



Conclusions

- ICME new field, strongly needed for innovation.

- Integrated use of computational and experimental techniques is crucial, but brings in many challenges

- In MPIE, we couple
  - crystal plasticity & in-situ deformation experiments
  - diffusion simulations & alloy design
  - atomistic simulations & alloy design
  - ...