

Design and micromechanics of metal-matrix-composites and high-throughput mechanical testing for alloy design

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Course for Master students on Micromechanics of Materials at RWTH Aachen



Outline

Metal-matrix-composites

Motivation

Basics of MMC's

Challenges – micromechanics

Alloy design strategies

High-throughput mechanical testing

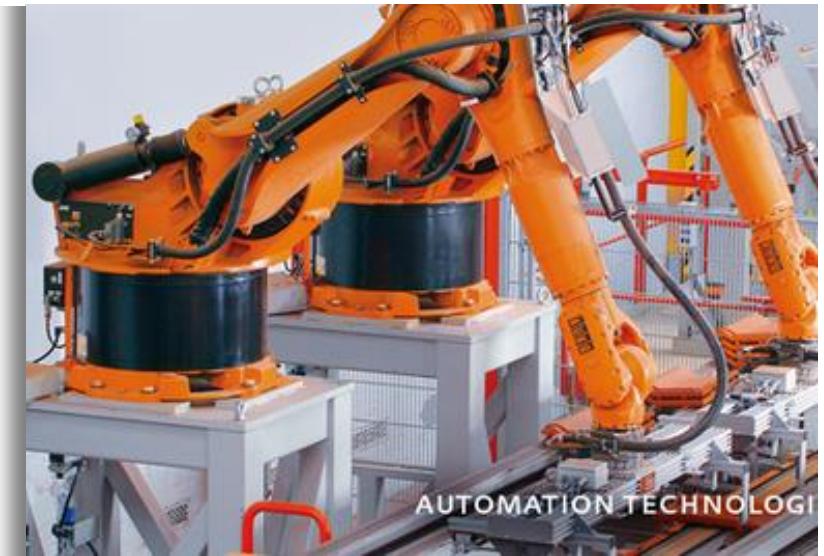
Motivation and challenges

Examples

Why MMCs?

Weight saving as major challenge

Performance, efficiency,
environmental, ...





How to save weight?

(1) Reduce density

	IA	IIA	VIIA
1	H Hydrogen		He Helium
2	Li Lithium	B Boron	
3	Na Sodium	Mg Magnesium	
4	K Potassium	Ca Calcium	Sc Scandium
5	Rb Rubidium	Sr Strontium	Y Yttrium
6	Cs Cesium	*	Hf Hafnium
7	Fr Francium	Rf Rutherfordium	**
* lanthanides			
89 (227)	La Lanthanum	Ce Cerium	Pr Praseodymium
90 (232)	Th Thorium	Pa Protactinium	U Uranium
91 (231)	Ac Actinium	Pm Promethium	Np Neptunium
92 (238)	Th Thorium	U Uranium	U Uranium
93 (237)		Pu Plutonium	Am Americium
94 (244)		Pu Plutonium	Cm Curium
95 (243)		Am Americium	Bk Berkelium
96 (247)		Cm Curium	Cf Californium
97 (251)		Bk Berkelium	Es Einsteinium
98 (259)		Cf Californium	Fm Fermium
99 (252)		Es Einsteinium	Md Mendelevium
100 (257)		Fm Fermium	No Neptunium
101 (258)		Md Mendelevium	Lr Lawrencium
102 (259)		No Neptunium	Lu Lanthanum
103 (262)			

Material $\rho / \text{g cm}^{-3}$

Fe 7.85

Ti 4.50

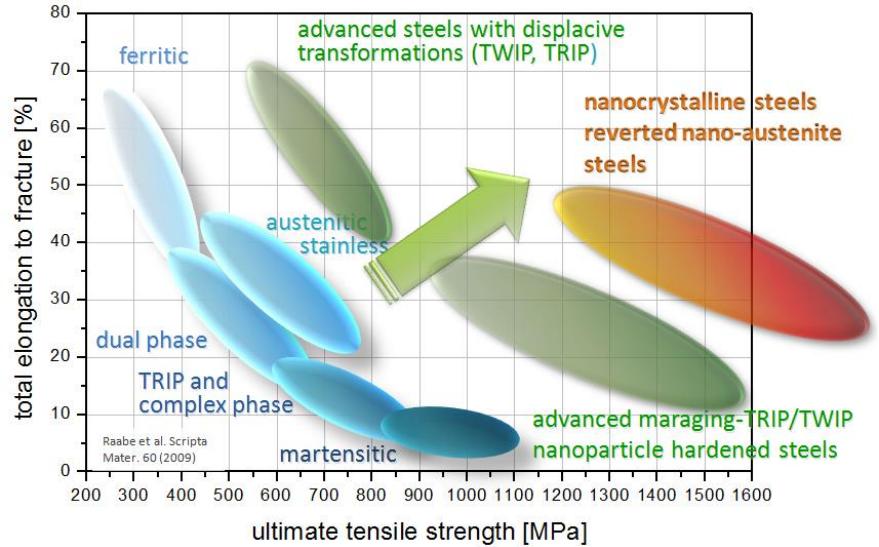
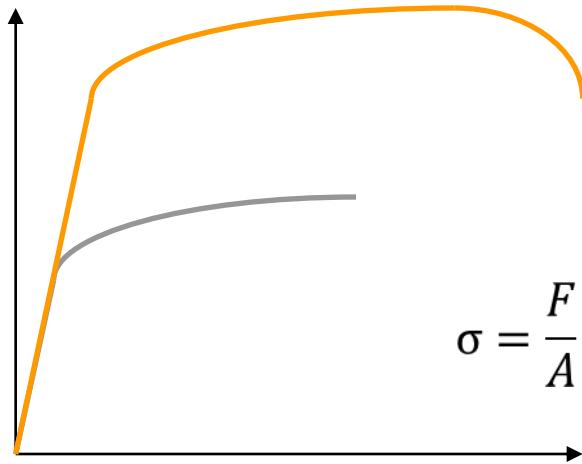
Al 2.70

Mg 1.74

PE-LD 0.95

How to save weight?

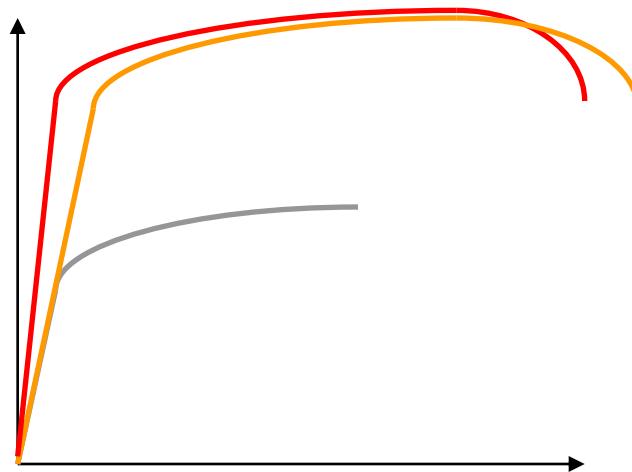
(2) Increase specific strength



Material	$\rho / \text{g cm}^{-3}$	UTS / MPa
UHS steel	7.85	> 1500
Ti 6 4	4.50	~ 800
Al #7000	2.70	~ 450
Mg AZ31	1.74	~ 200
PE-LD	0.95	~ 10

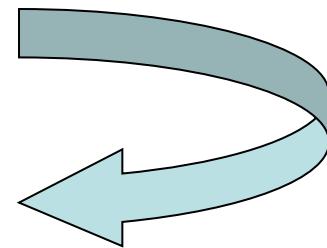
How to save weight?

(3) Increase stiffness



Deflection

$$f_b = \frac{Fl^3}{3EI_{xx}}$$



Resonance

$$f_R = \sqrt{\frac{c}{m}}$$

Material	$\rho / \text{g cm}^{-3}$	UTS / MPa	E / GPa
UHS steel	7.85	> 1500	~ 200
Ti 6 4	4.50	~ 800	~ 110
Al #7000	2.70	~ 450	~ 70
Mg AZ31	1.74	~ 200	~ 45
PE-LD	0.95	~ 10	~ 0.2

→ Lightweight design

Most important material properties

High (Yield)Strength

no plastic deformation under load

High Youngs-Modulus

high stiffness and resonance

Low density

low mass

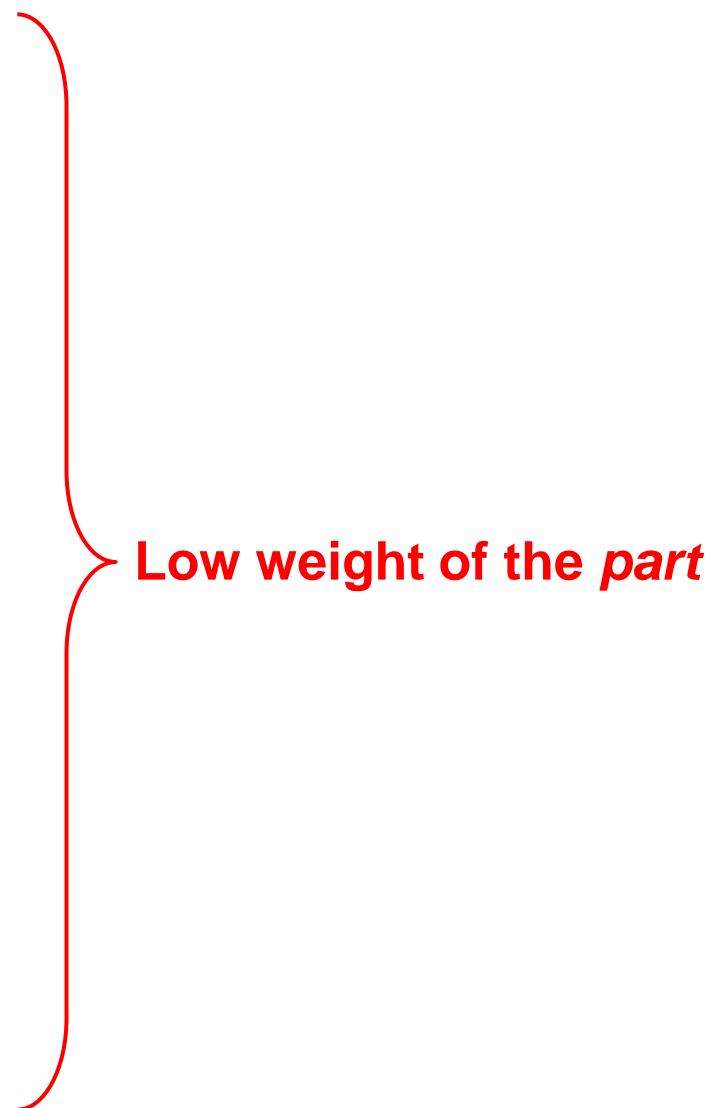
sufficient ductility

production → energy-absorption special case

More

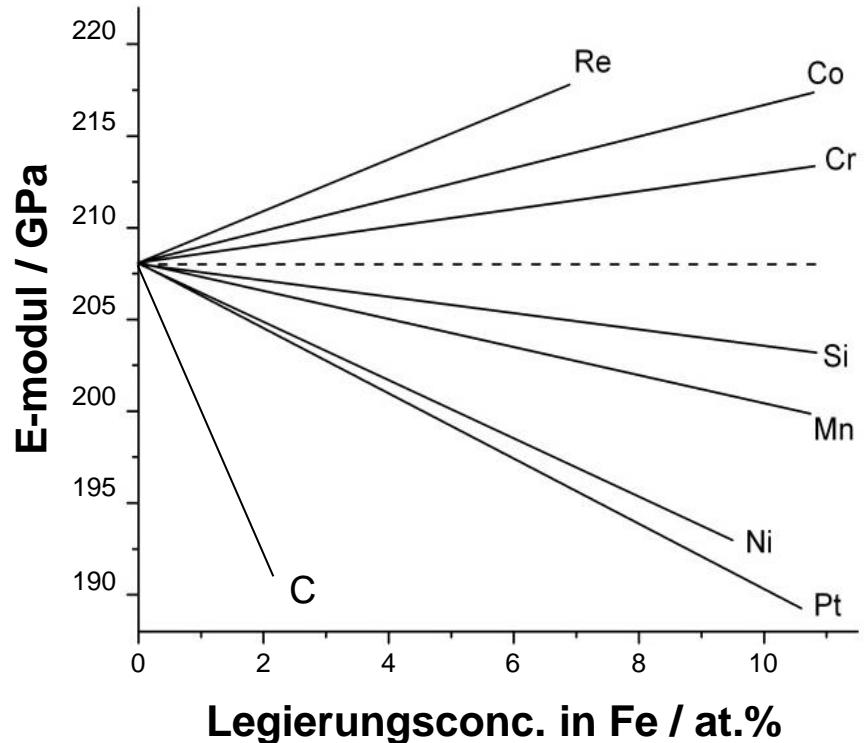
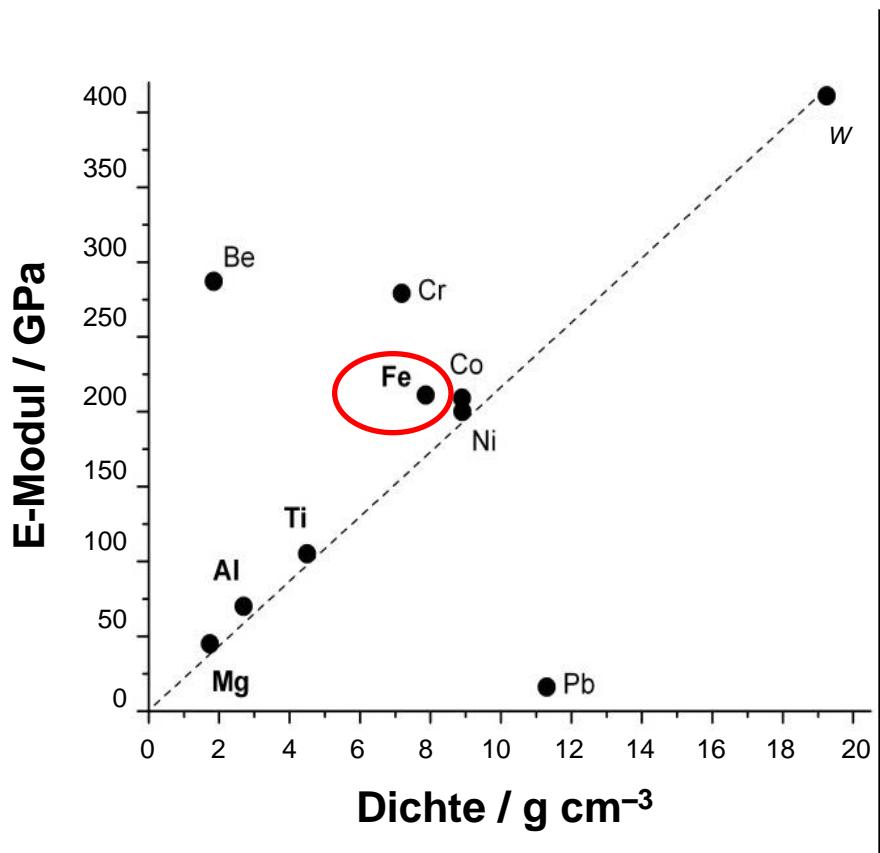
Fatigue- & corrosion resistance, welding

... @ low costs – steels!



Light steels?

Common metals have similar E/ρ ratio



Alloying often detrimental

→ defects, lattice distortion (**austenite, martensite?**)

Example: drive shaft design

Strength $\sigma_B = \frac{F l y}{J_{xx}} < R_p \text{ 0.2 } \nu$

Deflection $f_b = \frac{F l^3}{3EJ_{xx}}$ $J_{xx} = \frac{\pi r^4}{4}$



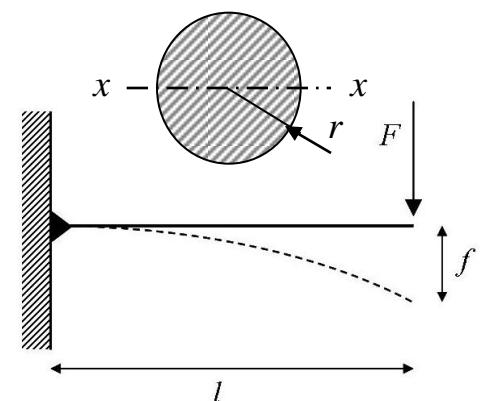
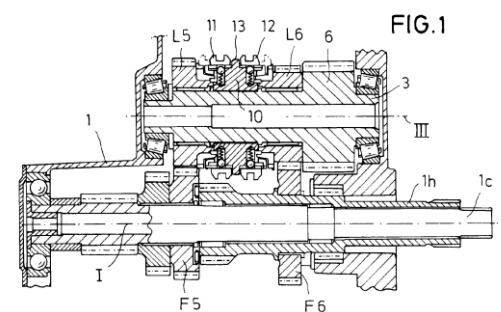
→ Mass of part

$$m = \frac{\rho l \pi r^2}{4}$$

Comparison ($F, f_b, l = \text{constant}$)

Material	E / GPa	$\rho / \text{g cm}^{-3}$	$\Delta \text{Mass / \%}$
42CrMo4	208	7.90	/
30Mn-1.2C-5Al	175	7.14	- 0.84

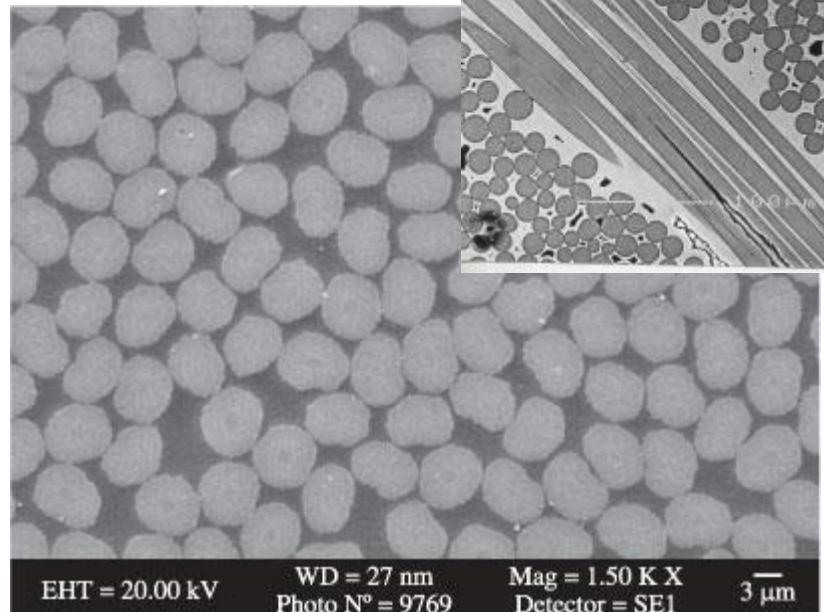
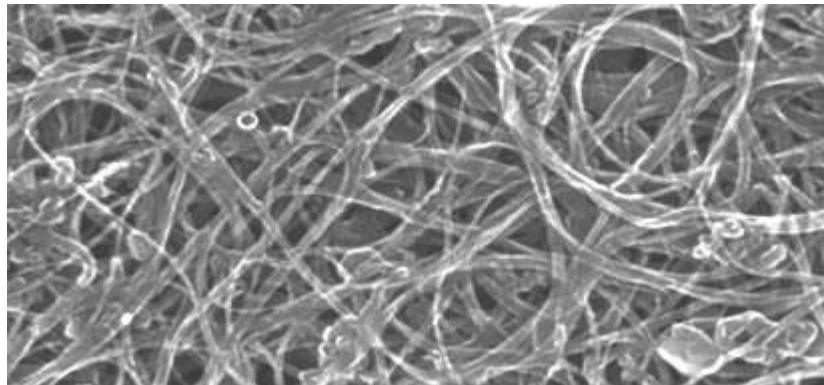
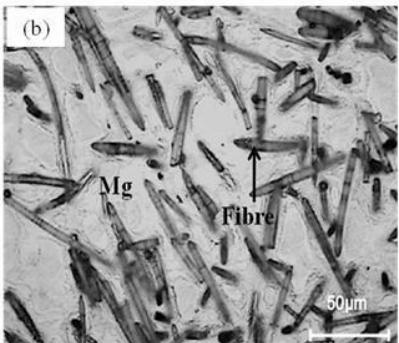
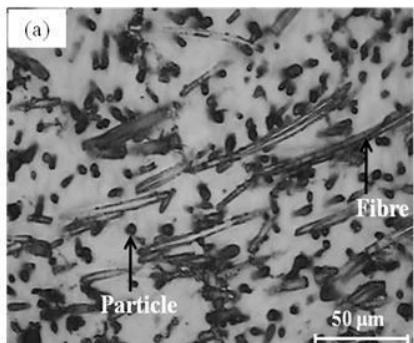
→ Only minimum saving!



What do do?

Implement stiff and light particles (spheres, fibres, flakes ...)

→ Known (M)MC applications?



(a)

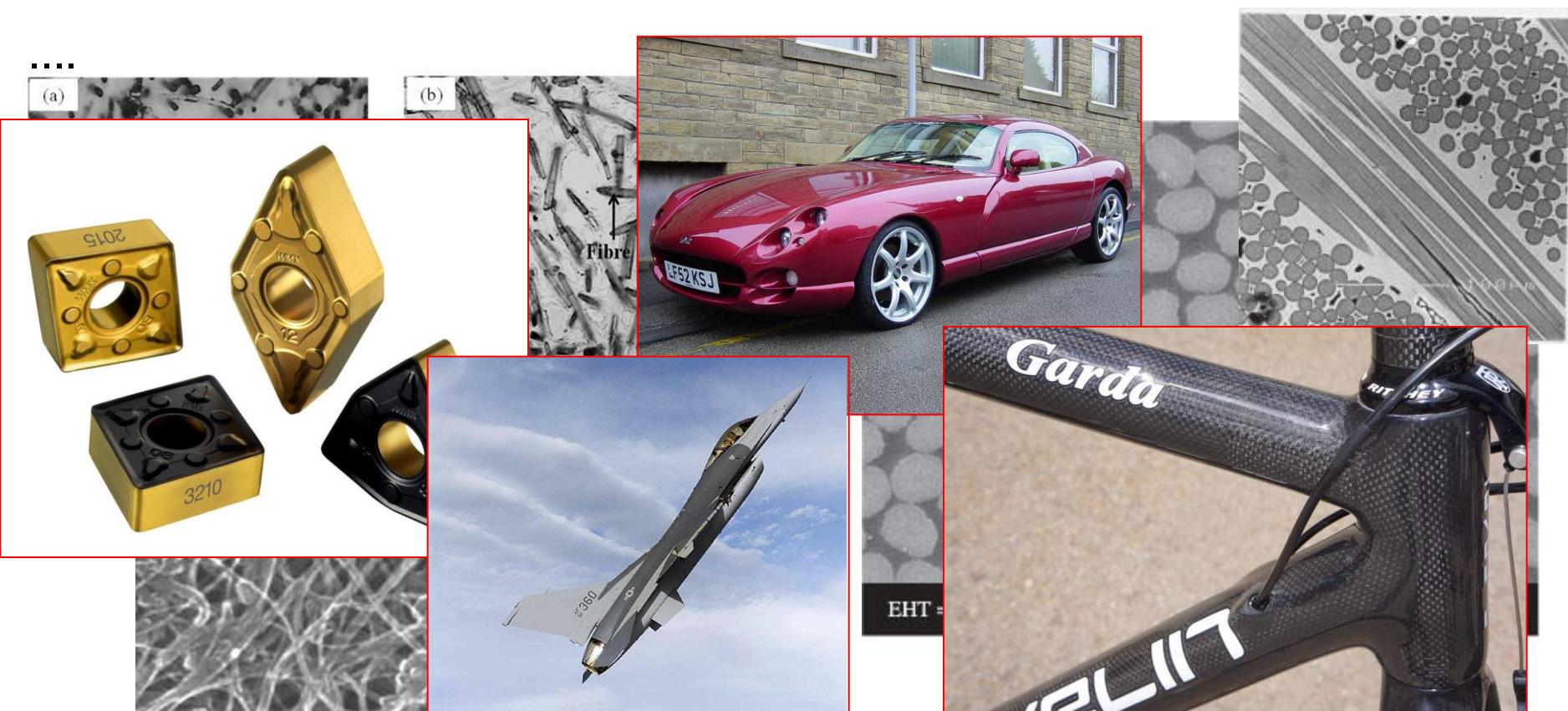
What do do?

Implement stiff and light particles (spheres, **fibres**, flakes ...)

Cutting plates (WC-Co)

GFRP

CFRP $\rightarrow \rho \sim 1.5 \text{ g cm}^{-3}$; $E \sim 200 \text{ GPa}$ (**non-isotropic!**)



„No“ fibres in MMC´s for isotropic behaviour

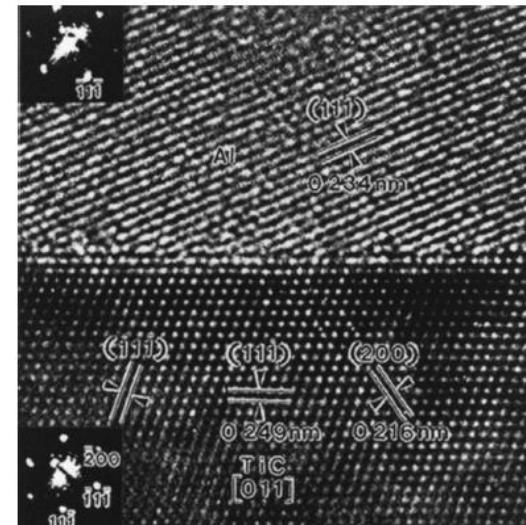
Desired property profile

High efficiency (E , ρ)

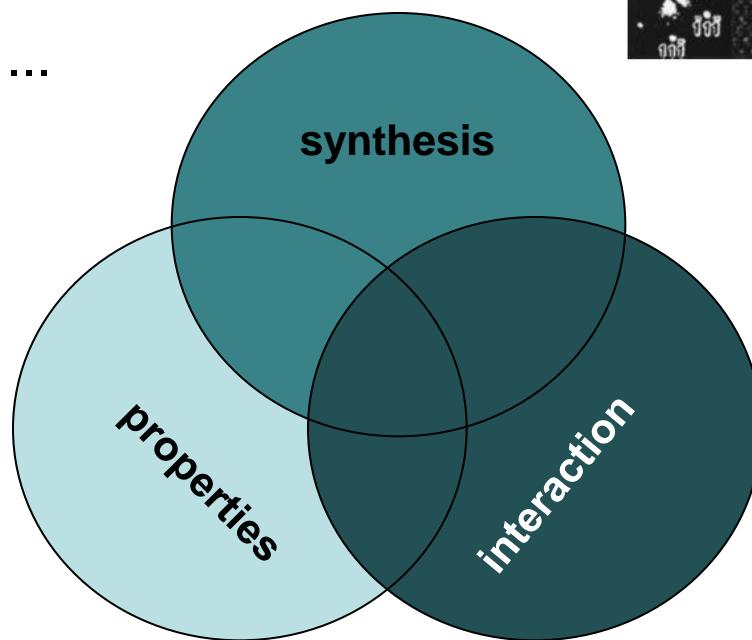
Strong interface (d_{Misfit} , wetting angle)

High ductility (K_{IC} , B/G)

Stable, cost effective, α_{therm} , ...



→ Balance required:





Particle selection

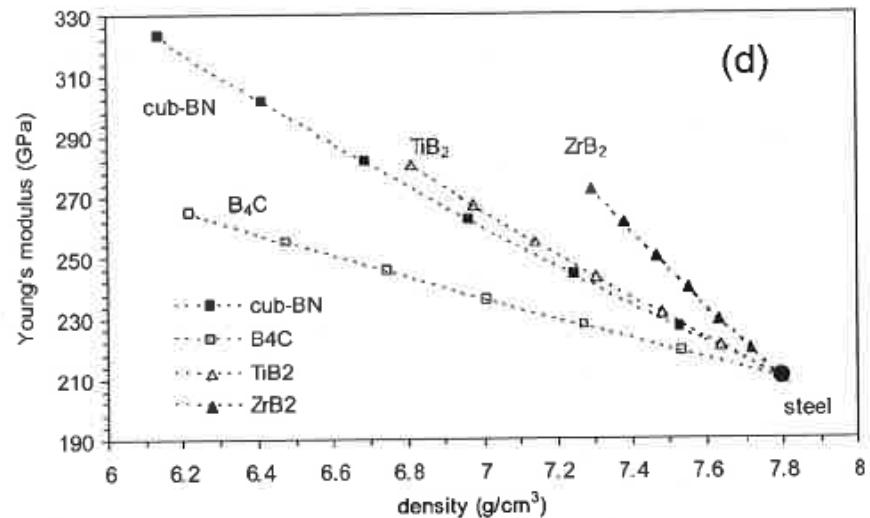
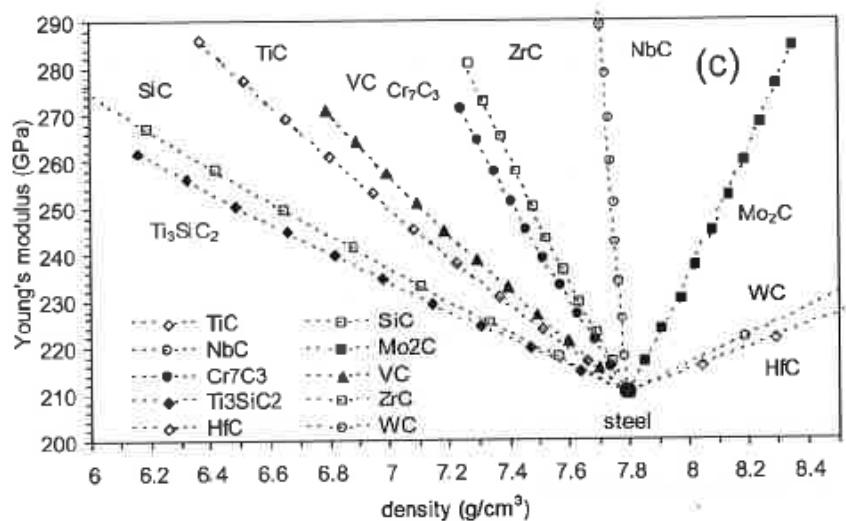
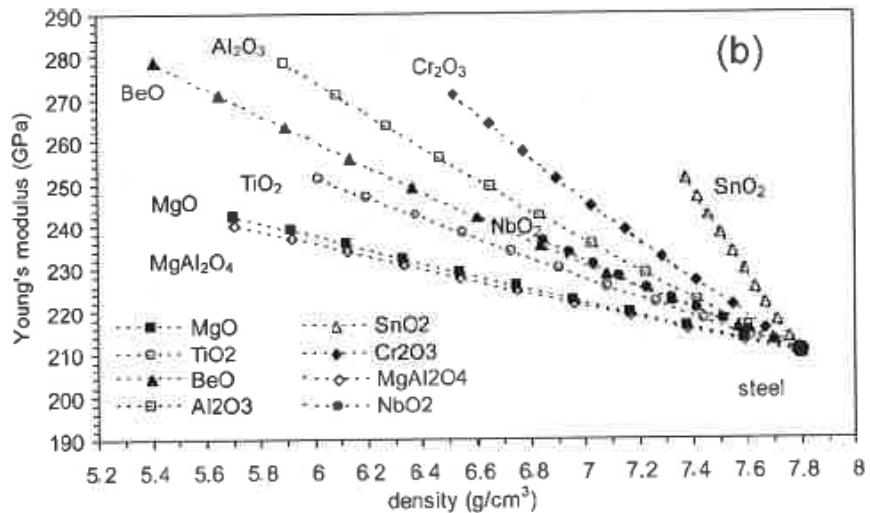
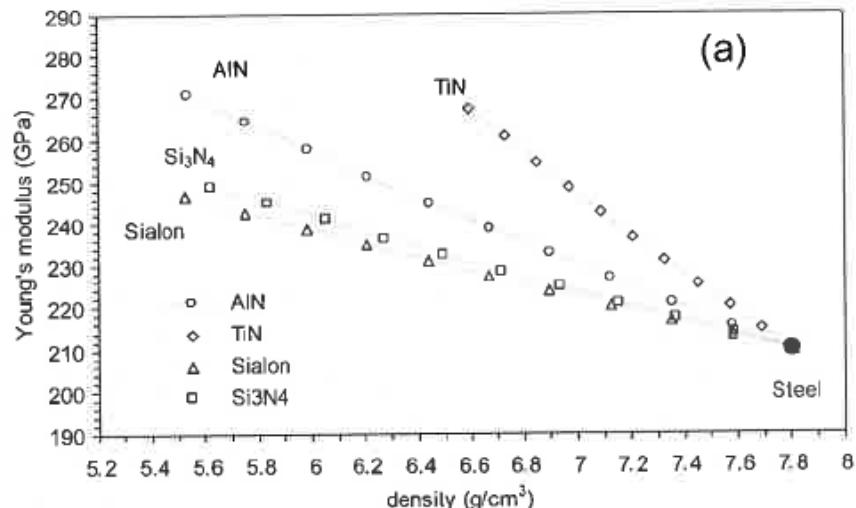
Types of particles: Borides, Carbides, Nitrides, Oxides, Intermetallics

Kind	Component	T _{Liq} [°C]	[Lit]	Bulk modulus [GPa] 20 - 25 °C	G Shear modulus [GPa] 25 °C	[Lit]	B / G	Hardness [GPa] 25 °C	[Lit]	Density [g cm ⁻³]	[Lit]	Poisson 25 °C	[Lit]	E Young's [Gpa] 20 - 25 °C	[Lit]	Specific modulus [GPa / gcm ⁻³]
	AlB₂	915	[71Eck]	190	95	[12Dvs]	2.00	23.6	[63Sha]	[3.19]	[63Sha]	0.29	[12Dvs]	244.4	[12Dvs]	76.6
	BeB₂	>1970	[71Eck]	215		[06ls]		31.2	[80Ssm]	2.32 - 2.48	[04Bur]					
	BeB₃	~ 1700	[64Ssm]					25.3	[80Ssm]	2.35 / [2.33]	[64Sam]					
	BeB₅	~ 2100	[71Eck]													
	CrB	2300	[64Ssm]													
		1515 / 1550+-50	[63Sha]					20.3	[63Sha]	6.05	[63Sha]					
		~ 2060	[71Eck]					13.2 - 22.3	[850ks]	6.04 / [6.11]	[71Eck]					
		2050	[64Ssm]					11.8 - 12.7	[64Sha]	6.05 / [6.11]	[80Ssm]					
	CrB₂	2280	[71Eck]	239.2	133.3	[12Dvs]	1.71	17.7	[63Sha]	[5.6]	[63Sha]	0.26	[12Dvs]	415.4	[12Dvs]	74.2
		1360 / 1390 / 1850+-50	[63Sha]					20.3 - 22.5	[850ks]	5.22 / [5.60]	[64Sam]					
		2200+-50	[64Ssm]					20.6	[64Sam]							
	CrB₄	1400 - 1600	[80Ssm]	265	261	[12Niu]	1.02	48.0	[12Niu]							
	CrB₂	1960	[63Sha]							6.13 / 6.7	[63Sha]					
	ErB₂	-														
		1363	[13Fen]	243.73	60.24	[09Xis]	4.15	13.1+-0.5	[80Sal]	7.15	[13Fen]					
	Fe₂B	1363	[71Eck]	154	67	[09Xis]	2.90			~ 7.0	[71Eck]					
		~ 1390	[63Sha]	331	152.8	[09Xis]	2.17									
	FeB₄	-		253	177	[12Niu]	1.43	24.2	[12Niu]							
	GdB₂	-		131.2	113.5	[12Dvs]	1.16					0.16	[12Dvs]	264	[12Dvs]	
		3100 / 3060 - 3065 / 3250 +-100	[63Sha]	260.3	233	[12Dvs]	1.12	28.4+-4.3	[80Ssm]	11.2	[63Sha]	0.16	[12Dvs]	538.7	[12Dvs]	48.1
		3250	[80Ssm]	215	233	[08Zha]	0.92			28.0	[08Zha]	0.12	[08Zha]	514	[08Zha]	45.9
	HfB₂	3380	[05Nar] p.203	265 - 288	240 - 273	[08Zha]	0.97	21.2 - 28.4	[05Nar] p.211	10.5 / [11.2]	[71Eck] / [64Sam]	0.124 - 0.153	[08Zha]	554 - 614	[08Zha]	49.5
		3250	[71Eck]					28.4	[64Sam]			0.12	[05Nar] p.211	530	[05Nar] p.211	
		> 2100	[63Sha]					27.2	[80Ssm]	[4.72]	[63Sha]					
	LaB₆	2530	[71Eck]							4.74	[71Eck]					
	LeB₂	-		178.4	173.3	[12Dvs]	1.03			4.76 / [4.72]	[64Sam]					
		-								[9.656]	[80Ssm]	0.13	[12Dvs]	392.7	[12Dvs]	40.7
		-		151.5	116.4	[12Dvs]	1.30	-		[9.76]	[64Sam]					
	MgB₂	-		120	[06ls]	[06ls]				2.48 - 2.67 / [2.63]	[71Eck]					
		151	[06ls]							[2.63]	[71Eck]					
	MaB₂	1968	[80Ssm]	220.1	121.6	[12Dvs]	1.81	16.7+-0.5	[80Ssm]	[5.344]	[80Ssm]	0.31	[12Dvs]	318.4	[12Dvs]	59.6
			[06ls]							[5.37]	[64Sam]					
	MaB₄	2160	[80Ssm]	270	245	[12Niu]	1.10	41.5	[12Niu]							
		151	[06ls]					35.3+-1	[80Ssm]							
	MoB₂	2100 / 2250+-50	[63Sha]	302.5	186	[12Dvs]	1.63	11.7 / 12.6 / 13.5	[63Sha]	[7.78]	[64Sam]	0.24	[12Dvs]	463.1	[12Dvs]	59.5
		2350	[80Ssm]							[7.78] / [7.81]	[63Sha]					
	MoB₄	< 1600	[71Eck]	287	239	[12Niu]	1.20	36.7	[12Niu]	4.8 / [4.96]	[64Sam] / [71Eck]					
		2000 / 2165	[63Sha]							[9.31] / [9.31]	[63Sha]	0.19	[12Dvs]	278	[12Dvs]	104.1
										[9.26]	[71Eck]					
	Mo₂B	decompose to MoB ₂ & 1600 - 1650	[63Sha]							9.1 / [9.31]	[64Sam]					
		< 1600	[71Eck]													
		2300	[63Sha]	286.3	210.4	[12Dvs]	1.36	16.7 / 25.4	[63Sha]	6.97	[64Dom]	0.2	[12Dvs]	512	[64Dom]	73.5
	NbB₂	~ 3000	[71Eck]					25.5	[80Ssm]	6.4 / 6.5 / 6.6 / 6.97	[63Sha]			507	[12Dvs]	71.2
		3000	[64Sam]							6.6	[71Eck]			637.5	[80Ssm]	
	NbB₄	-		243	194	[12Niu]	1.25	30.4	[12Niu]	7.13	[71Eck]					
	NiB	330	[71Eck]					15.2	[80Ssm]	6.5 / [7.13]	[64Sam]					

Particle selection

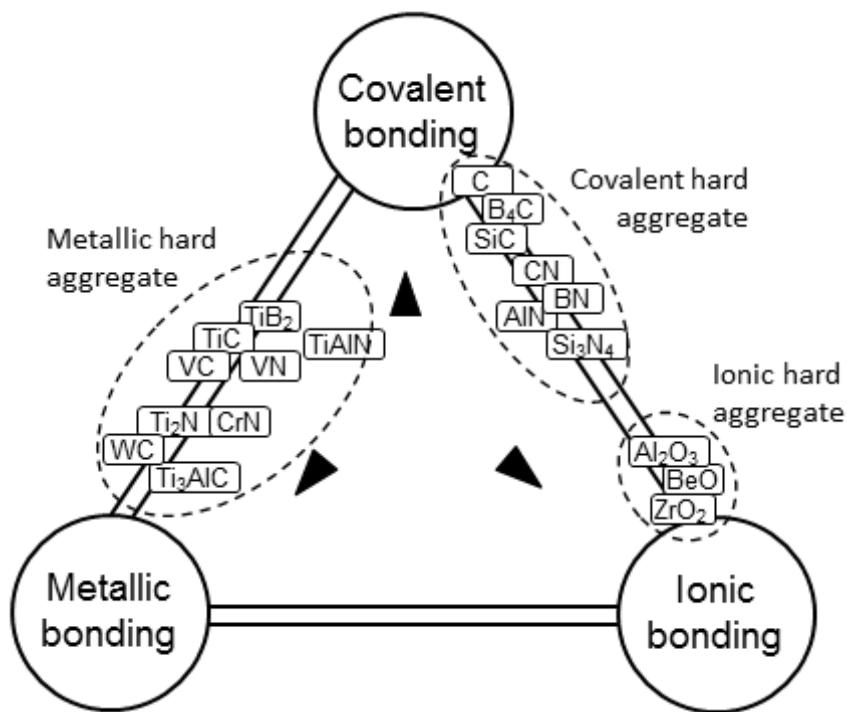


Types of particles: Borides, Carbides, Nitrides, Oxides, Intermetallics



Why these types of compounds?

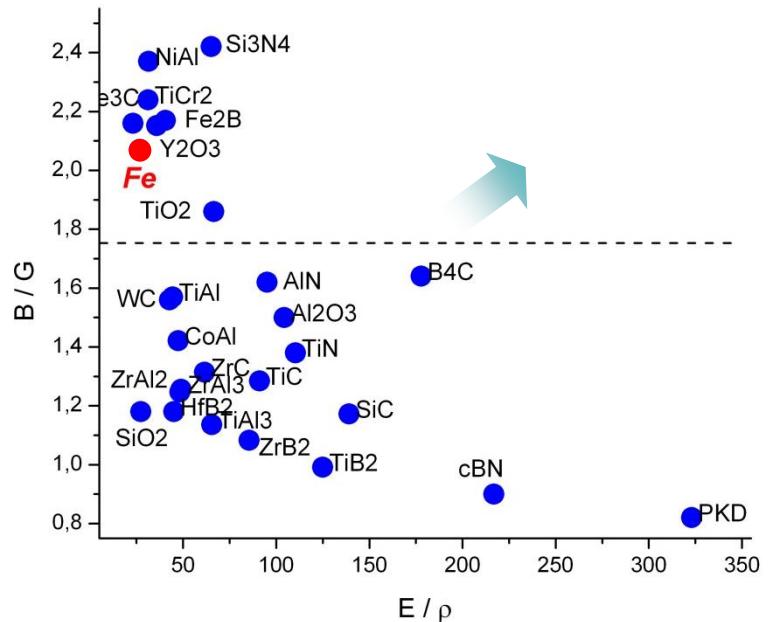
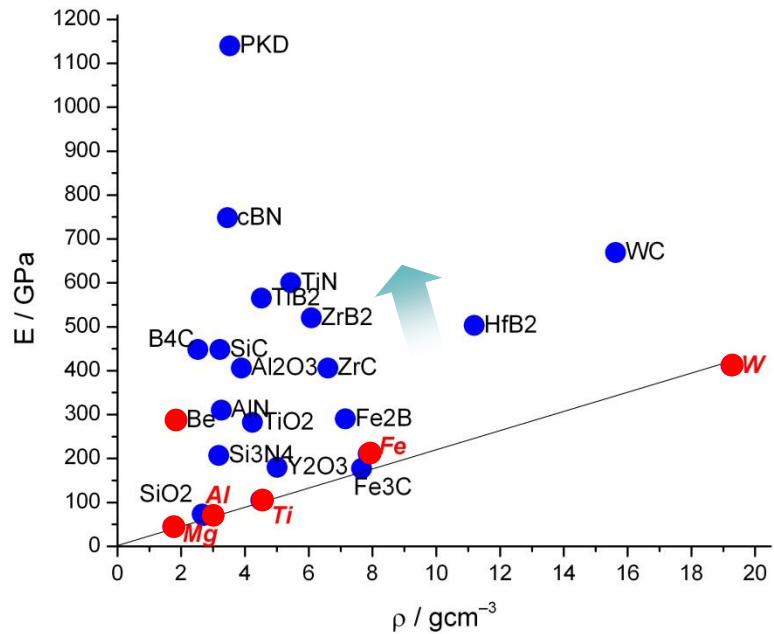
Types of particles: Borides, Carbides, Nitrides, Oxides, Intermetallics



- Light elements for density reduction
- Strong bonding by covalent and ionic contribution for stiffness

Particle selection

Types of particles: Borides, Carbides, Nitrides, Oxides, Intermetallics



Optimisation (again)

Not all particles are stable in liquid Fe (example?)

Production is often difficult – how to introduce particles?

Production strategies

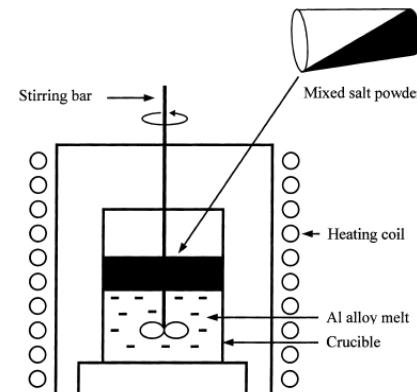
Powder metallurgy

Sintering

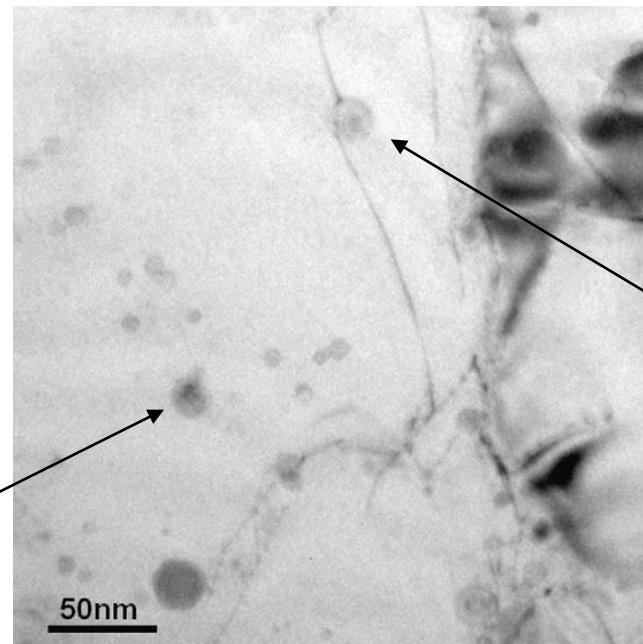
Melt injection

Infiltration

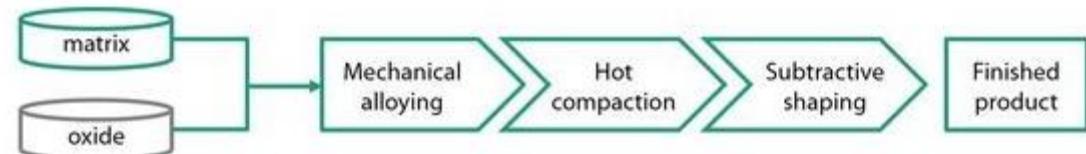
...



Often expensive and difficult to control → **in-situ liquid metallurgy favourable!**

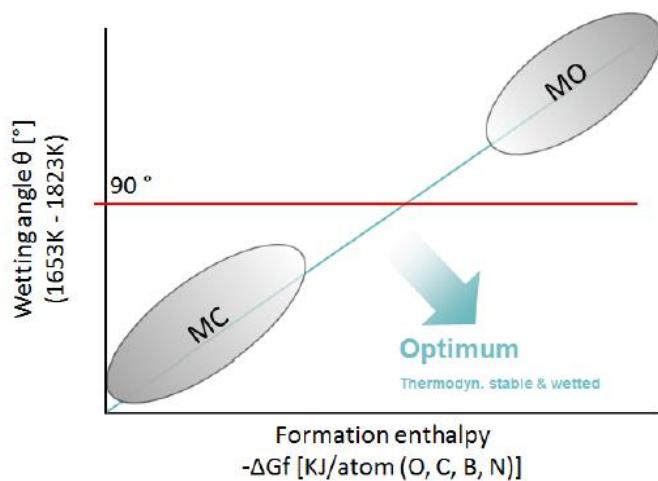


Example ODS steel:
Agglomeration, clustering, decohesion

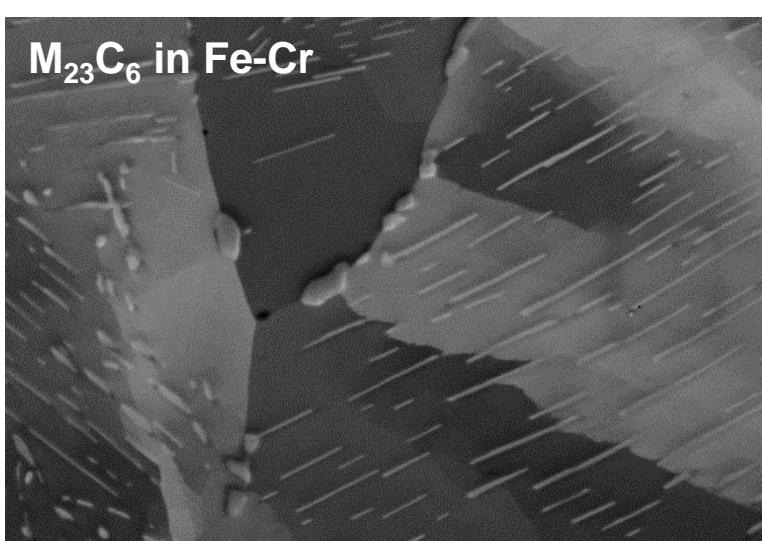
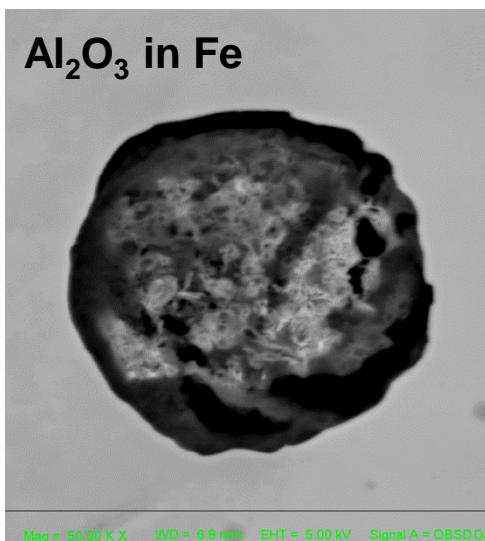
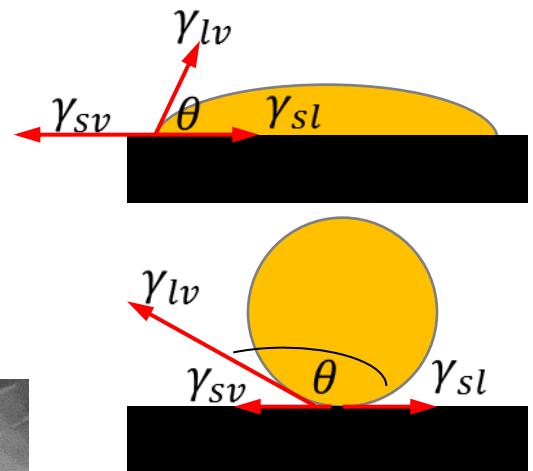


Particle selection

Wetting often controls interfacial properties



$$\cos\theta = \frac{\gamma_{sv} - \gamma_{sl}}{\gamma_{lv}}$$



Model System Fe – TiB₂

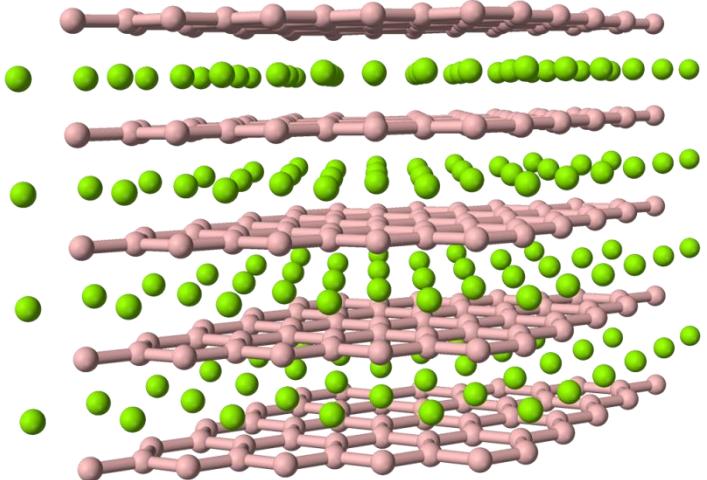
Effective particle

$E = 515 \text{ GPa}$

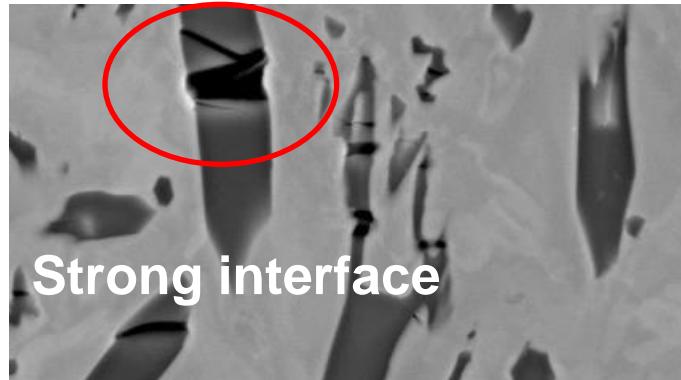
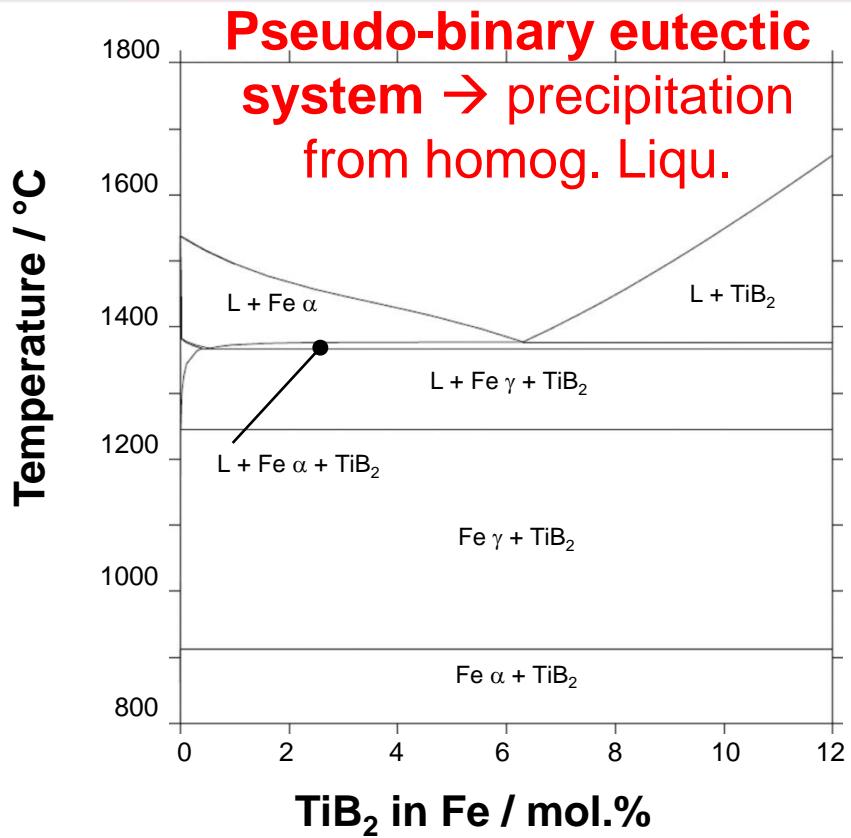
$\rho = 4.52 \text{ g cm}^{-3}$

SG P6/mmm (type MgB₂)

$c/a \sim 1.066$



→ Lecture S. Sandlöbes



Strong interface

Example: drive shaft design

Strength $\sigma_B = \frac{F l y}{J_{xx}} < R_p \text{ 0.2 } \nu$

Deflection $f_b = \frac{F l^3}{3EJ_{xx}}$ $J_{xx} = \frac{\pi r^4}{4}$



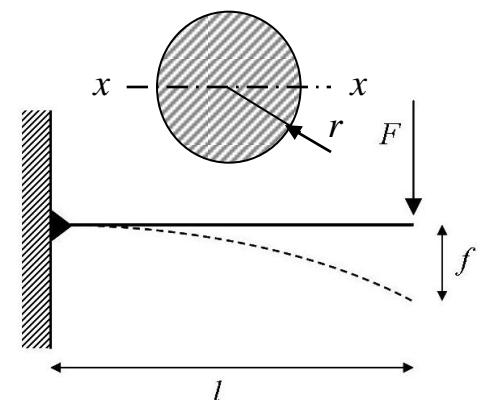
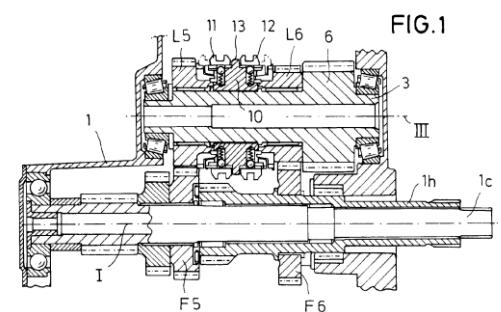
→ Mass of part

$$m = \frac{\rho l \pi r^2}{4}$$

Comparison ($F, f_b, l = \text{constant}$)

Material	E / GPa	$\rho / \text{g cm}^{-3}$	$\Delta \text{Mass} / \%$
42CrMo4	208	7.85	/
30Mn-1.2C-5Al	175	7.14	- 0.84
HMS + 20%TiB2	244	6.96	- 19.89

→ Story over?





Outline

Metal-matrix-composites

Motivation

Basics of MMC's

Challenges – Micromechanics

Alloy design strategies

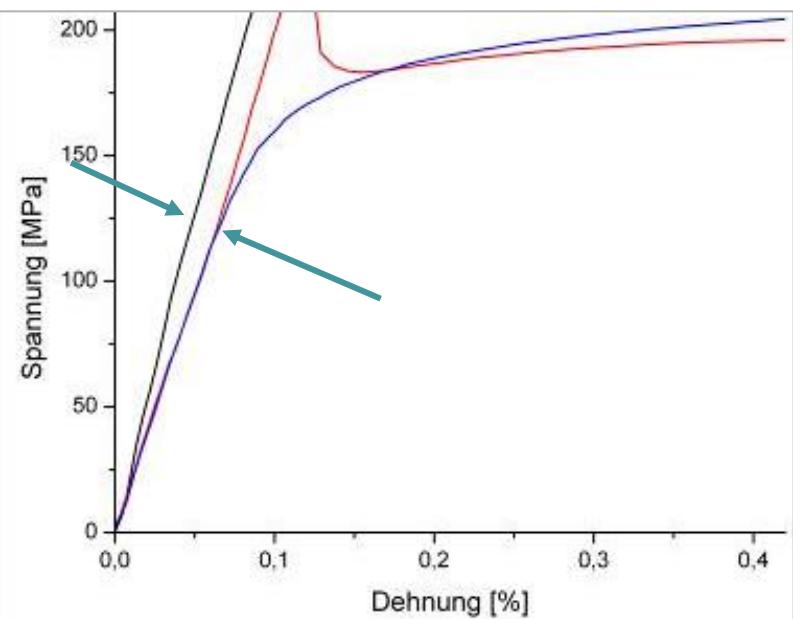
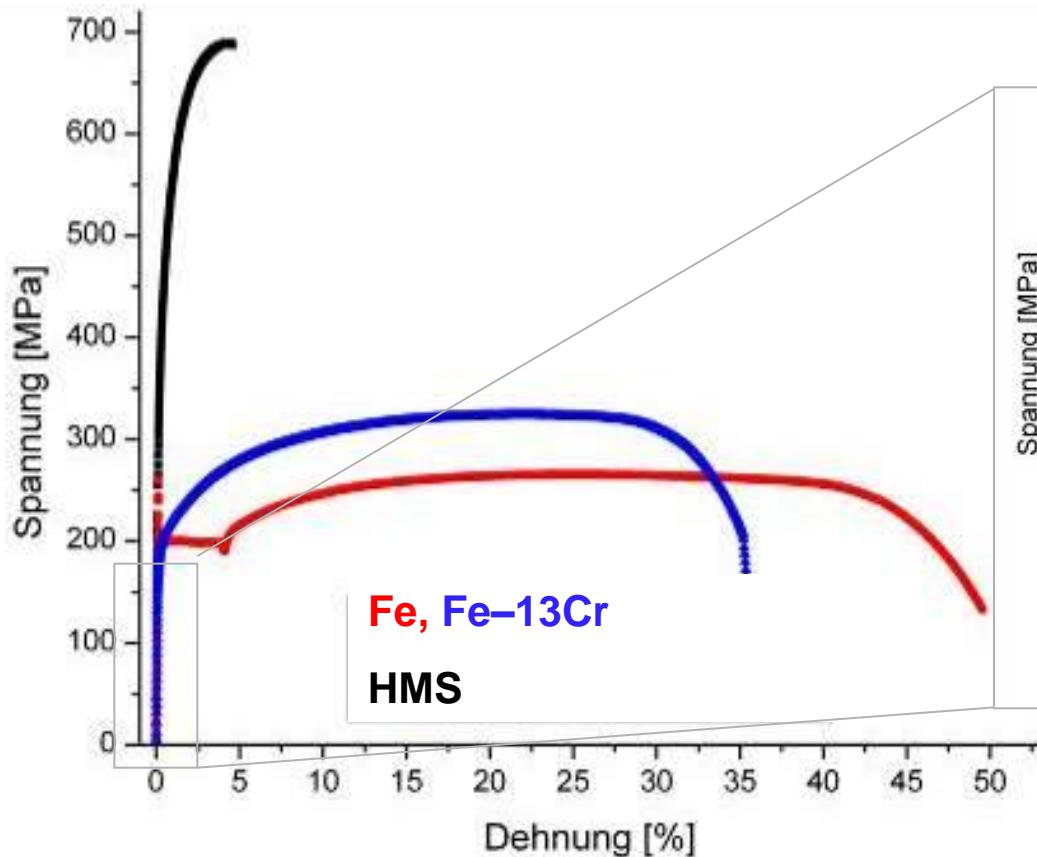
High-throughput mechanical testing

Motivation and challenges

Examples

In-situ fabrication feasible, physical properties achieved

Macro-mechanical behaviour not satisfactory (embrittlement):



→ Micro-mechanical reasons for material performance?

(1) Elastic mechanics – predict particle contribution

$$\begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{(C_{11} - C_{12})}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{(C_{11} - C_{12})}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{(C_{11} - C_{12})}{2} \end{bmatrix}$$

$$C_{11} = \frac{E(1-\nu)}{(1+\nu)(1-2\nu)}$$

$$C_{12} = \frac{E\nu}{(1+\nu)(1-2\nu)}$$

$$\times \begin{pmatrix} e_{11} \\ e_{22} \\ e_{33} \\ \gamma_{23} \\ \gamma_{13} \\ \gamma_{12} \end{pmatrix} - \begin{pmatrix} \alpha\Delta T \\ \alpha\Delta T \\ \alpha\Delta T \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

HOOKEs law
(isotropic) and relations
between properties

	Young's modulus E	Shear modulus G (or μ)	Poisson's ratio ν	Bulk modulus K	Lamé constant λ
E, G	E	G	$\frac{E-2G}{2G}$	$\frac{GE}{9G-3E}$	$\frac{G(E-2G)}{3G-E}$
E, ν	E	$\frac{E}{2(1+\nu)}$	ν	$\frac{E}{3(1-2\nu)}$	$\frac{\nu E}{(1+\nu)(1-2\nu)}$
E, K	E	$\frac{3KE}{9K-E}$	$\frac{3K-E}{6K}$	K	$\frac{K(9K-3E)}{9K-E}$
G, ν	$2G(1+\nu)$	G	ν	$\frac{2G(1+\nu)}{3(1-2\nu)}$	$\frac{2G\nu}{1-2\nu}$
G, K	$\frac{9GK}{3K+G}$	G	$\frac{3K-2G}{2(3K+G)}$	K	$K - \frac{2G}{3}$
G, λ	$\frac{G(3\lambda+2G)}{\lambda+G}$	G	$\frac{\lambda}{2(\lambda+G)}$	$\lambda + \frac{2G}{3}$	λ
ν, K	$3K(1-2\nu)$	$\frac{3K(1-2\nu)}{2(1+\nu)}$	ν	K	$\frac{3K\nu}{1+\nu}$
K, λ	$\frac{9K(K-\lambda)}{3K-\lambda}$	$\frac{3(K-\lambda)}{2}$	$\frac{\lambda}{3K-\lambda}$	K	λ

(1) *Elastic mechanics – predict particle contribution*

Different assumptions and models developed (volume changes, interfacial properties, geometry of reinforcement ...)

→ Good agreement for disc. reinf. by **Halpin–Tsai (Hashin) Equation:**

for discontinuous reinforcement in the Halpin–Tsai equation¹⁰¹

$$E_c = \frac{E_m(1 + 2sqV_p)}{1 - qV_p} \quad \dots \dots \dots \dots \dots \dots \dots \quad (17)$$

where

$$q = \frac{(E_p/E_m - 1)}{(E_p/E_m) + 2s} \quad \dots \dots \dots \dots \dots \dots \dots \quad (18)$$

and s is the particle aspect ratio. As seen from

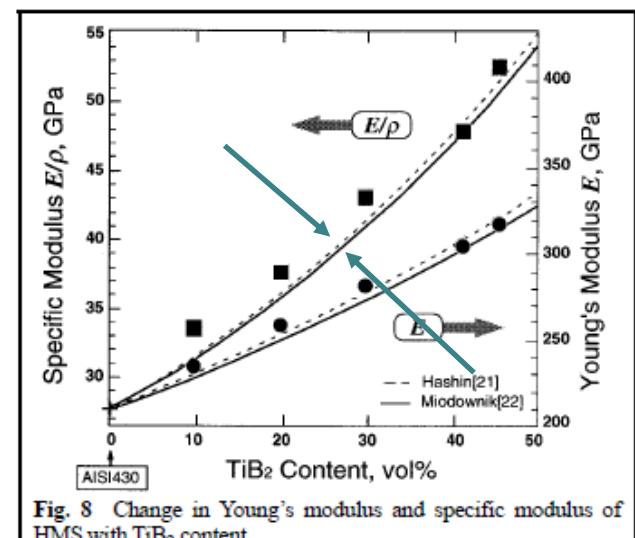
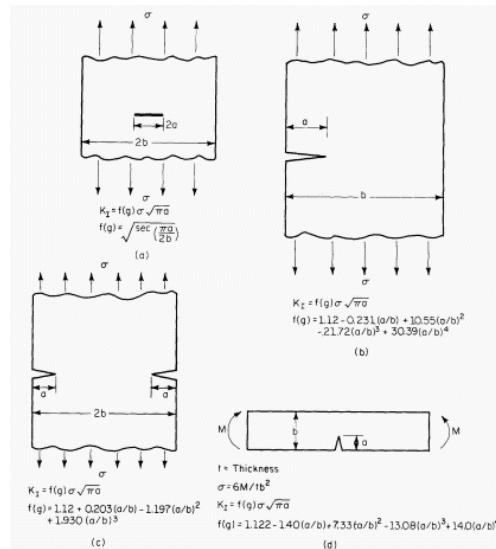
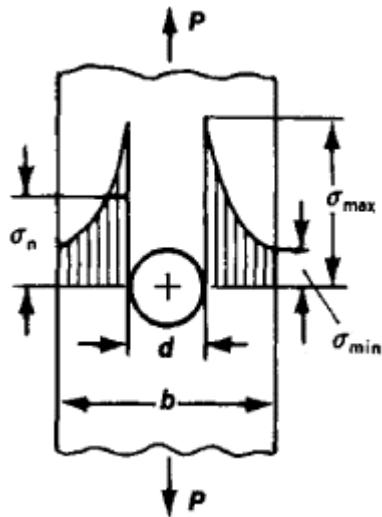


Fig. 8 Change in Young's modulus and specific modulus of HMS with TiB₂ content

Particles should be spherical → plastic behaviour!

About 20 vol.% of TiB₂ neccessary for 240 GPa

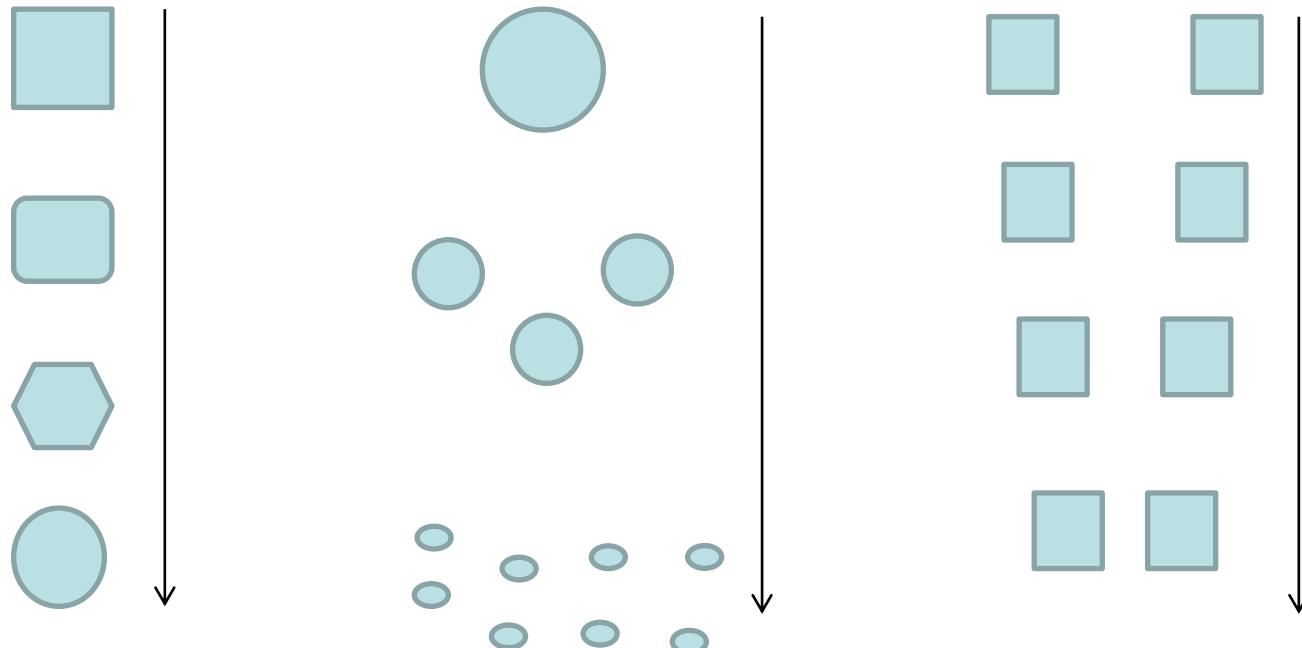
(2) „Plastic“ mechanics – damage



Particles represent stress/strain-concentrators: at interface and sharp edges (fracture mechanics) → spherical ideal (?)

→ Lectures P. Shanraj, C. Tasan

(2) Damage: initiation and propagation

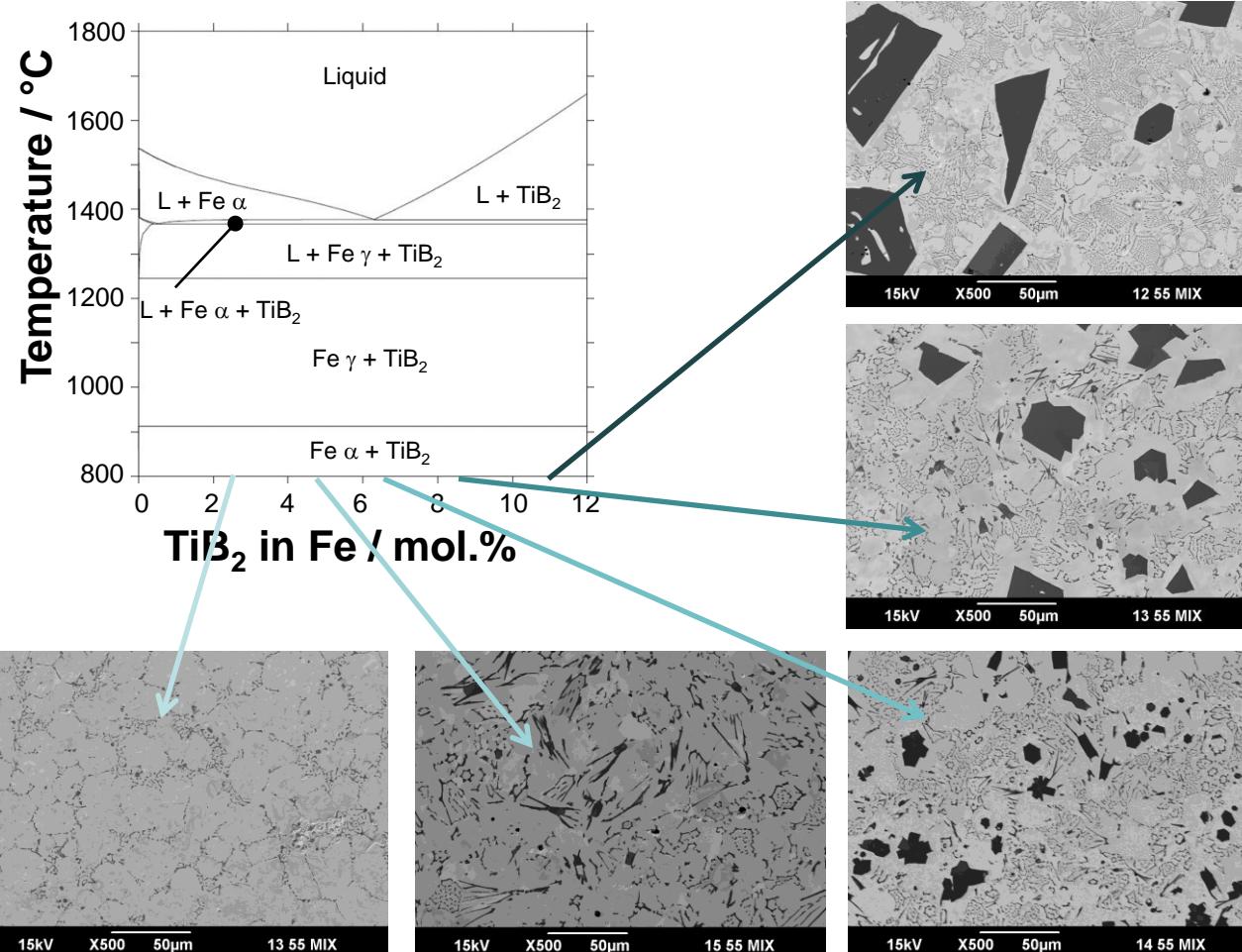


Complex scenario!

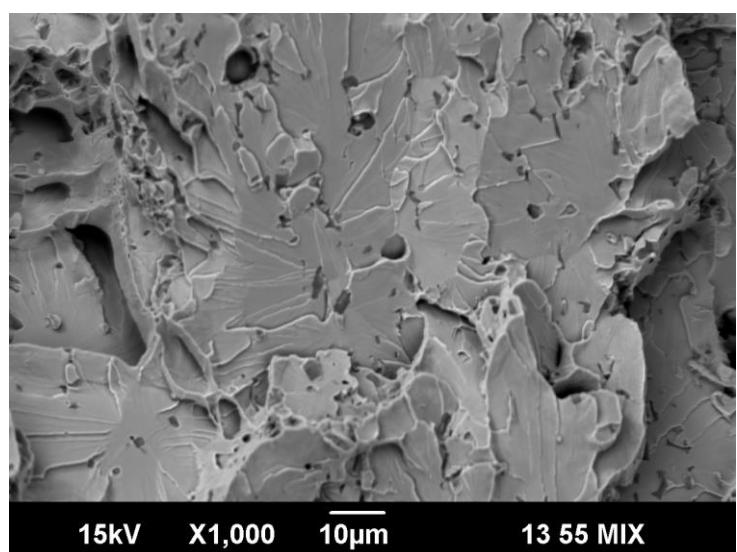
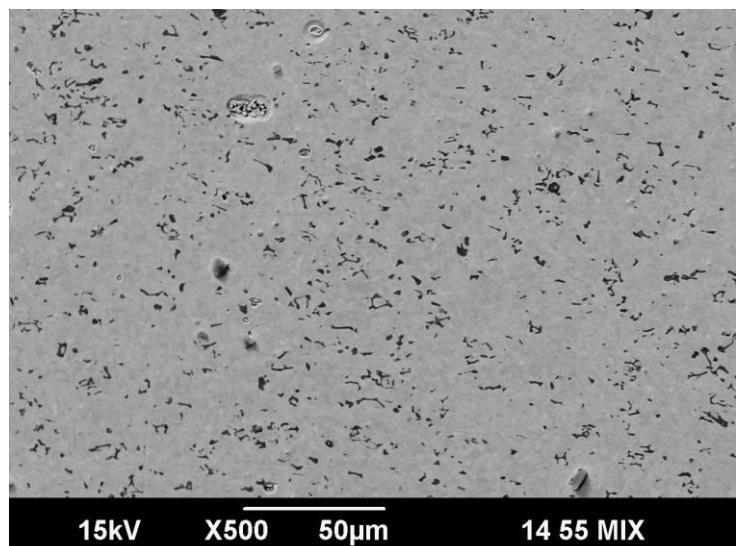
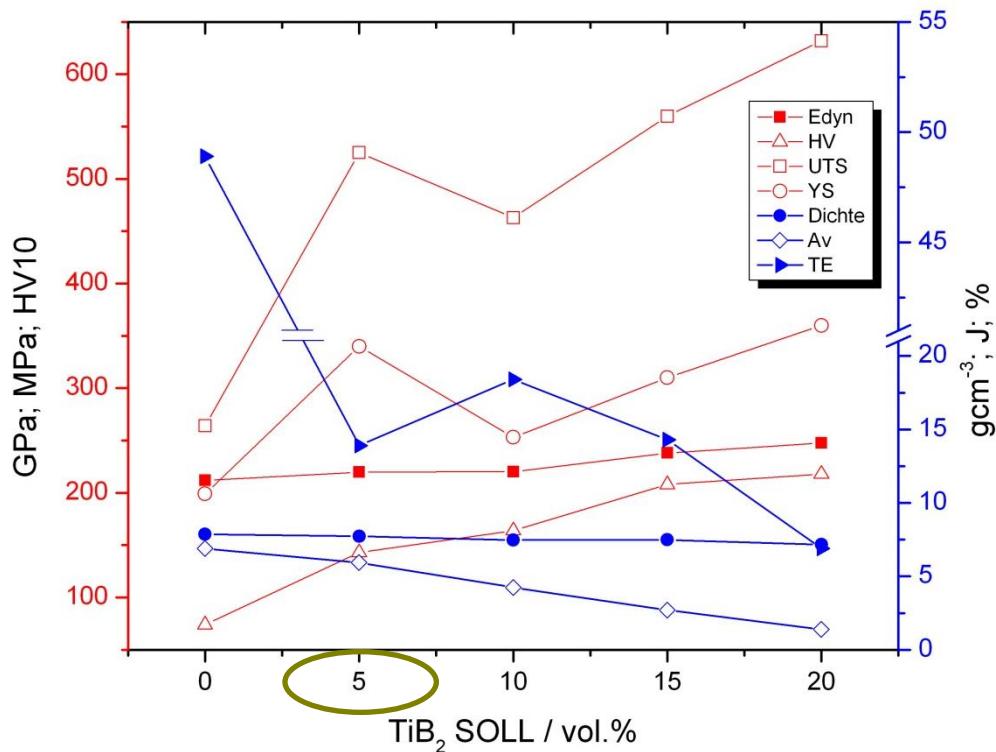
Behaviour depending on size, shape, relative crystallographic orientations, properties of *both* phases, dispersion, ... → modelling?

Example Fe – TiB₂

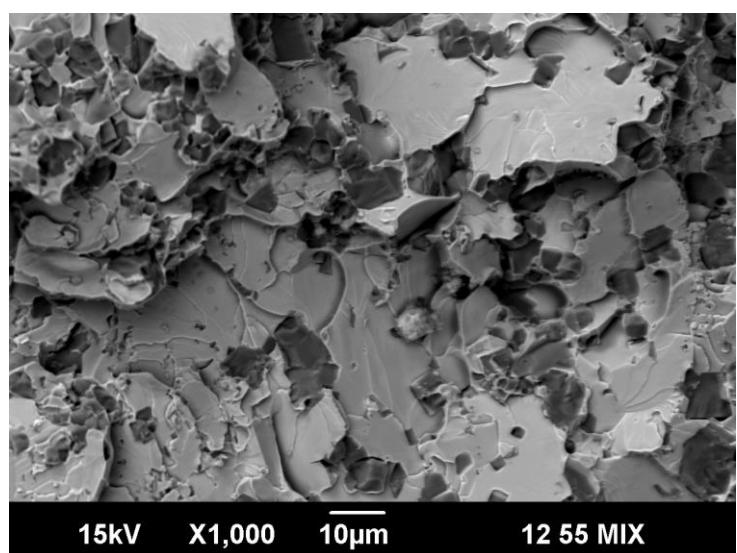
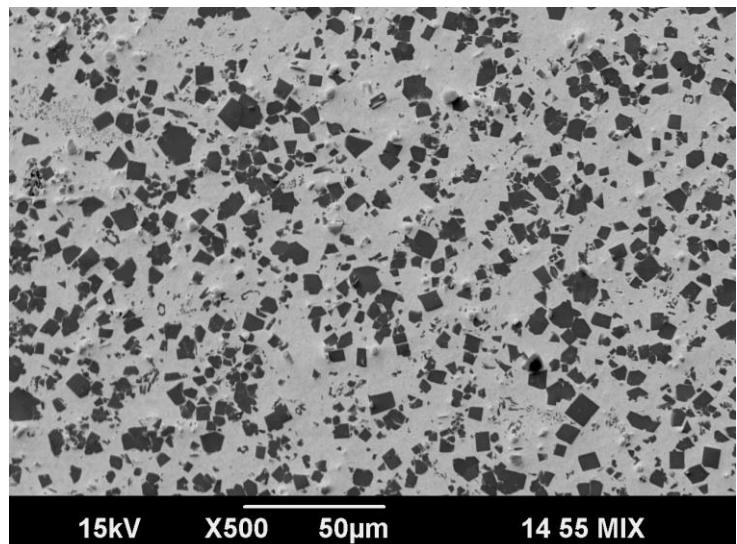
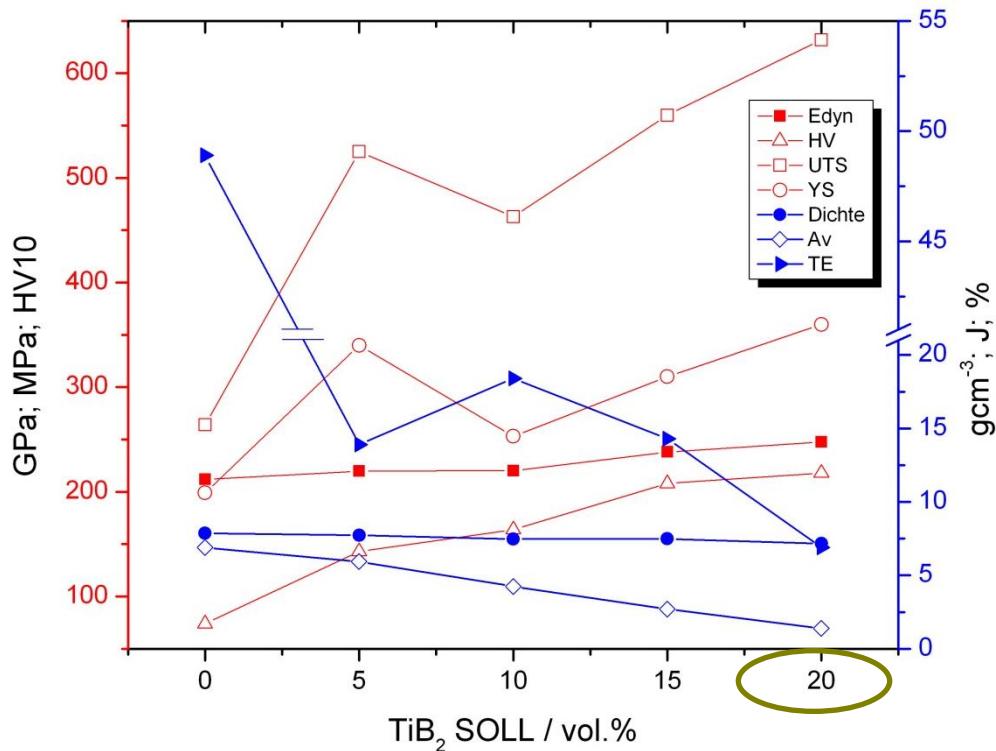
Increasing fraction leads to large (primary) particles with detrimental morphology



Improving physical properties deteriorates mechanical behaviour

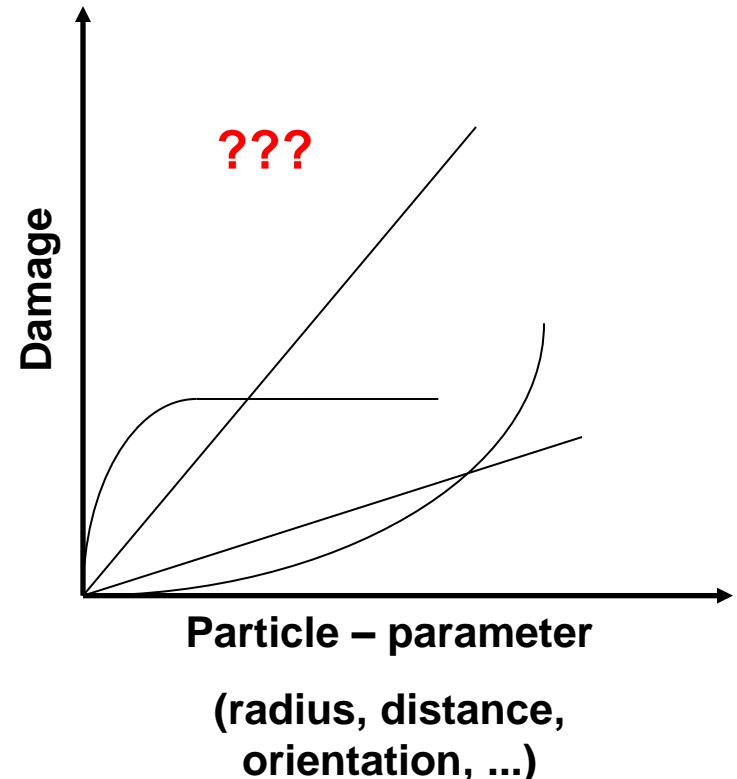
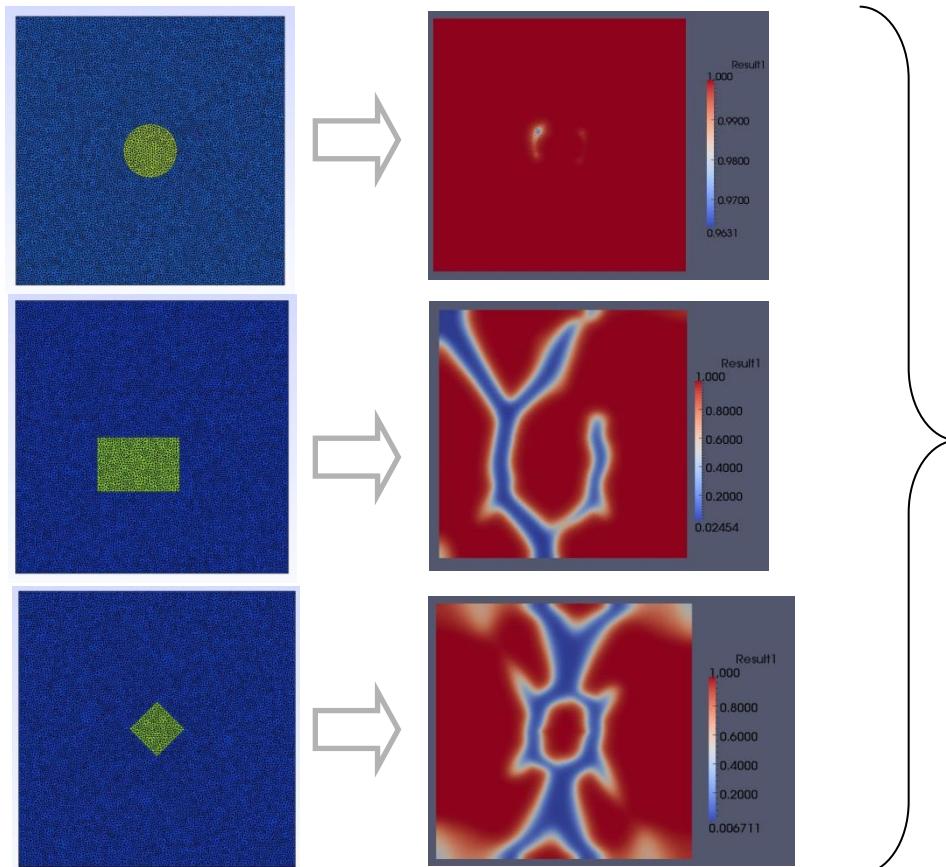


Improving physical properties deteriorates mechanical behaviour



What do do?

Modelling: get insight into crack initiation and propagation as a function of particle shape, dispersion and location, matrix properties



→ Knowledge-based guidelines for alloy/microstructure design

What to do?

Known boundary conditions for alloy design:

20 vol.% TiB₂ needed → hyper-eutectic alloy

Particles should be spherical (max. E , min. stress-concentration)

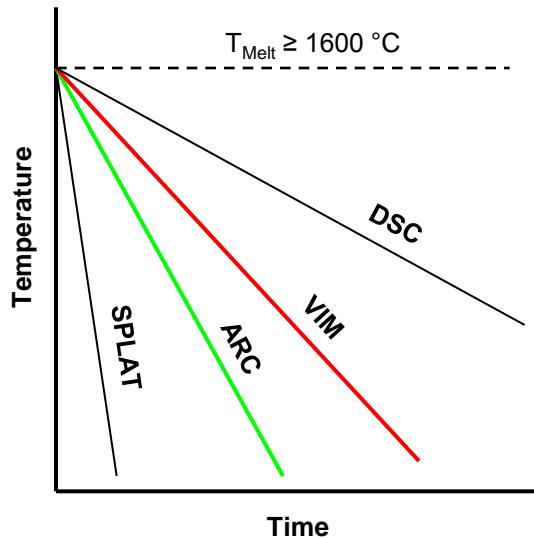
Particles should be small (strengthening) → size?

How to achieve this?

-
-
-
-

Example: solidification rate

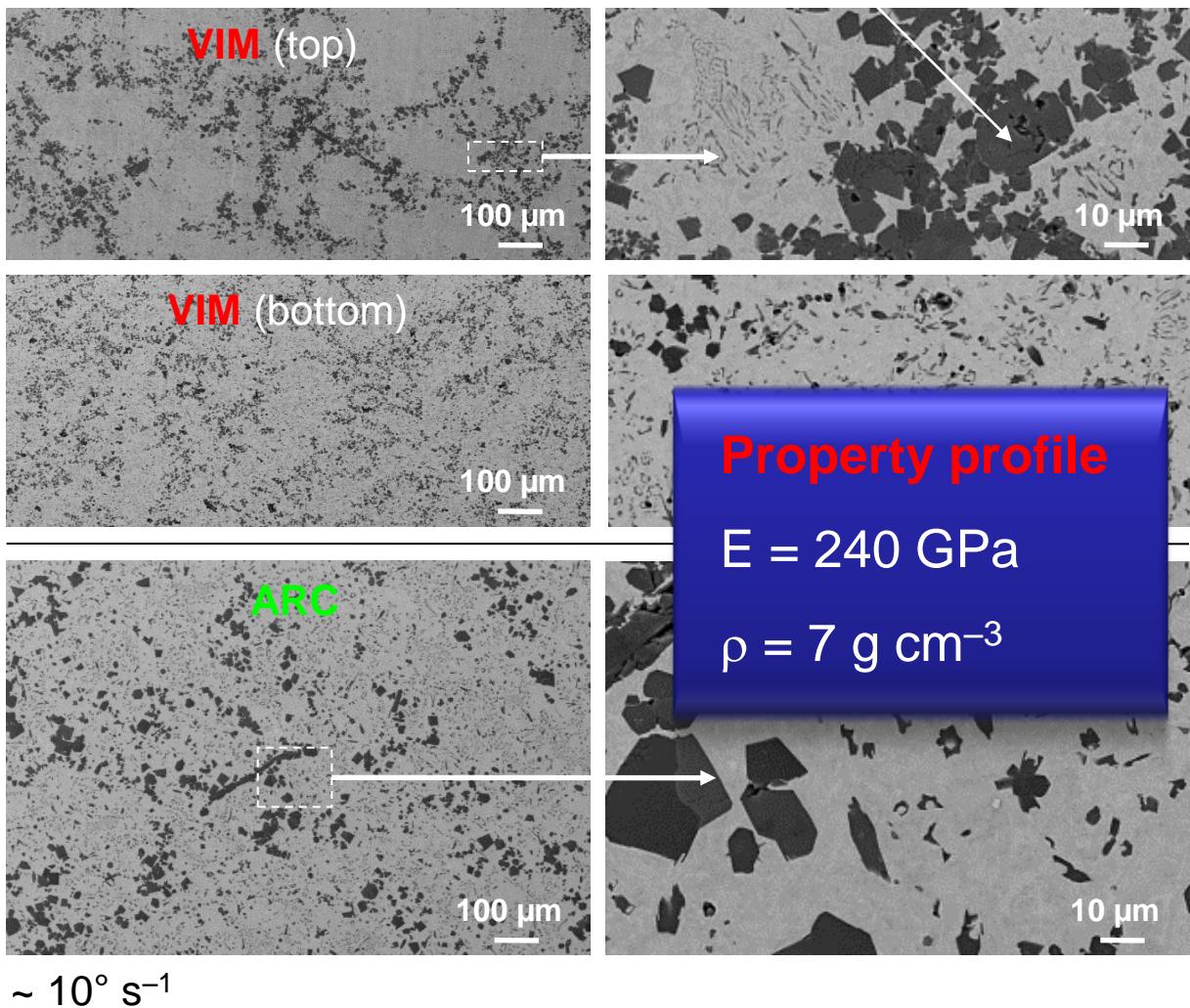
Hyper-eutectic Fe – Ti – B melt



**„industrial“
solidification
unfavourable**

floatation,
agglomeration

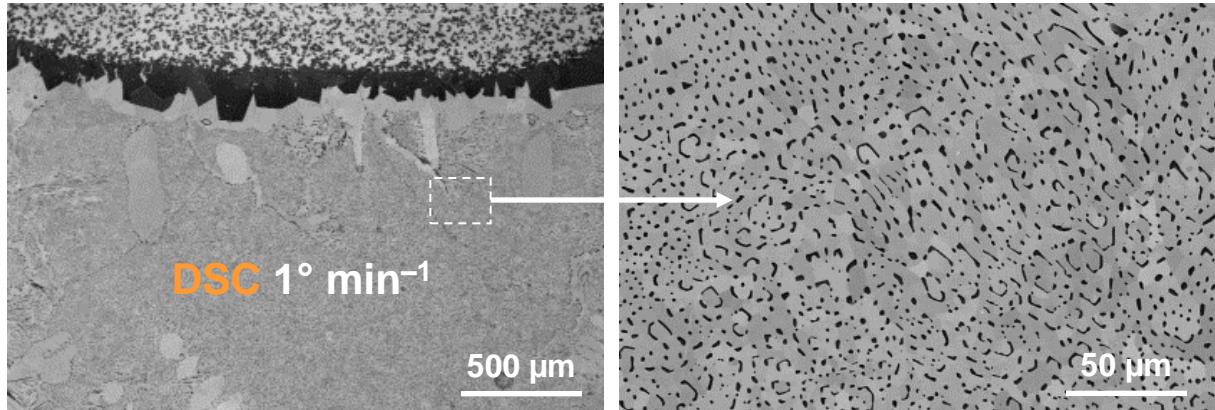
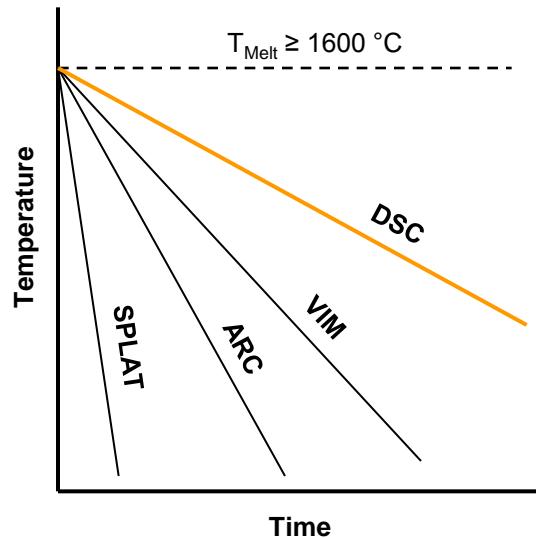
→ Embrittlement



$\sim 10^{\circ} \text{ s}^{-1}$

Example: solidification rate

Slow solidification close to equilibrium



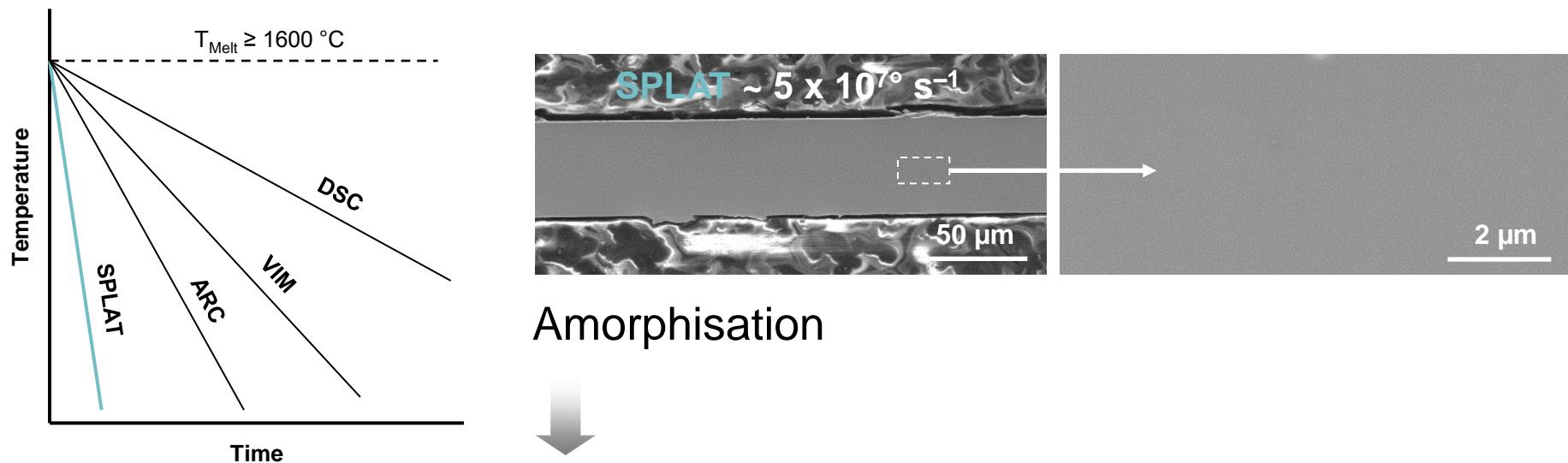
Separation of solidification products (primary, eutectic)

Homogenous areas fine grained **one order of magnitude** → ductile

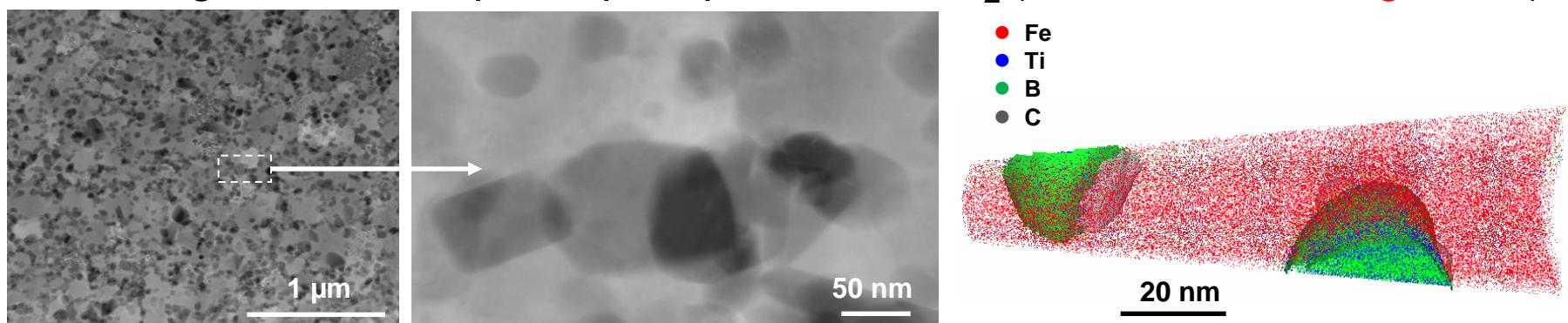
Primary layer for wear resistance

Example: solidification rate

Rapid solidification + reheating

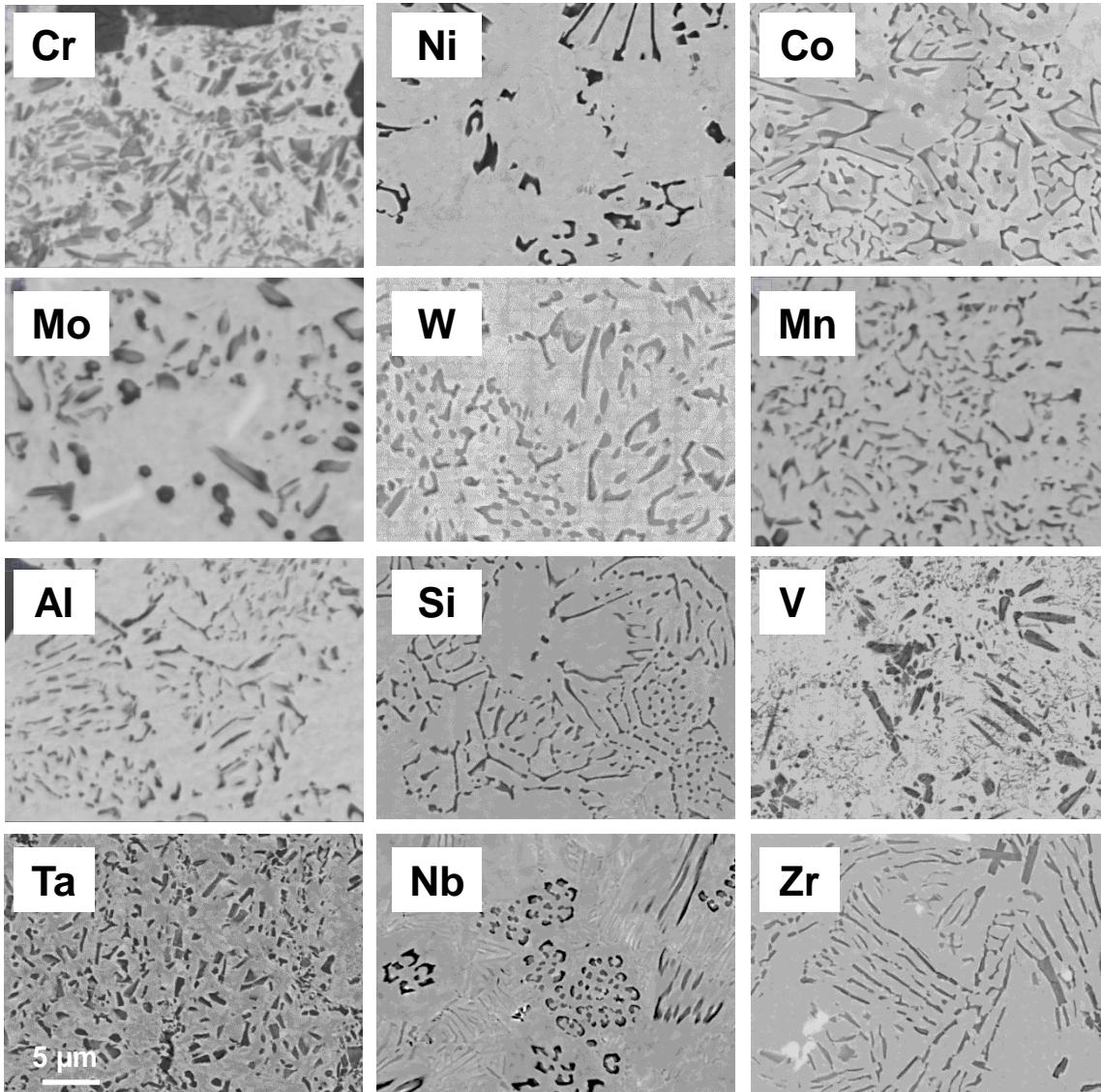


Annealing for nano-disperse precipitation of TiB_2 (100 orders of magnitude)



Example: alloying

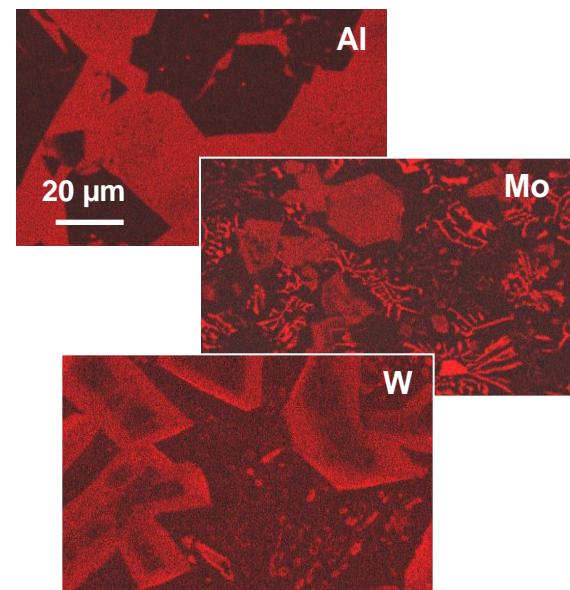
Hyper-eutectic Fe – Ti – B melt + 5 wt.% x



Strong change in morphology

reasons?

changed properties?



Superpositioning?



Outline

Metal-matrix-composites

Motivation

Basics of MMC's

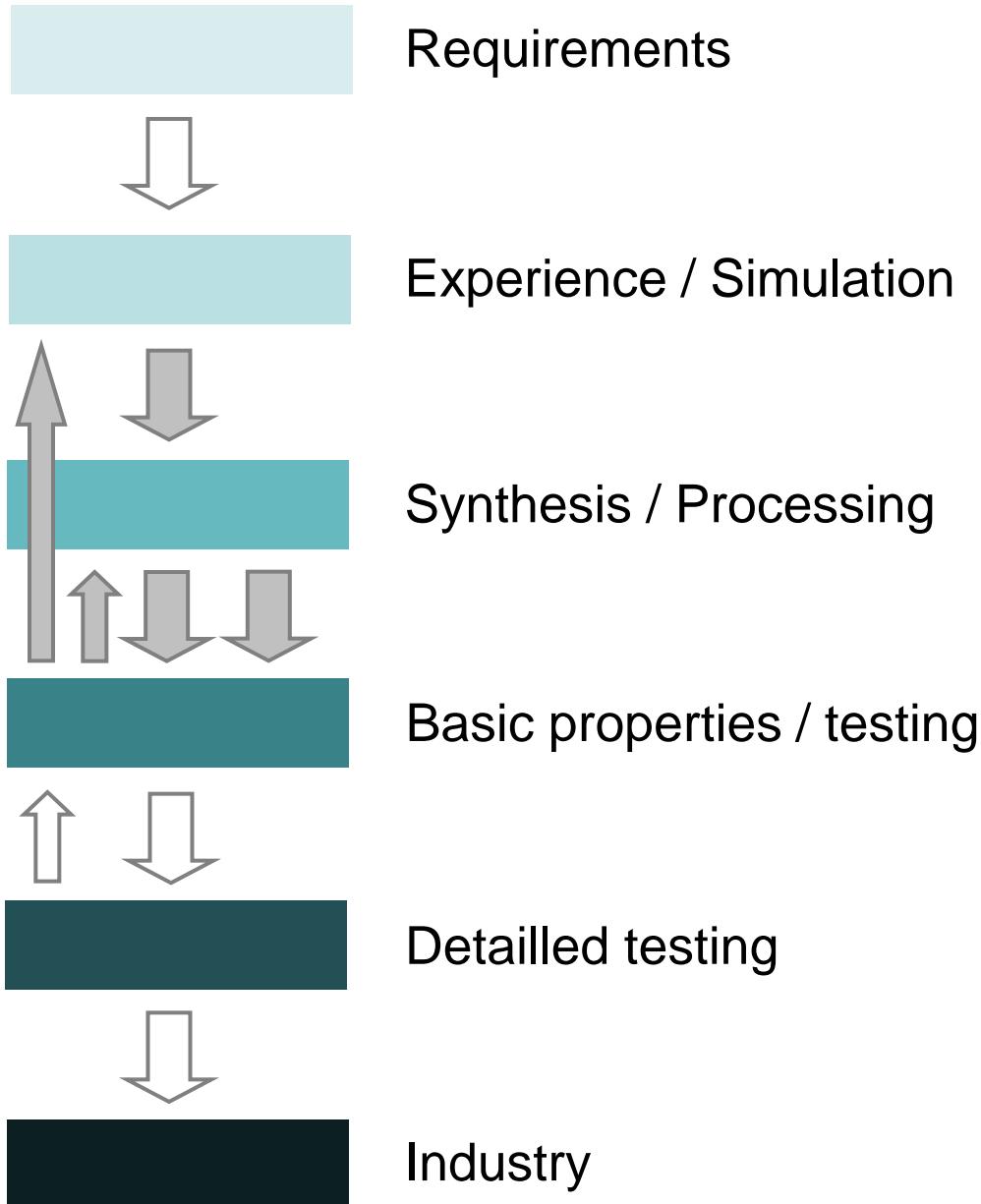
Challenges – Micromechanics

Alloy design strategies

High-throughput mechanical testing

Motivation and challenges

Examples

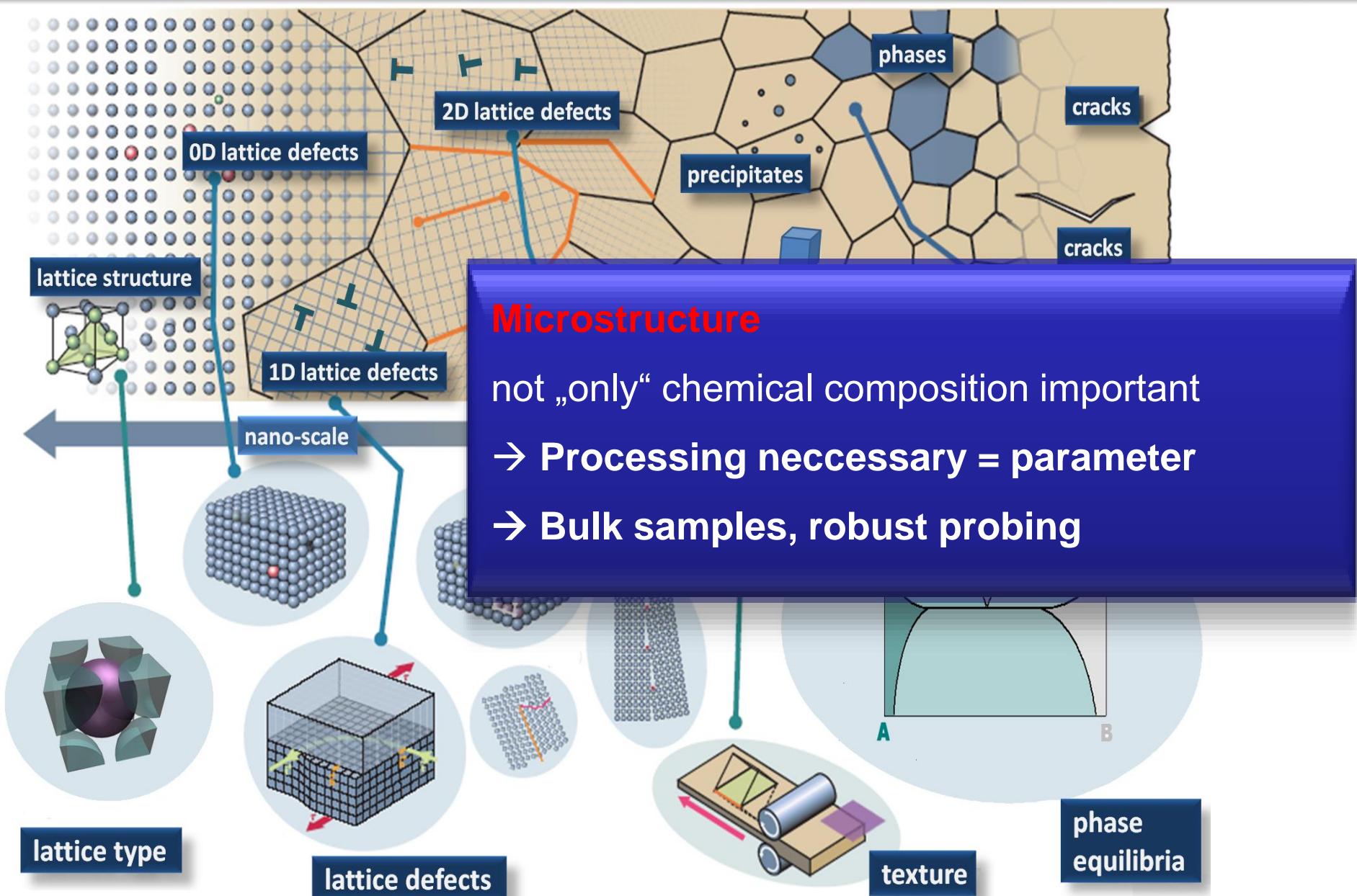


Iterations = Bottleneck



→ Acceleration through
combinatorics

Challenge → structural materials



Requirements



Experience / Simulation



Rapid Alloy Prototyping

Synthesis

Processing

Basic testing



Upscaling

Detailed testing



Industry

High throughput screening

Identify trends

Verify simulations

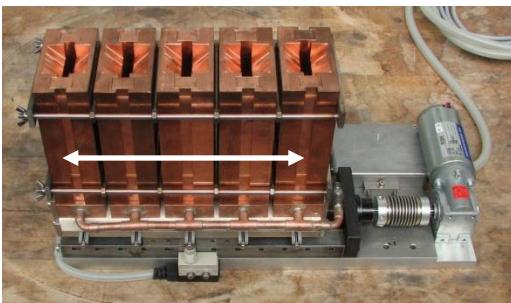
Study transients

How to test? → Properties depend on testing conditions!

Hardness indicates „strength potential“ (slow, compression), tensile and toughness (velocity!) more severe

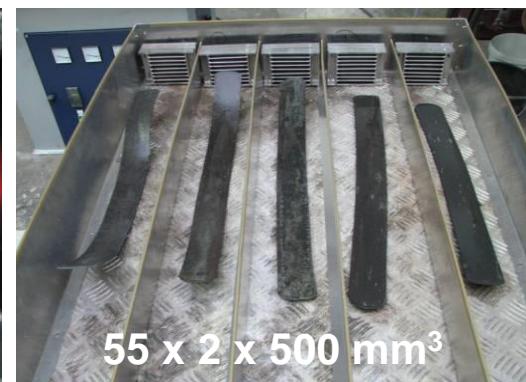
1. Multiple casting VIM

5 alloys



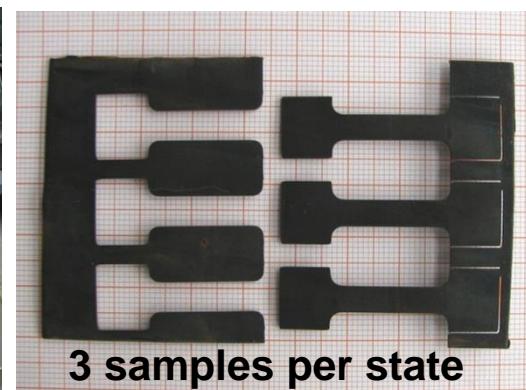
2. Hot rolling, cutting

10 segments / alloy



3. (heat) treatment

50 combinations (Matrix)



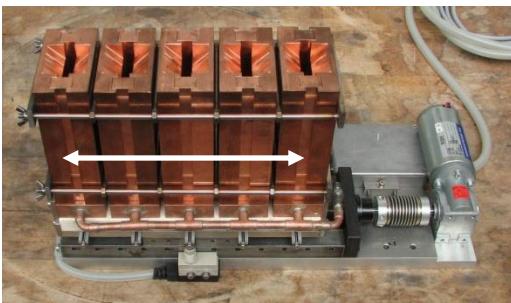
4. Sample preparation

5. Tensile tests

150 samples → Data management

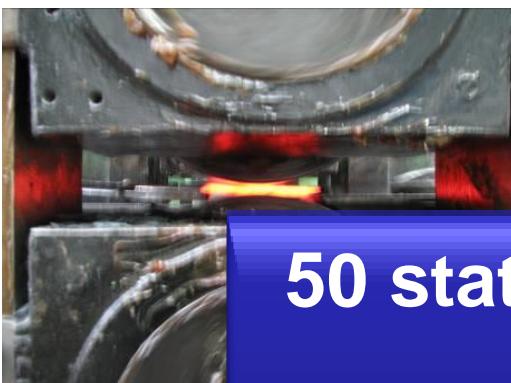
1. Multiple casting VIM

5 alloys



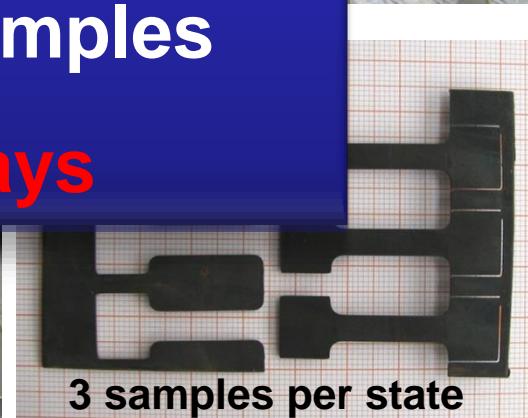
2. Hot rolling, cutting

10 segments / alloy



3. (heat) treatment

50 combinations (Matrix)



4. Sample preparation

50 states

150 samples

→ 5 days

5. Tensile tests

150 samples → Data management

3 samples per state

Program Triplex – lightweight steels



Compositions [wt.%]

Fe – 20Mn – 0.4C – 0...11Al

Fe – 20Mn – 0.8C – 0...11Al

Fe – 20Mn – 1.2C – 0...11Al

Fe – 25Mn – 0.4C – 0...11Al

Fe – 25Mn – 0.8C – 0...11Al

Fe – 25Mn – 1.2C – 0...11Al

Fe – 30Mn – 0.4C – 0...11Al

Fe – 30Mn – 0.8C – 0...11Al

Fe – 30Mn – 1.2C – 0...11Al

45 alloys

360 states

1080 tensile tests & hardness indents, 315 XRD measurements

Evaluation criteria?

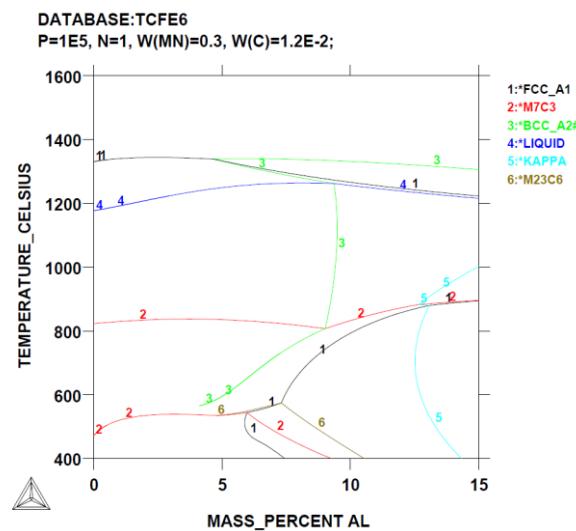
Treatments

aging variations (T & t)

cold rolling

cryogenic treatment

warm deformation



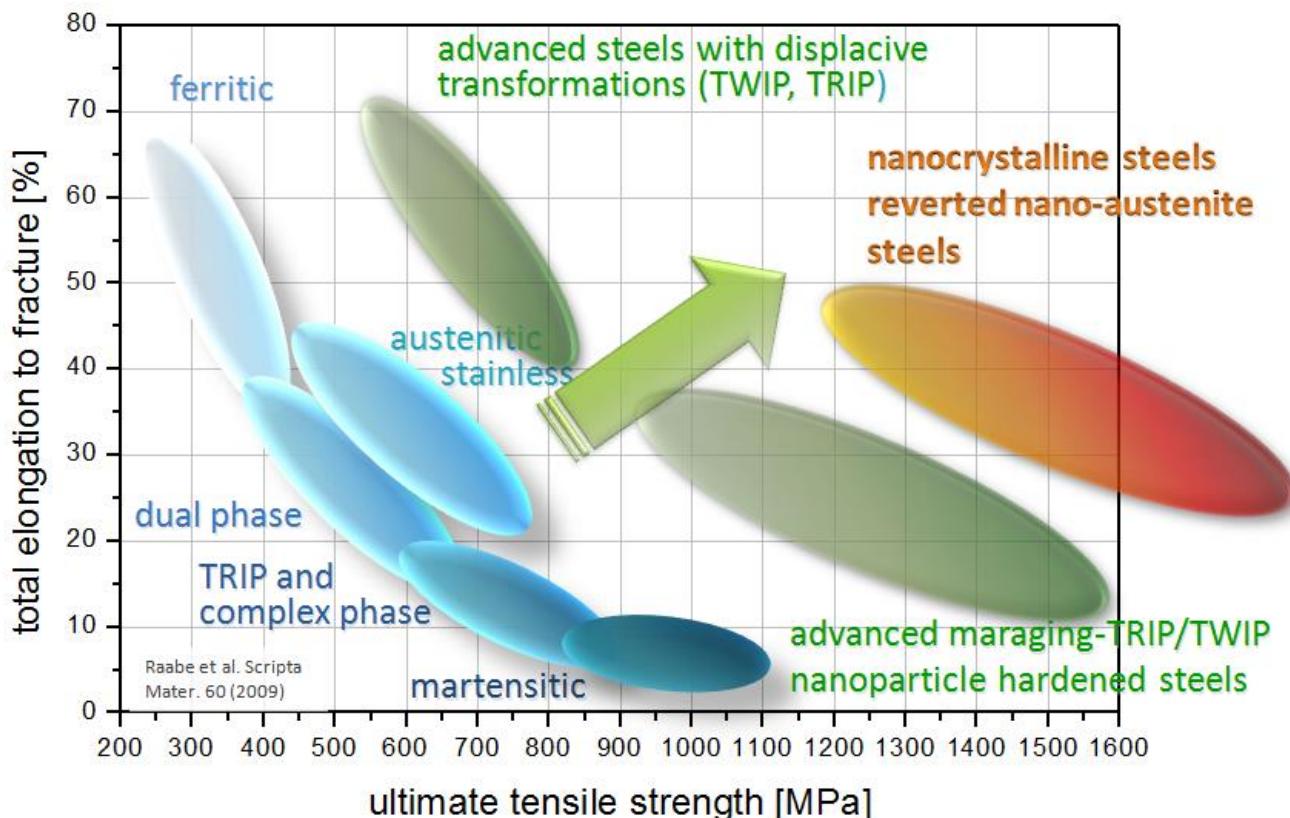
Program Triplex

Austenite stability / SFE

κ -carbide precipitation

Embrittling phases (ε , α' , M_7C_3 ...)

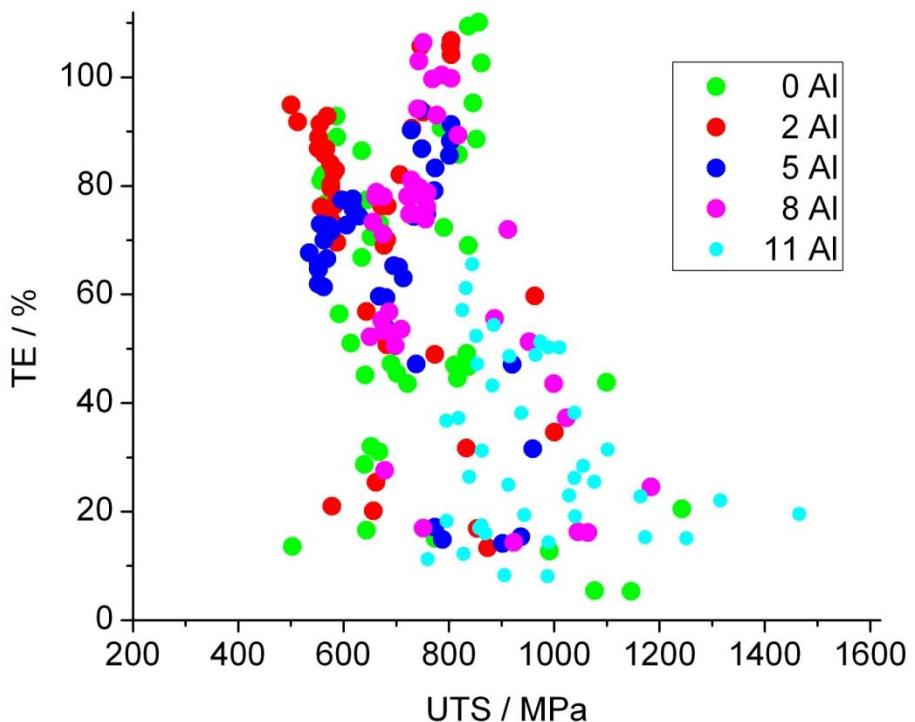
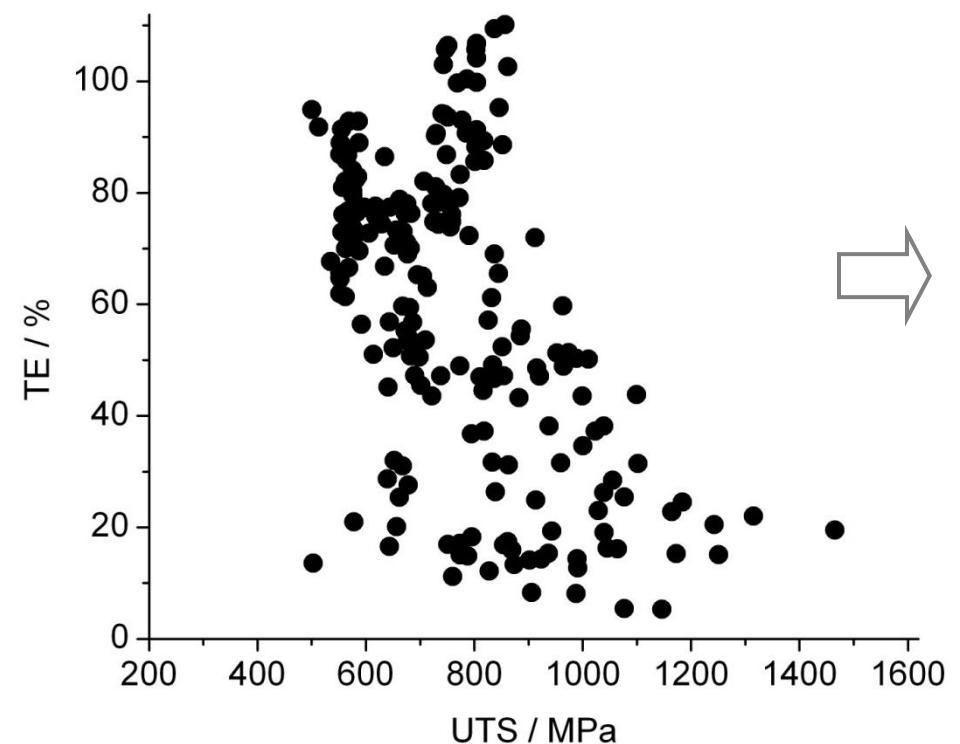
→ New alloys?



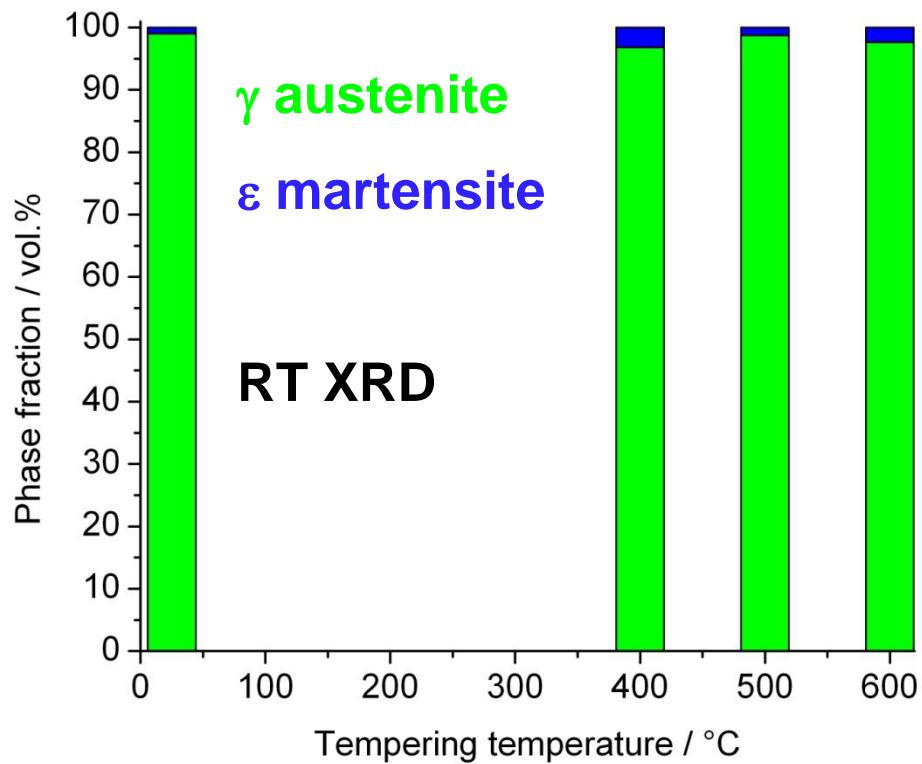
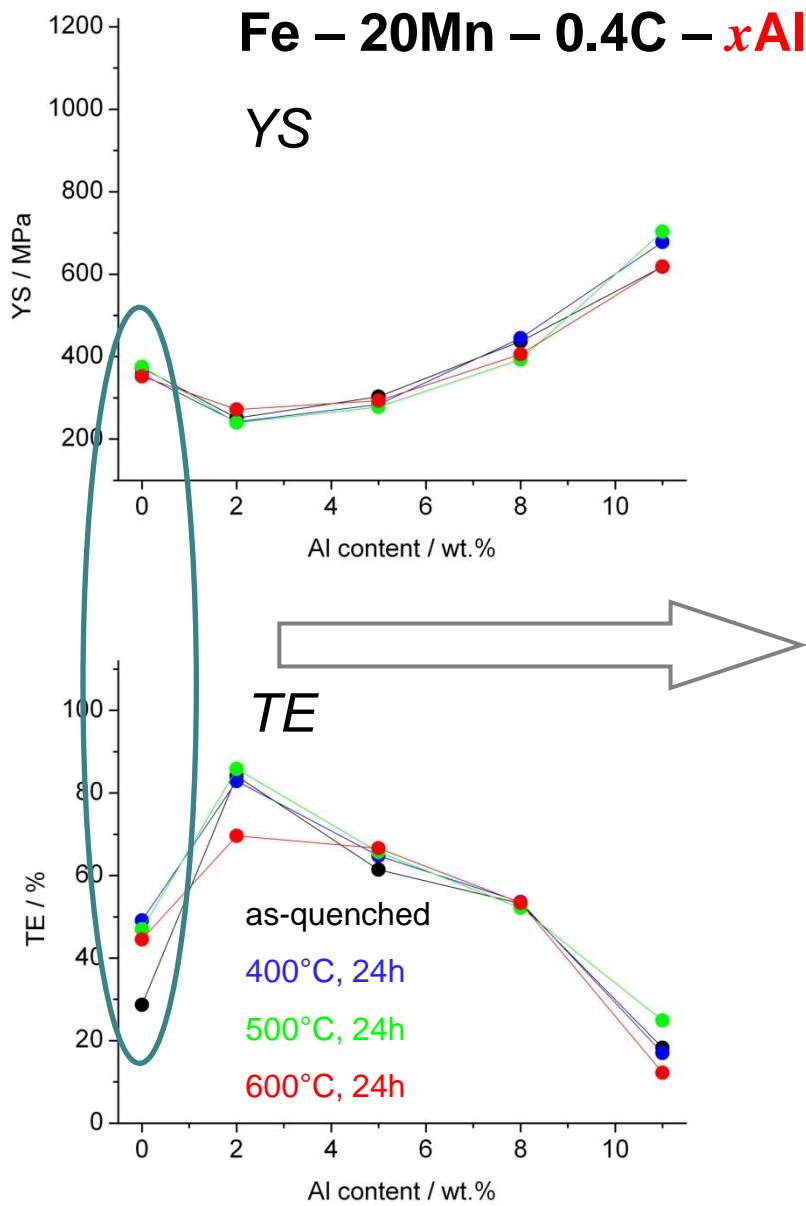
Results – overview

Material library

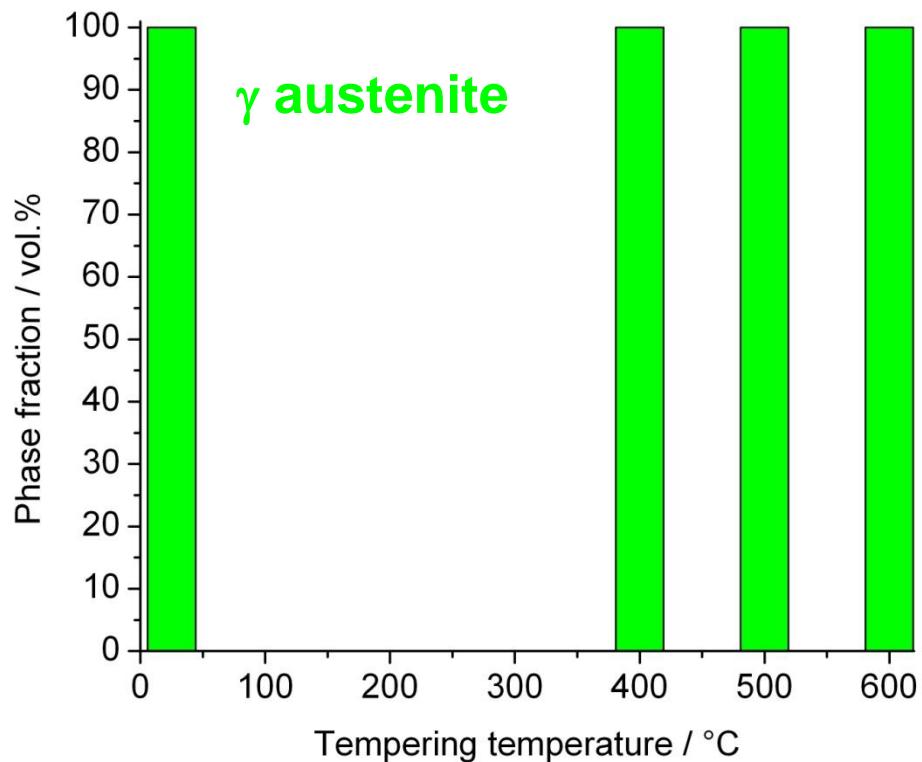
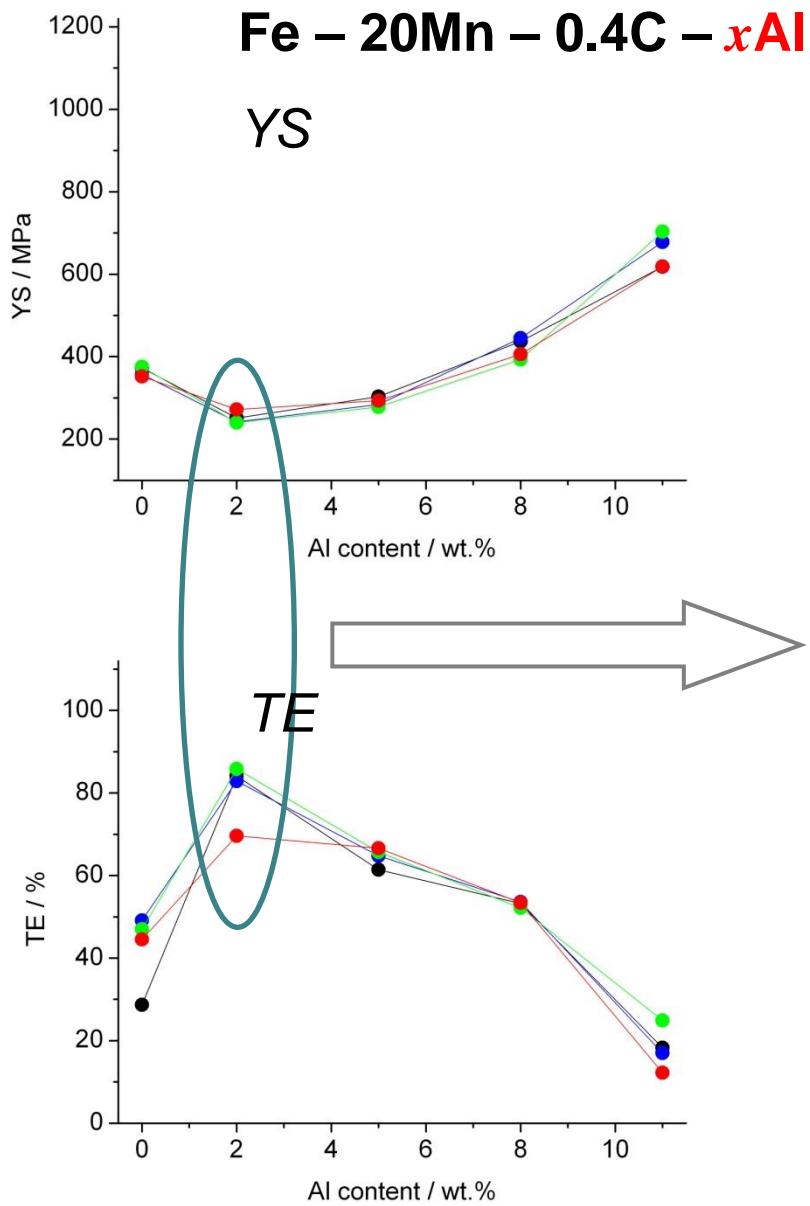
- recognize trends
- targeted alloy maturation



Link mechanical properties & constitution



Link mechanical properties & constitution

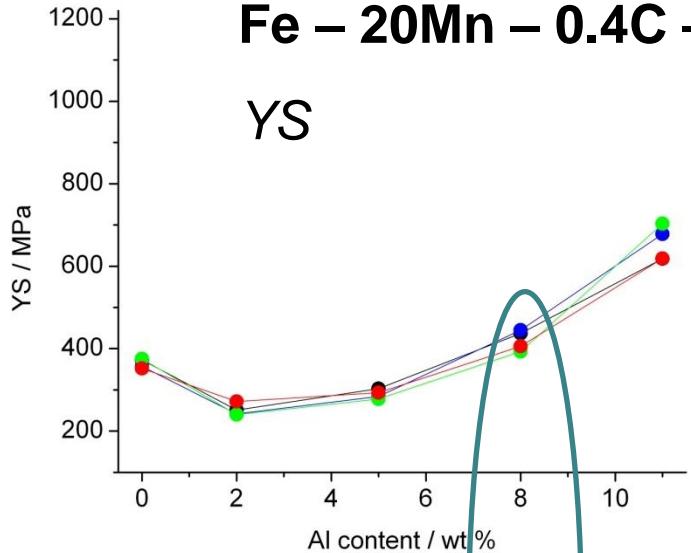


Link mechanical properties & constitution

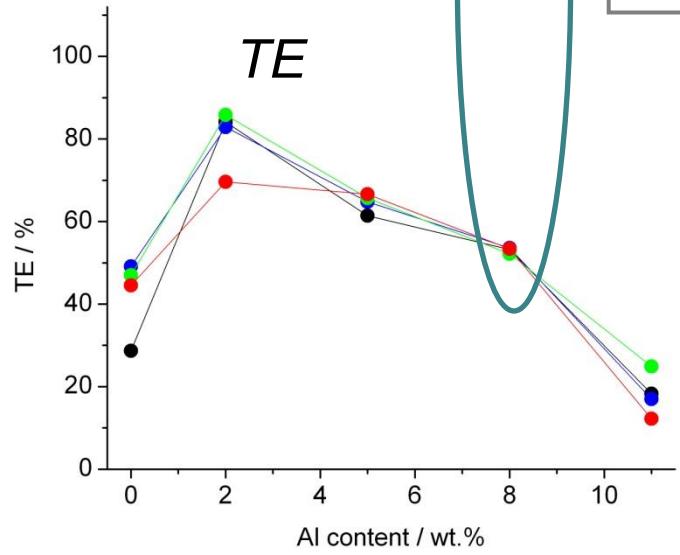


Fe – 20Mn – 0.4C – x Al

YS



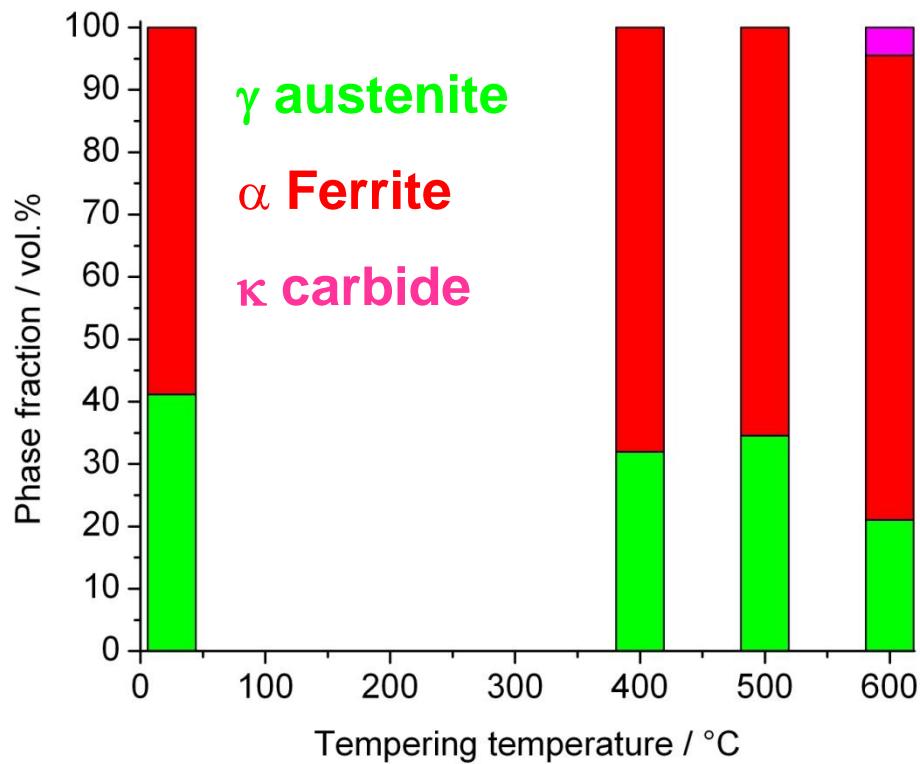
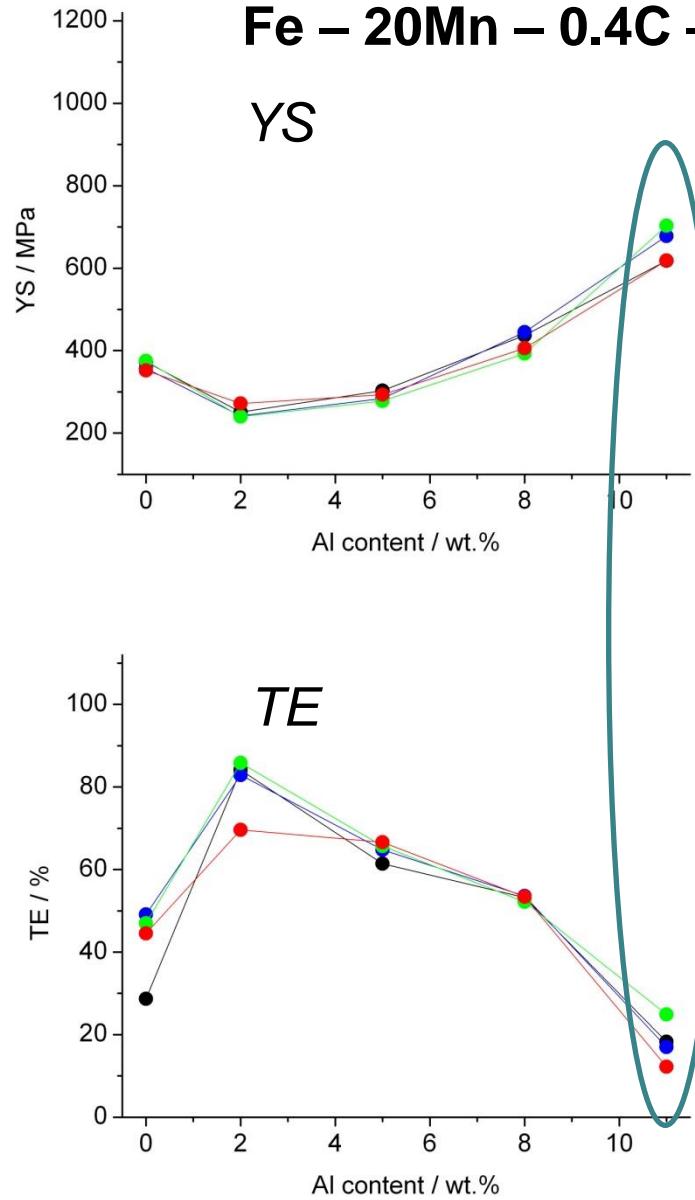
TE

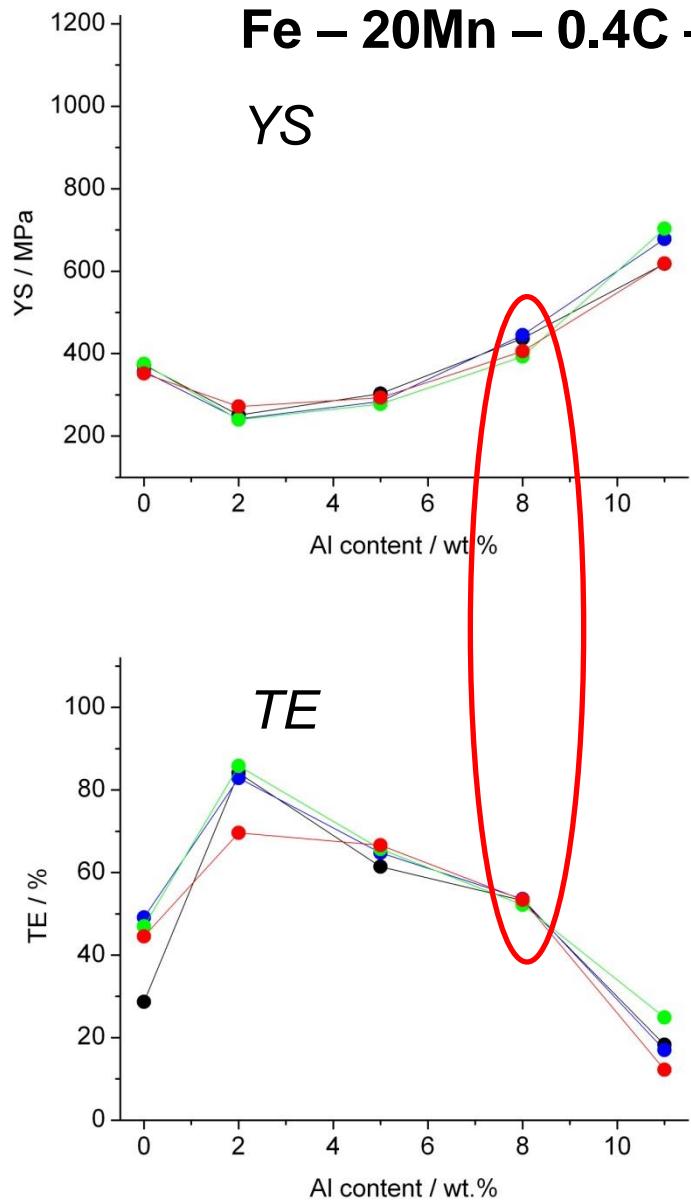


Link mechanical properties & constitution



Fe – 20Mn – 0.4C – x Al



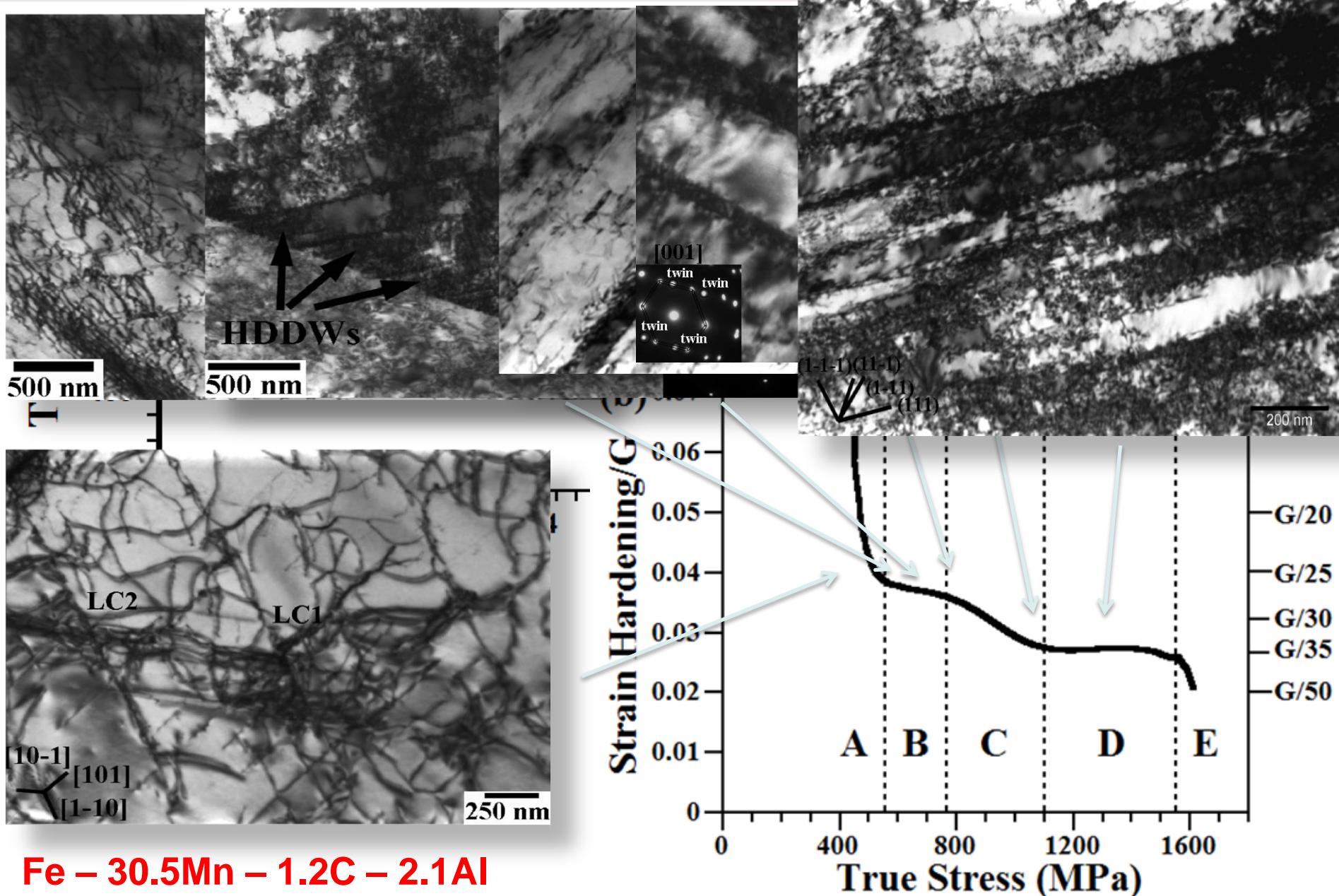


Embrittlement

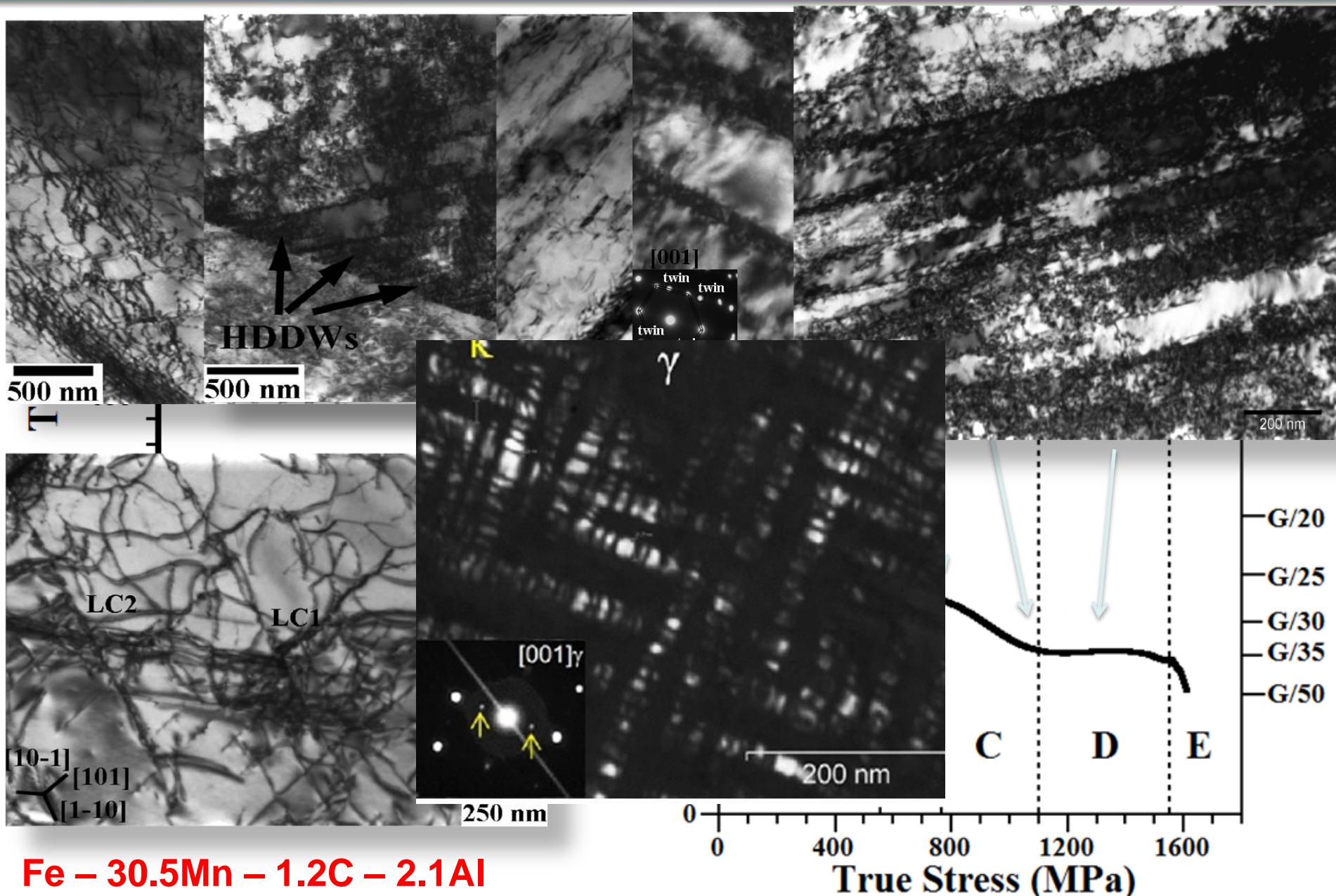
ε @ low Al, κ (+ α) @ high Al

→ 8 Al good balance of density, strength & ductility

Upscaling → detailed characterisation



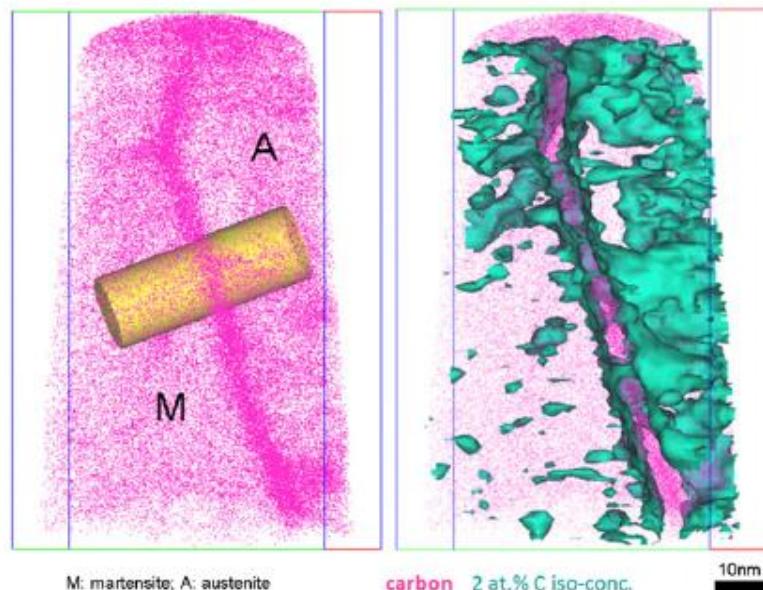
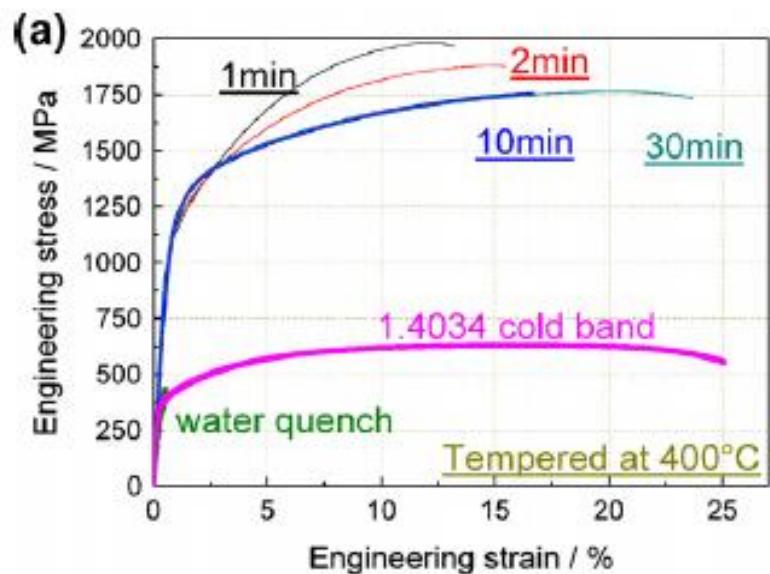
Upscaling → Details



Example – Lean & ductile martensitic steels



Optimum mechanical properties via nano-scaled austenite reversion

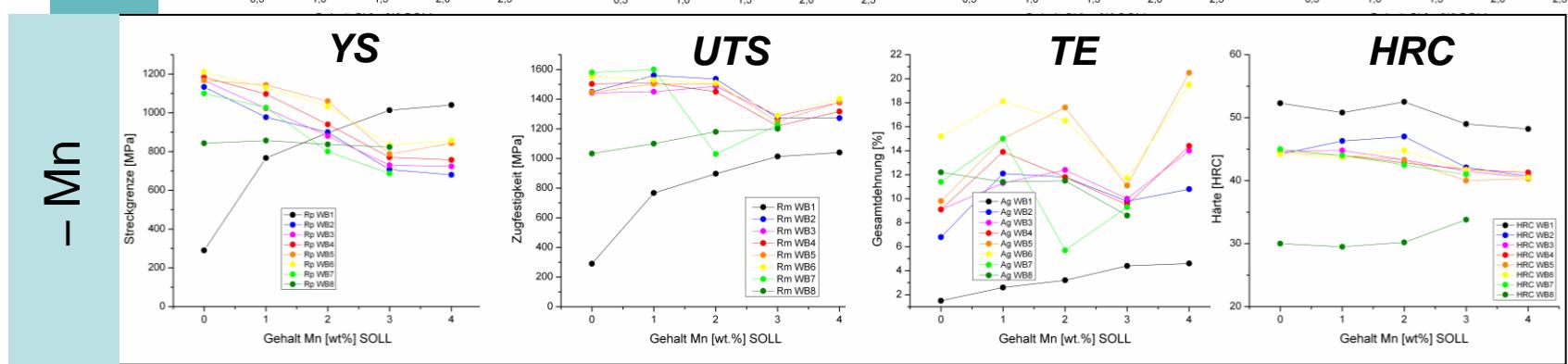
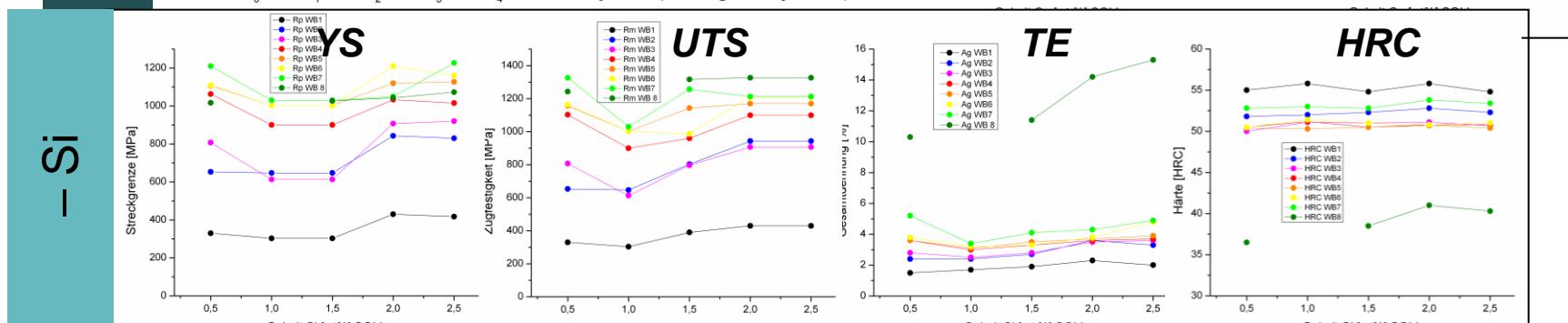
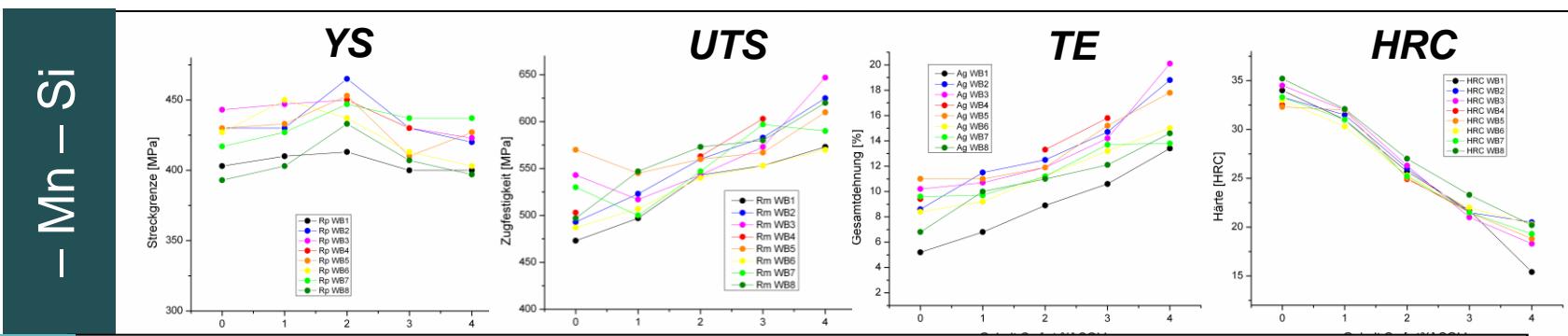


Steel 1.4034

influence of alloying elements?

Create material libraries

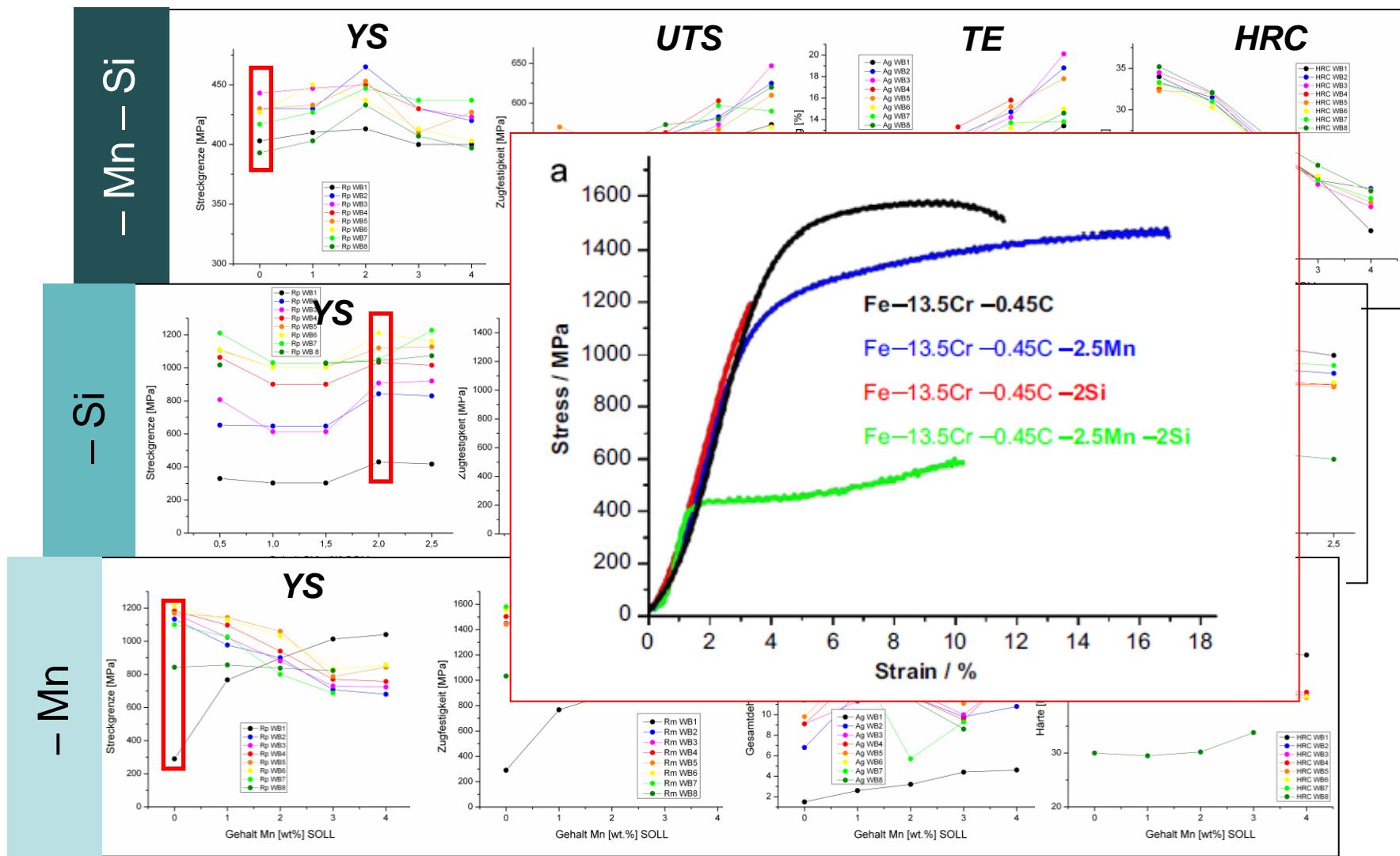
Fe – 13.5Cr – 0.45C...



Select interesting compositions / treatments



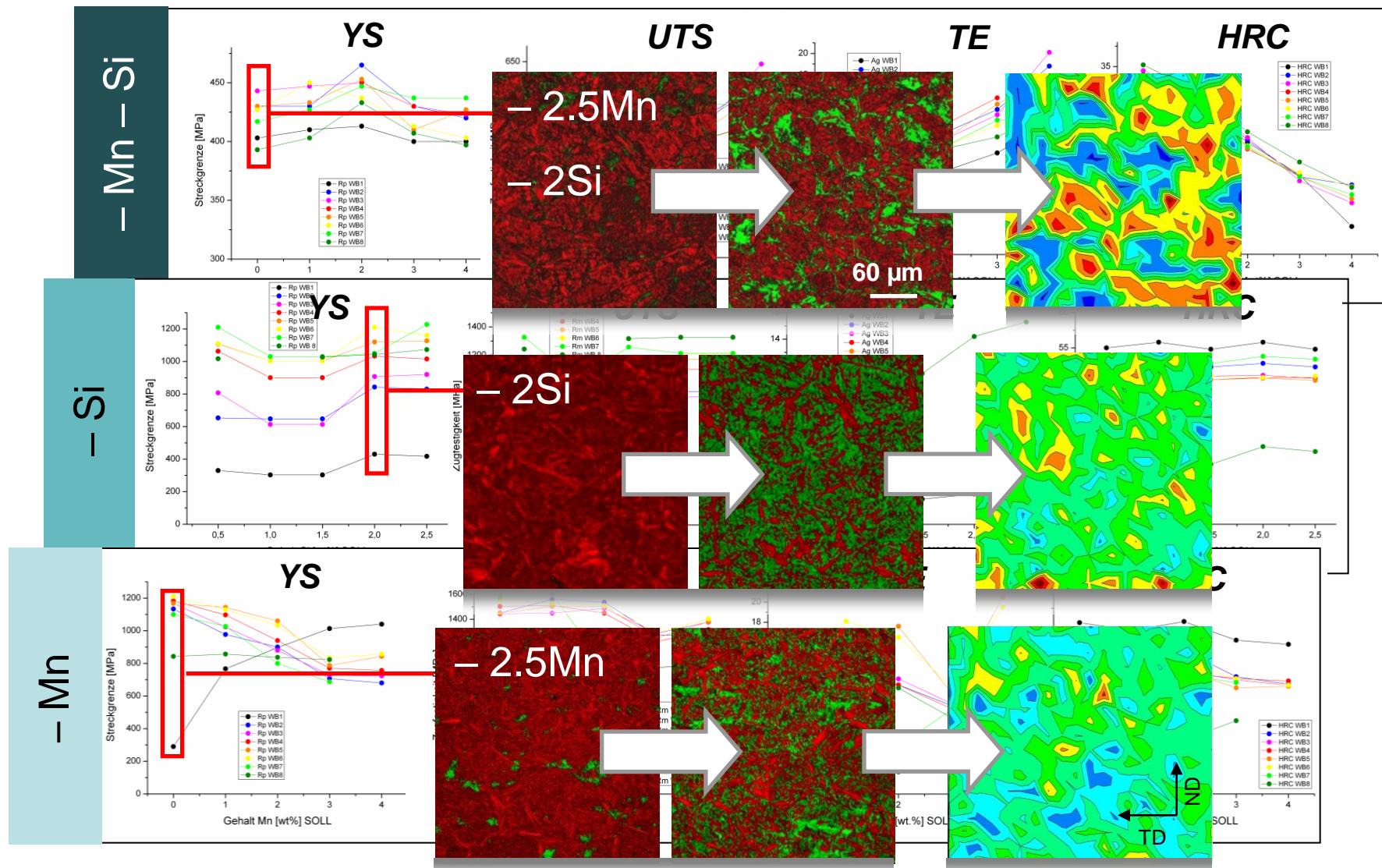
Fe – 13.5Cr – 0.45C...



Link microstructure / mechanical properties



Fe – 13.5Cr – 0.45C... → austenite reversion → mech. compliance



Thats it ...



... and thank you for your attention!

