ICME Design of Advanced Lightweight Steel

Jiayi Yan

Materials Design Engineer, QuesTek Europe AB

Advanced high-strength steels (AHSS) for lighter car body

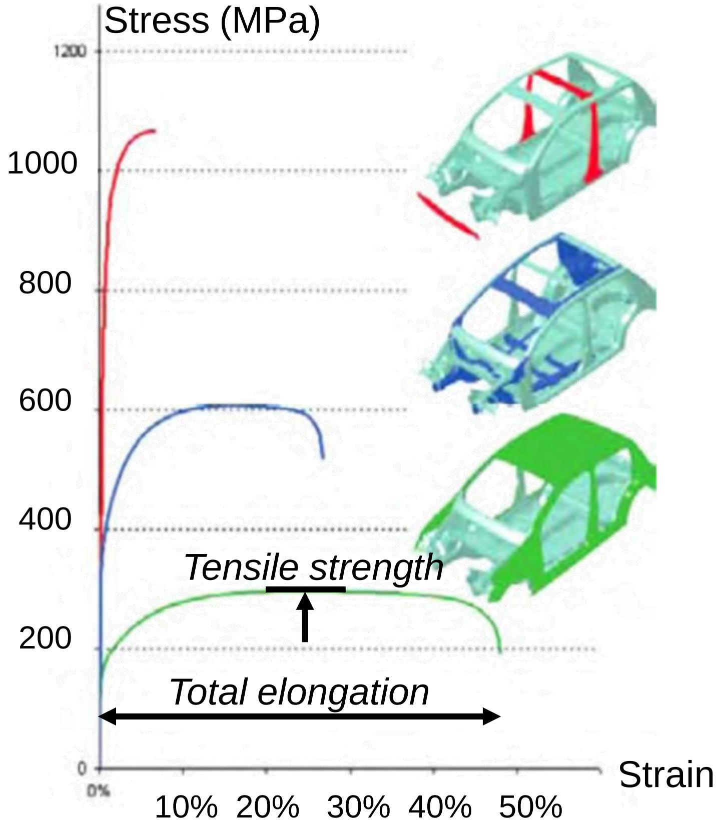
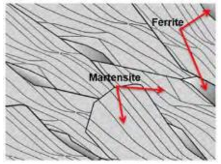
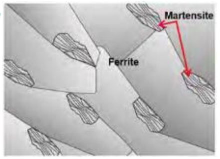


Figure 1.D-2: Stress (in MPa) vs. percent elongation for different steel types and their applications in body structure *[Adapted from C-5]*

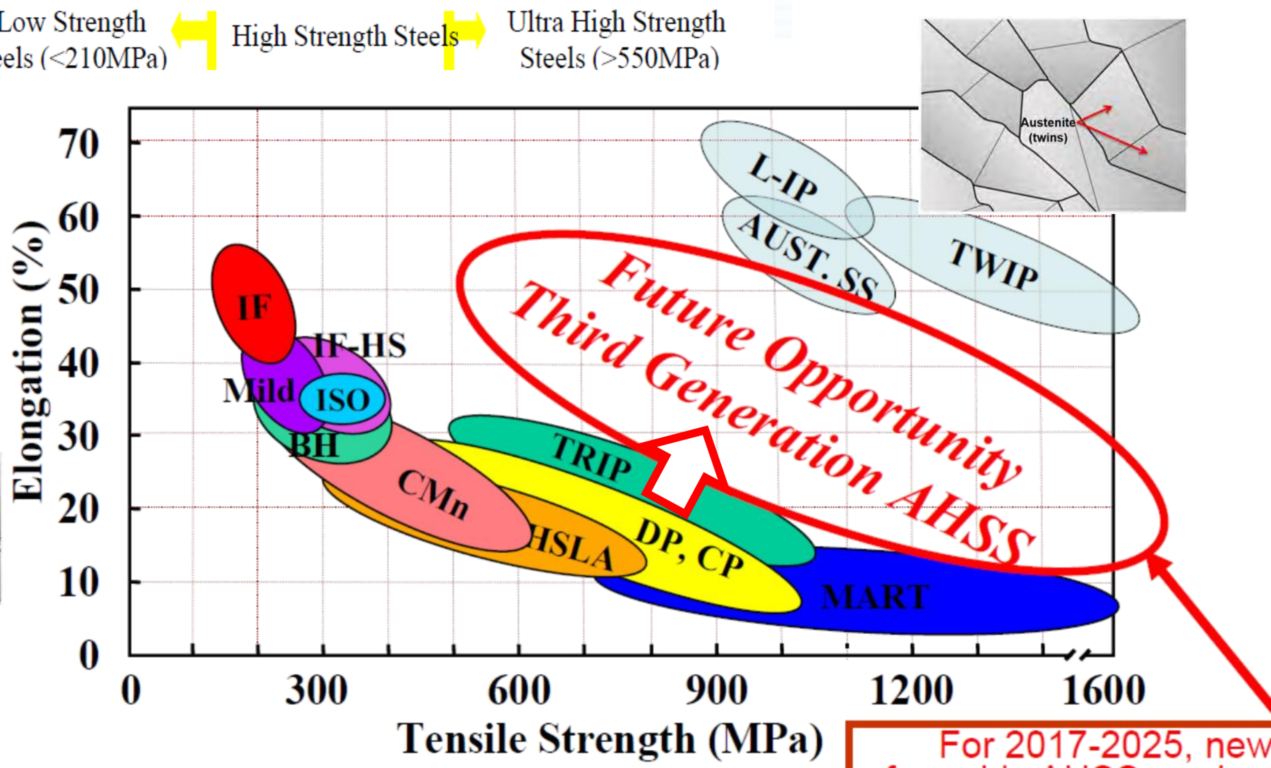
> Steels for safety-critical parts, especially for maintaining a passenger survival space in crash events



> High-strength steels with a good balance of strength, formability, energy absorption and durability



> Steels with excellent formability (eg. for deep drawing)



Hall (2011), WorldAutoSteel (2017)

For 2017-2025, new formable AHSS grades enable more steel mass reduction

Properties determined by microstructure

Microstructure design to break strength–ductility trade-off

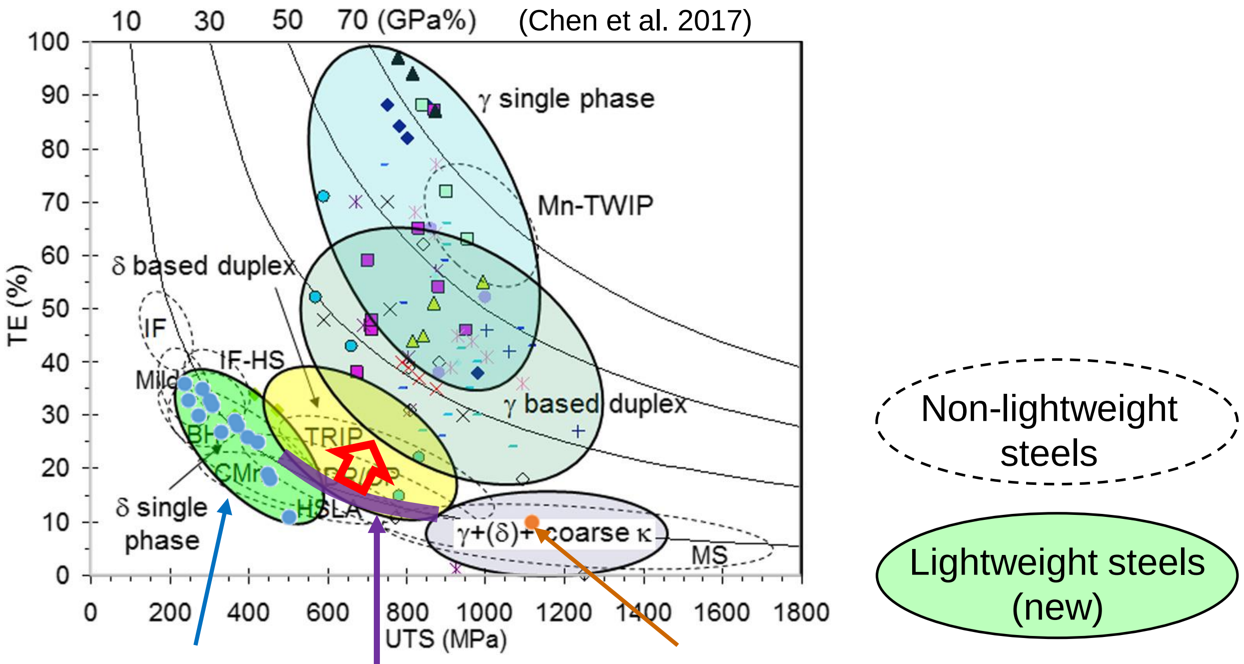
Significance of our LIGHTer Small Company Project (feasibility study)

- Demonstrate ICME modeling and design
  - What can be done in a short time (several weeks)

- Efficient evaluation of feasibility and potential of a design concept
  - Minimize trial-and-error

- Suggest most promising directions for research and prototyping
  - Based on a gap analysis
  - Based on potential of design concept

- Project plan:
  - Evaluate state of the art
  - ICME materials design process
  - Gap analysis



A2 binary Fe-Al
(Herrmann et al. 2003)

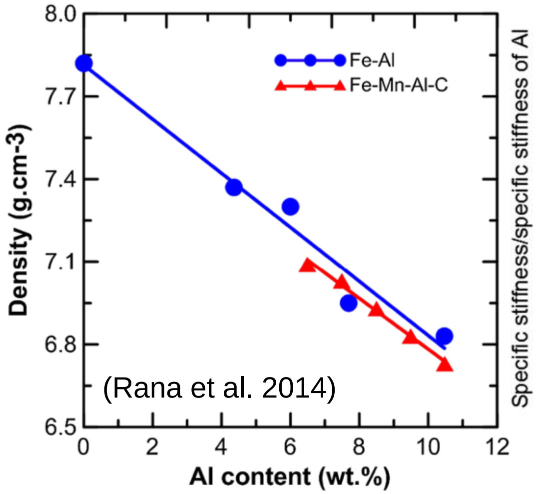
A2+B2 Fe-Al-Ni-Cr-Mo
(Teng et al. 2011, 2012)

Fe-Al-Ni design
(expected, this work)

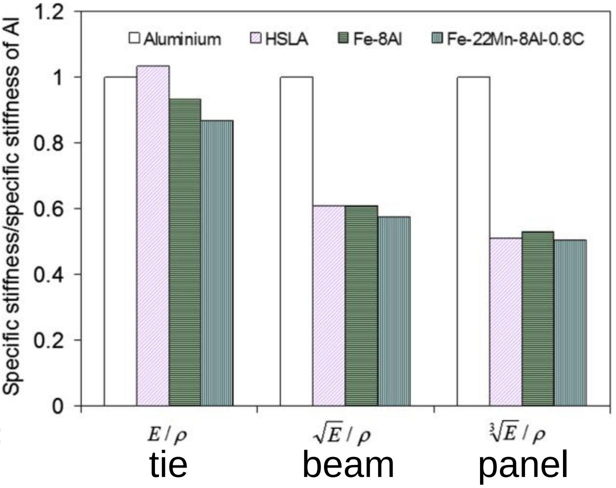
Motivation: lightweighting steel itself

- High-Al steels have lower density
- Comparable properties to non-Al steels
  - Specific stiffness
  - Tensile strength
  - Total elongation
- Large variety of microstructures

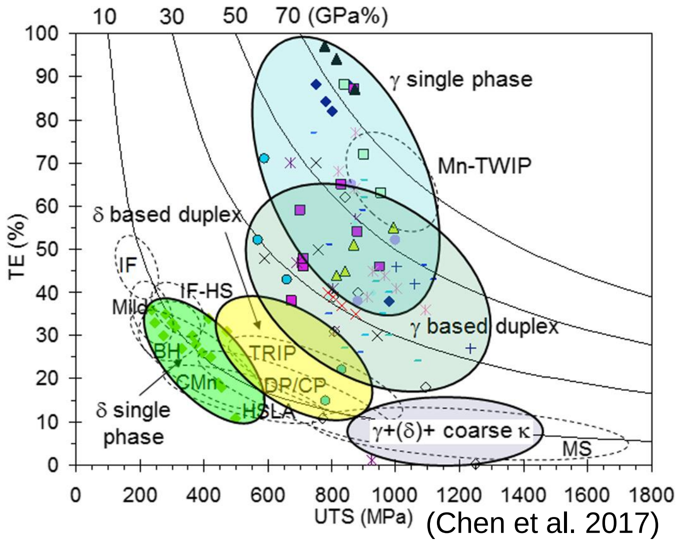
- Challenges in processing
  - Viscosity (castability)
  - Oxidation
  - Possible brittleness
- New phase relations and deformation mechanisms (austenite)



(Rana et al. 2014)



(Chen et al. 2017)

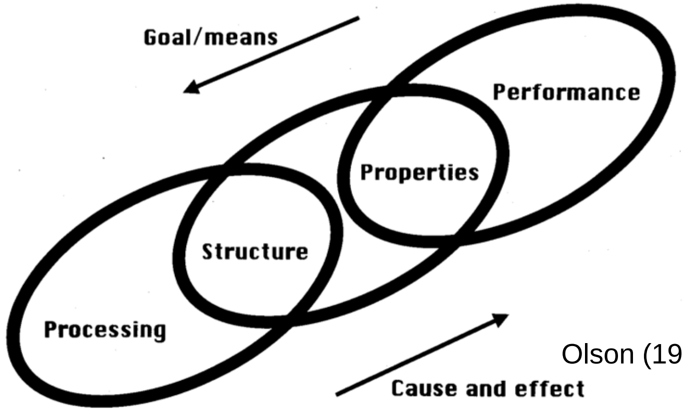


(Chen et al. 2017)

How can ICME accelerate materials development?

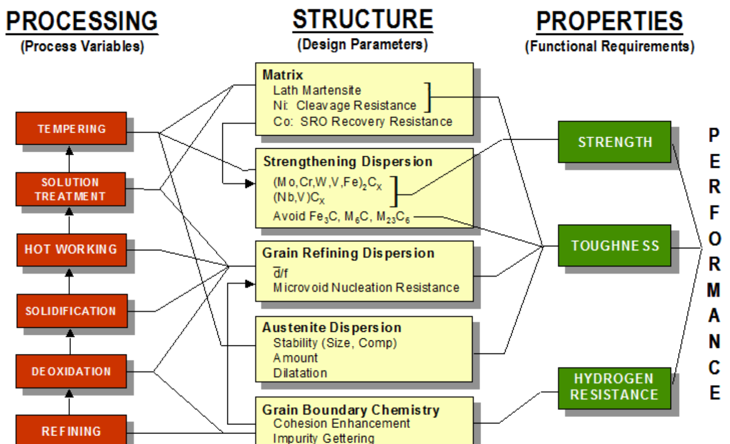
ICME materials design: an overview

- Materials Science and Engineering

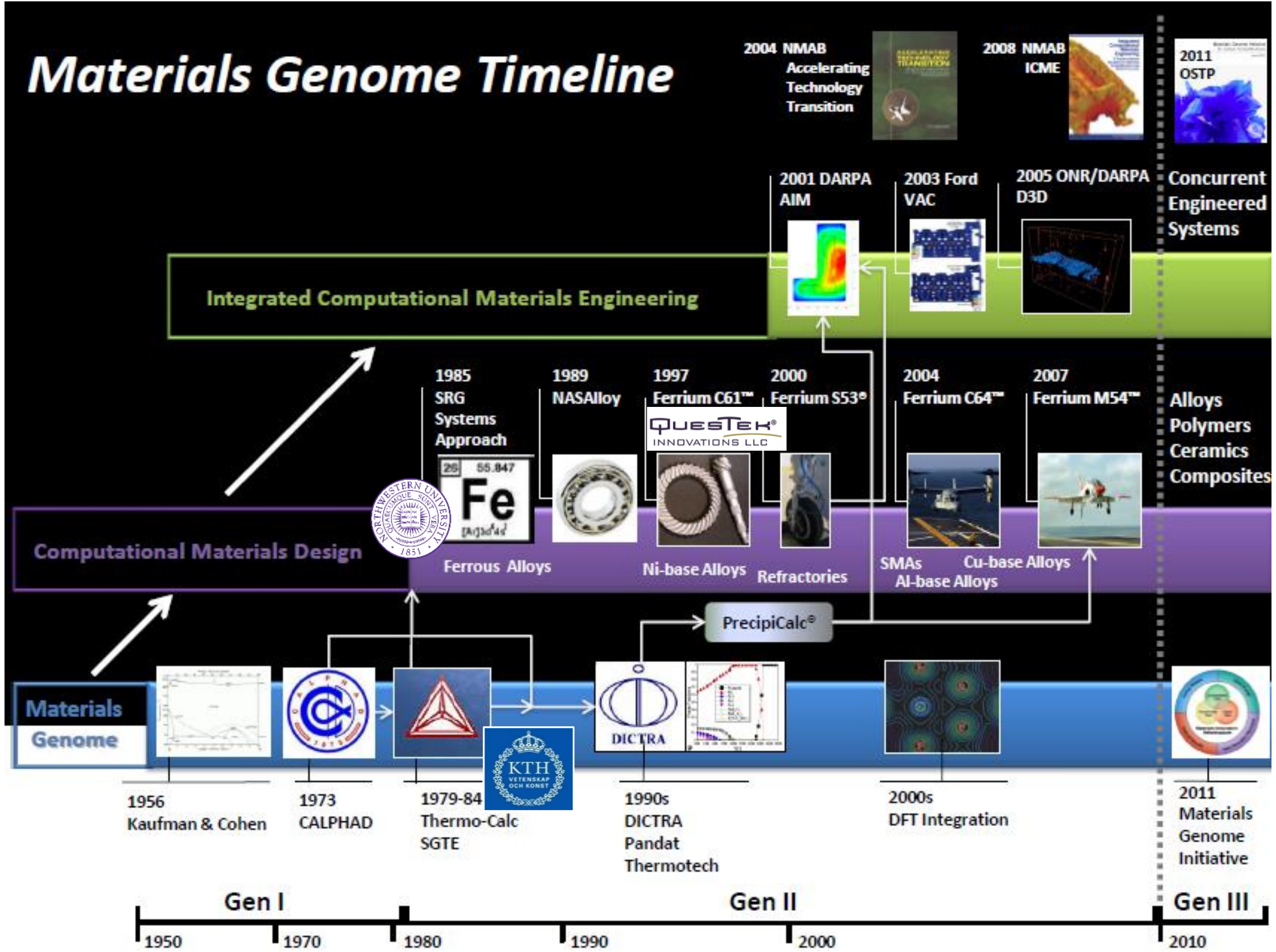


Olson (1997)

- Systems approach, materials design



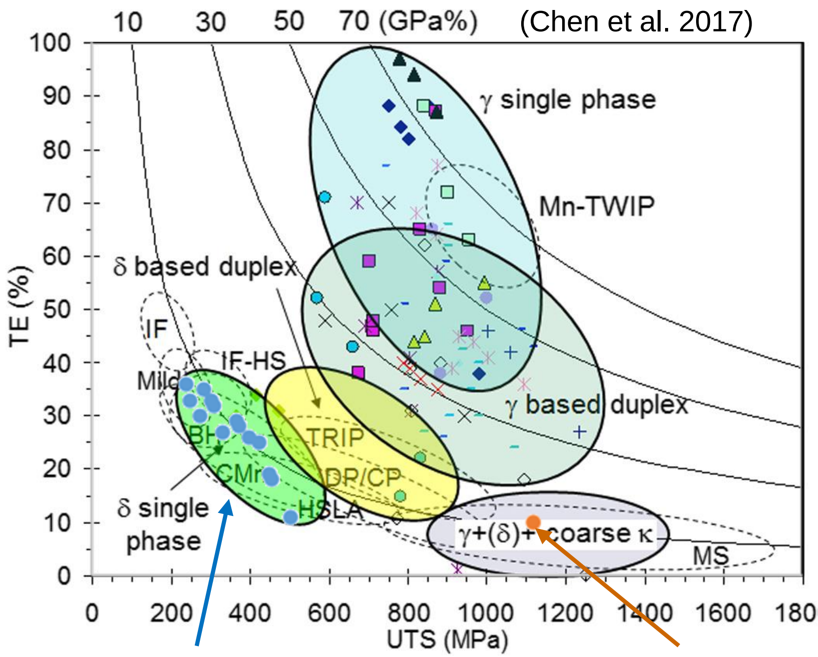
Olson (1997, 2013)



Materials design scope

- Consider Fe-Al ferrite + B2 precipitation strengthening
- Aiming for balanced strength and ductility

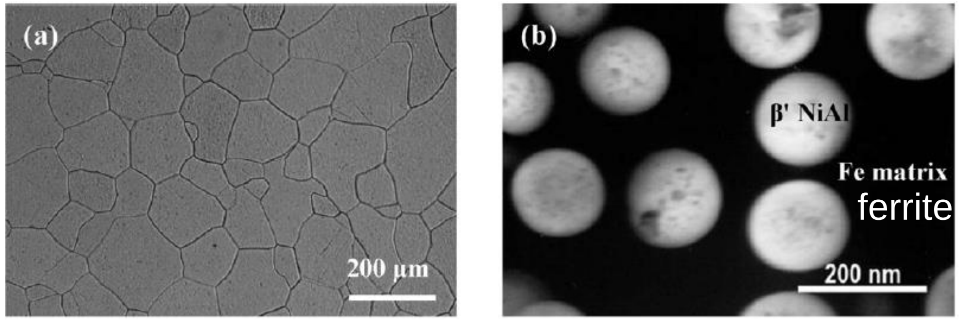
- Design methodology is transferrable to other materials scopes too



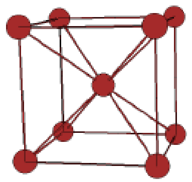
(Chen et al. 2017)

A2 binary Fe-Al
(Herrmann et al. 2003)

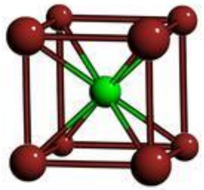
A2+B2 Fe-Al-Ni-Cr-Mo
(Teng et al. 2011, 2012)



(Teng et al. 2012)

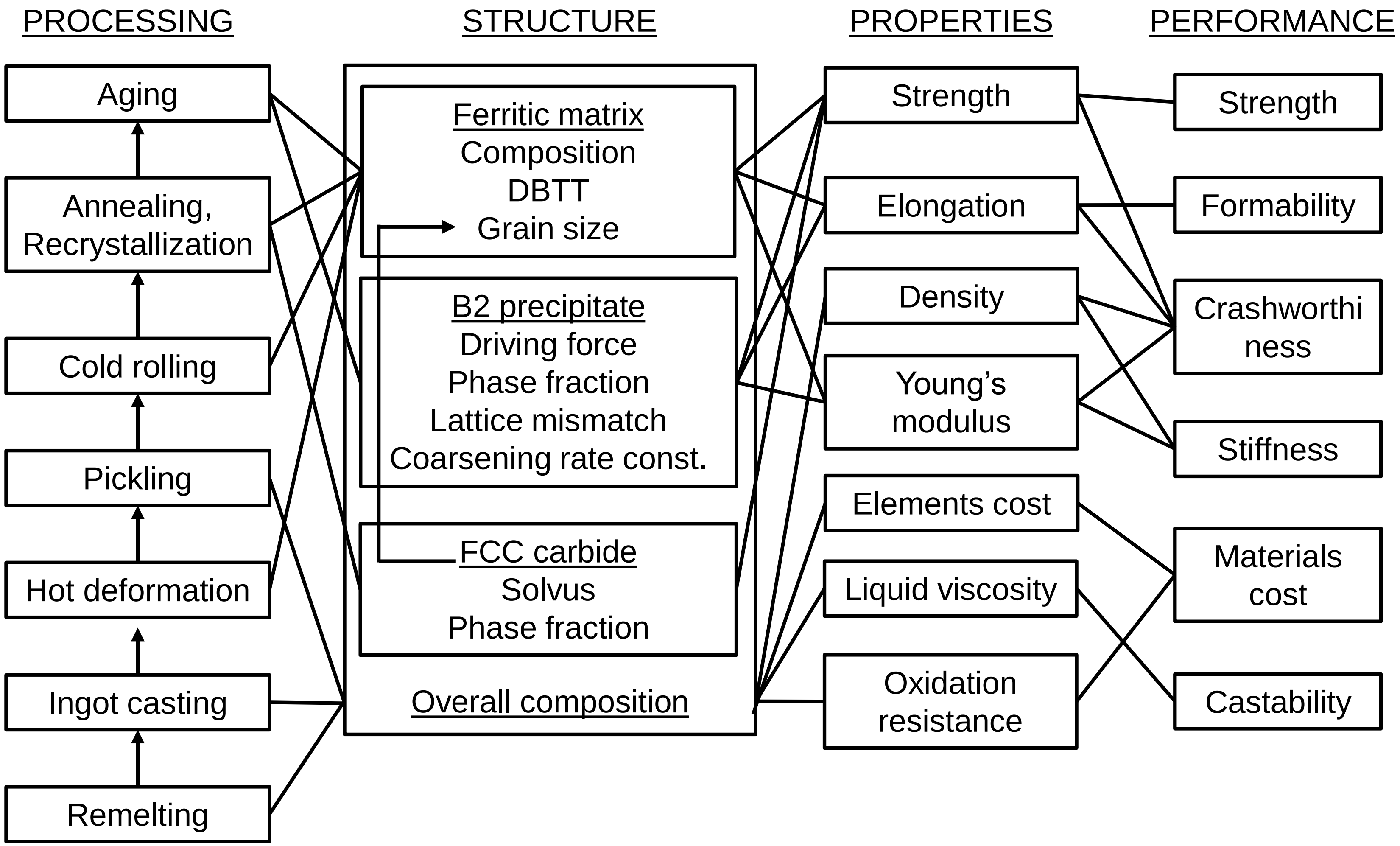


A2(bcc, ferrite)



B2(CsCl)

Systems design chart for the lightweight steel



PROCESSING

Aging

Annealing, Recrystallization

Cold rolling

Pickling

Hot deformation

Ingot casting

Remelting

STRUCTURE

Ferritic matrix
Composition
DBTT
Grain size

B2 precipitate
Driving force
Phase fraction
Lattice mismatch
Coarsening rate const.

FCC carbide
Solvus
Phase fraction

Overall composition

PROPERTIES

Strength

Elongation

Density

Young's modulus

Elements cost

Liquid viscosity

Oxidation resistance

PERFORMANCE

Strength

Formability

Crashworthiness

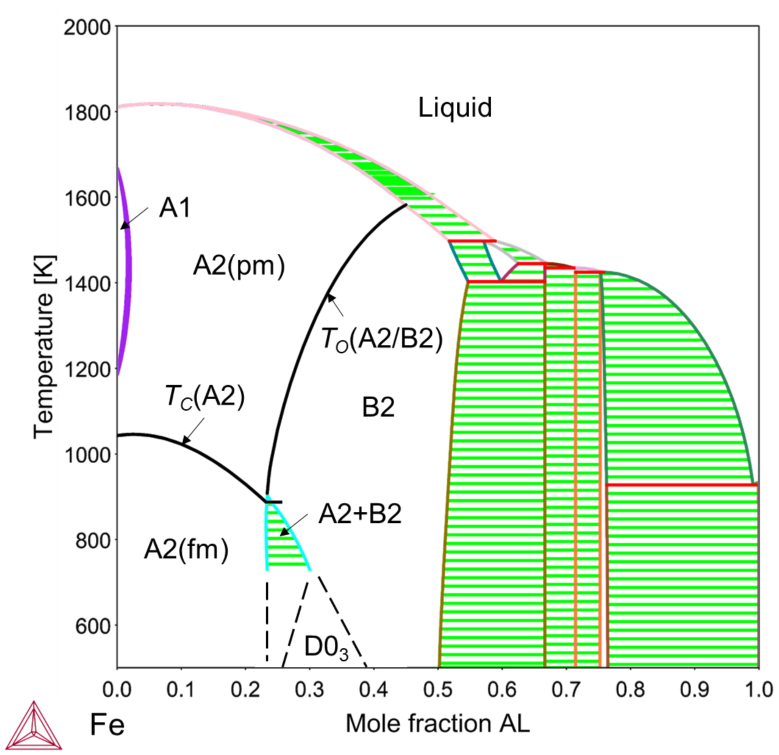
Stiffness

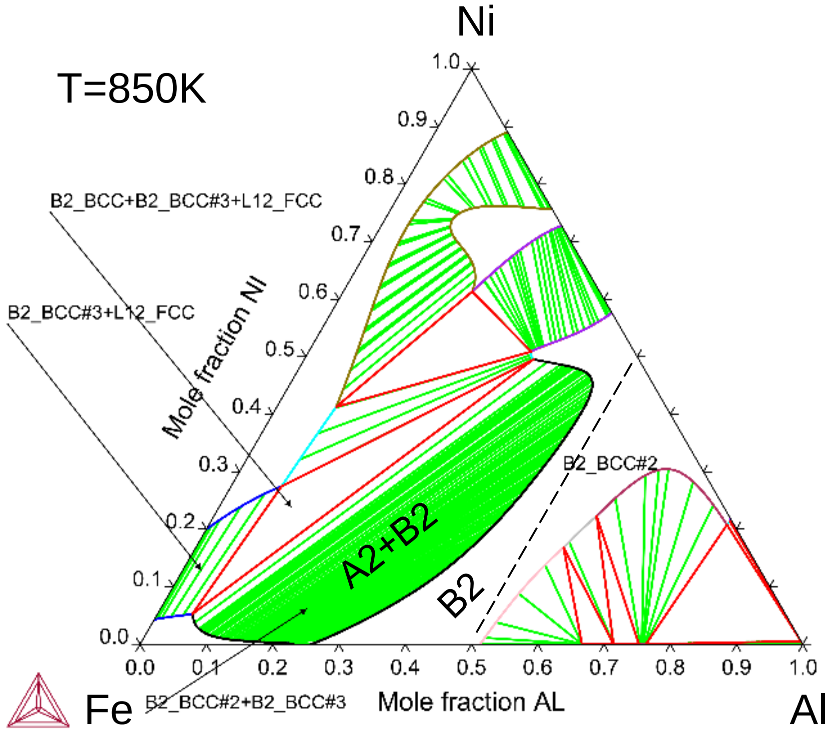
Materials cost

Castability

Fe-Al-X phase relations: a computational survey

- The narrow two-phase field A2+B2 in Fe-Al is broadened most efficiently by Ni

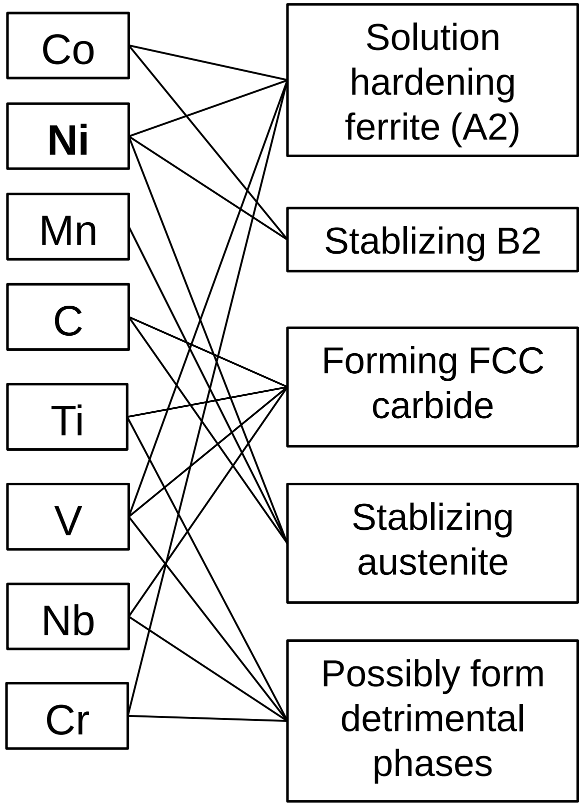




TCFE9 database

Ni identified as the best element to add after a computational survey of elements

- Roles of other elements identified from phase diagram calculations



Co

Ni

Mn

C

Ti

V

Nb

Cr

Solution hardening ferrite (A2)

Stablizing B2

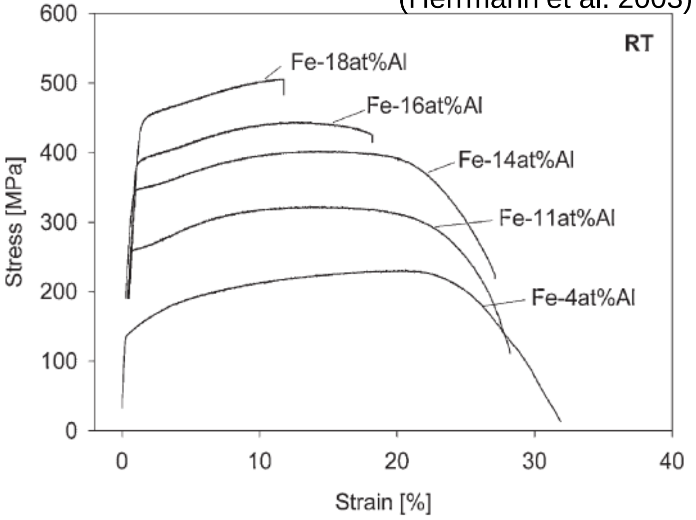
Forming FCC carbide

Stablizing austenite

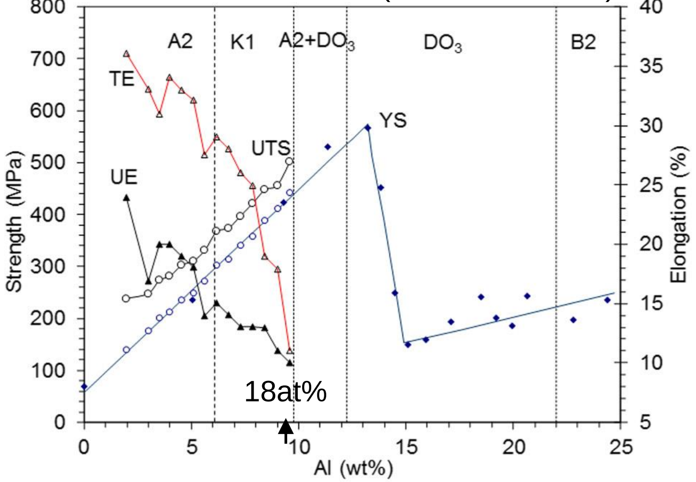
Possibly form detrimental phases

RT mechanical properties, Fe-Al ferrite as a baseline

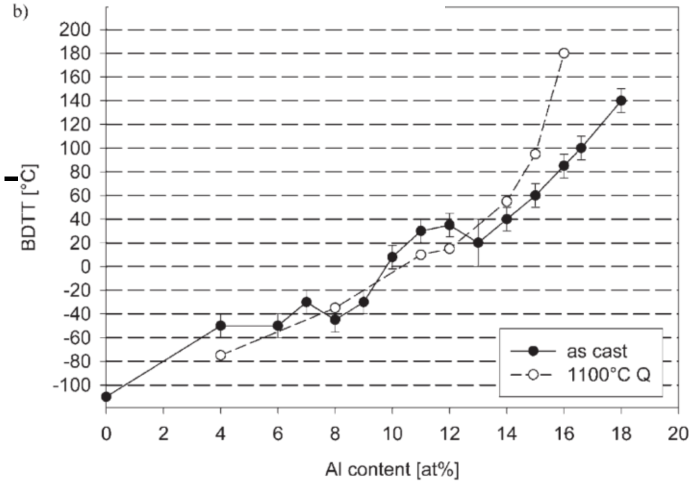
(Herrmann et al. 2003)



(Chen et al. 2017)



(Herrmann et al. 2003)



- Higher Al content gives higher strength and lower ductility
- Ductility can be understood from ductile-to-brittle transition temperature (DBTT)
  - The lower DBTT the better ductility

Need other element(s) to break strength-ductility trade-off

RT mechanical properties, B2-hardened ferritic steels

- Fe-Al-Ni-Cr-Mo B2-hardened steels (Teng et al.)

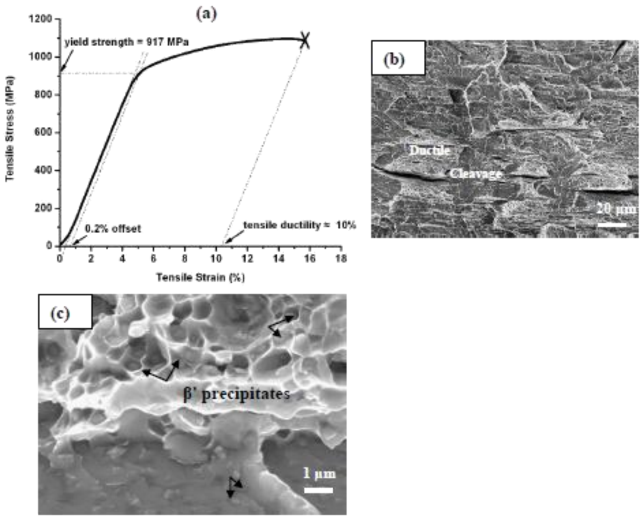
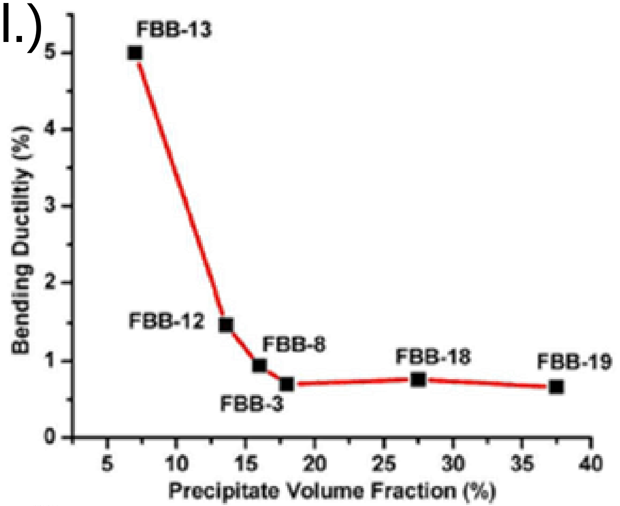
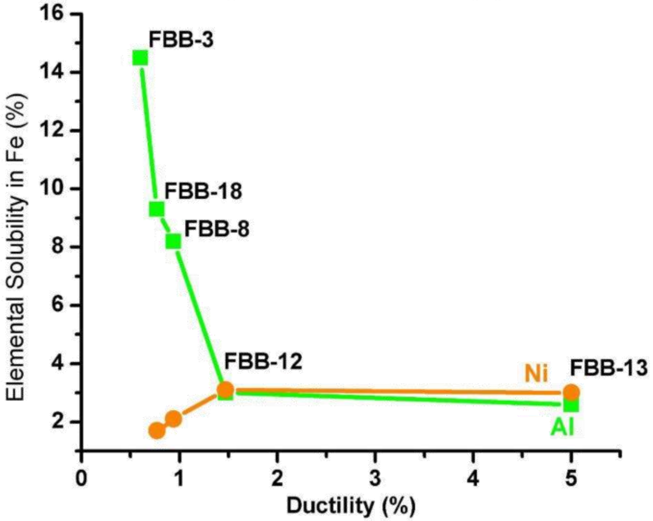


Figure 7.7 (a) Tensile stress vs. strain curve of hot rolled FBB-8, (b) fracture surface showing a mixture mode of cleavage and ductile rupture, and (c) high magnification image of the fracture surface in both ductile and cleavage areas.



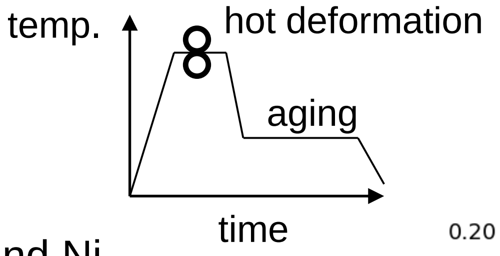


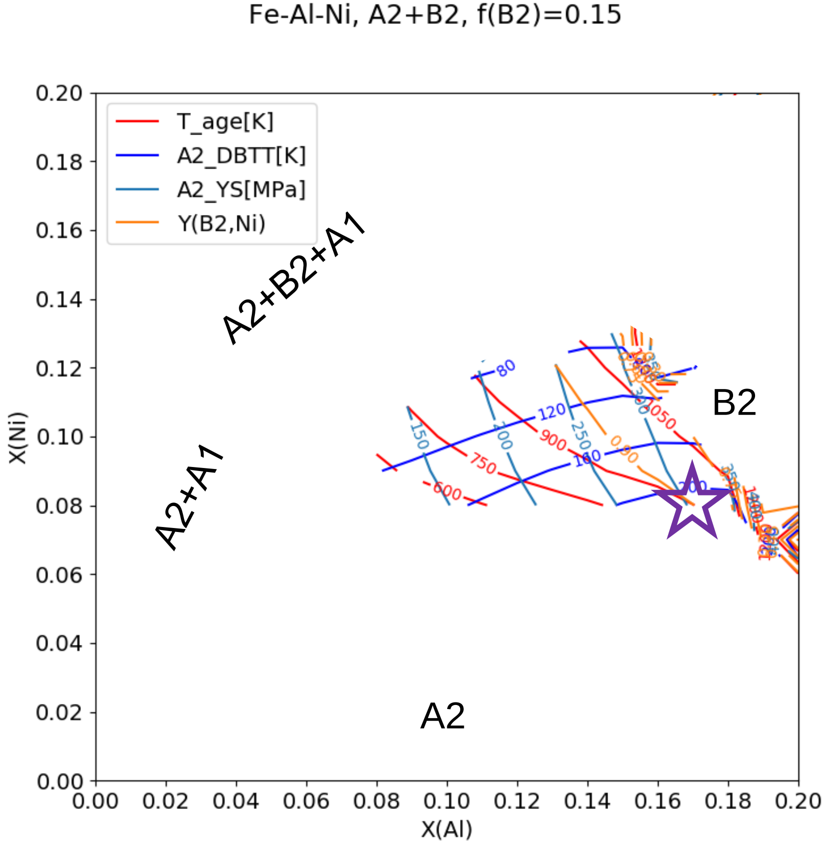
- RT bending ductility is higher with…
  - Less B2 phase
  - Lower Al content in matrix
  - Higher Ni content in matrix

Design space opened up

Design for balanced strength-ductility with processability

- Ductility
  - A2 (ferrite): Keep DBTT<=RT-40K
  - Fraction of B2 <= 15%
- Strength
  - A2 (ferrite): solution strengthening from Al and Ni
  - B2 precipitation strengthening: control fraction and mean radius
- Fe-Al-Ni system calculation
  - Avoid having to hot deform in B2 phase region
    - B2 is more difficult to hot deform than A2 (ferrite)
  - Find T_age which gives f(B2)=15%, 10%, 5%
  - At the T_age, extract A2 and B2 compositions and calculate DBTT and YS
- Design can be done
  - Fe-17Al-8Ni, aged at 900K for 15% B2
  - Composition bound by the requirement not to solutionize in B2 single-phase region

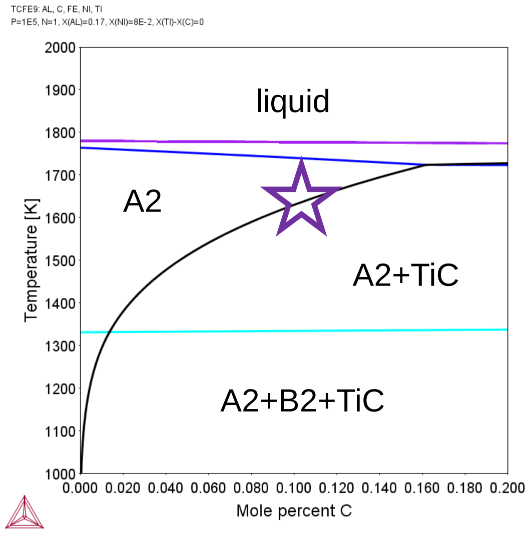




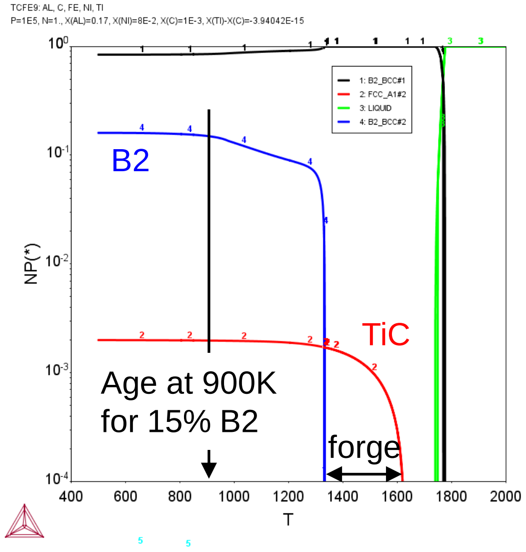
Grain size and control of carbides: an further improvement

- High-Al ferritic steels usually have large grains because ferrite directly solidifies from liquid
- To introduce FCC carbide as grain pinner and strengthener
- To have sufficiently high solvus of FCC carbide but not connected to solidus
  - Avoid interdendritic continuous FCC carbide films

Fe-17Al-8Ni-x(TiC), at%

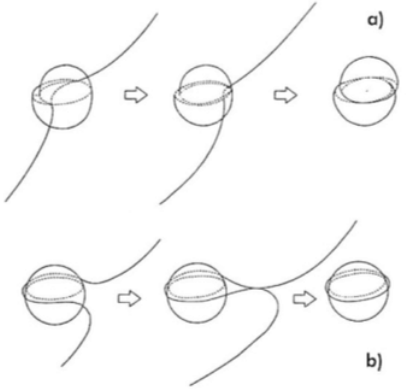


Fe-17Al-8Ni-0.1(TiC), at%



Finding optimal aging time by model calibration to experiments

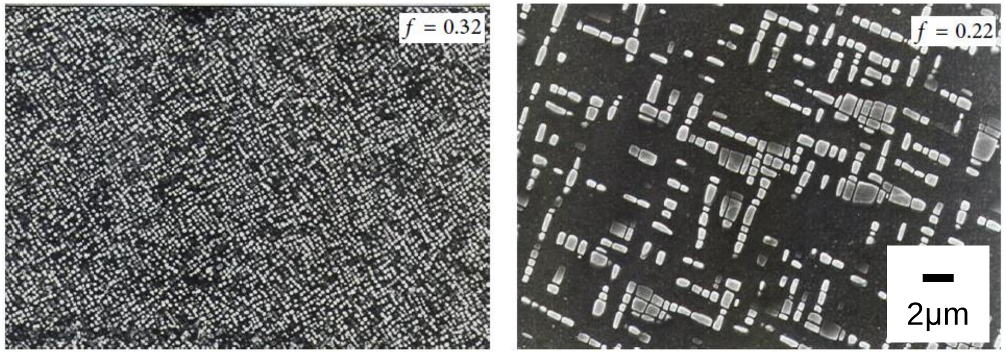
- TC-PRISMA simulation of B2 from A2
  - Fe-15Al-10Ni (at%) at 1023K (750C)
  - Precipitate radius and hardness from Cayetano-Castro et al. (2015)
  - Cuboidal morphology neglected, taken as equivalent spheroid
  - Interfacial energy=0.06J/m^2



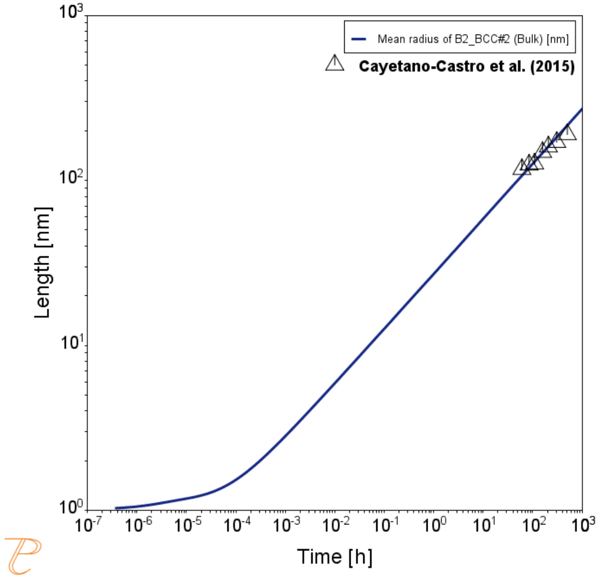
$r < r_c$: Shear

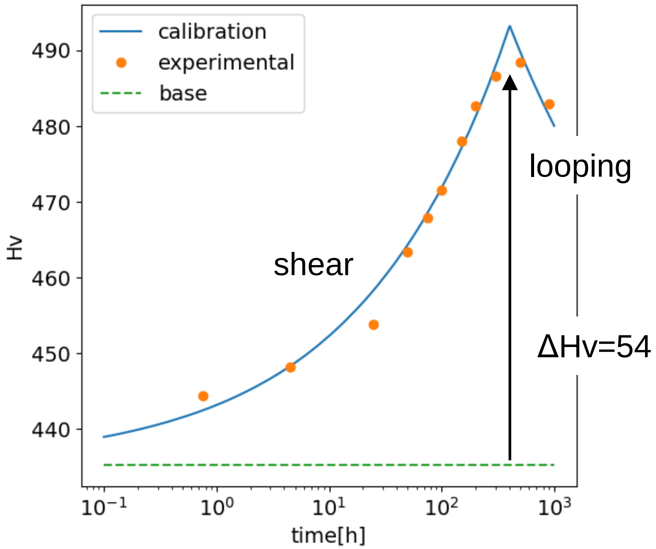
$r > r_c$: Looping

- Calibration of precipitation hardening model
  - Friedel shear and Orowan looping
  - Peak aged condition in coarsening regime



(a) Cayetano-Castro et al. (2015) (b)





Design and analysis

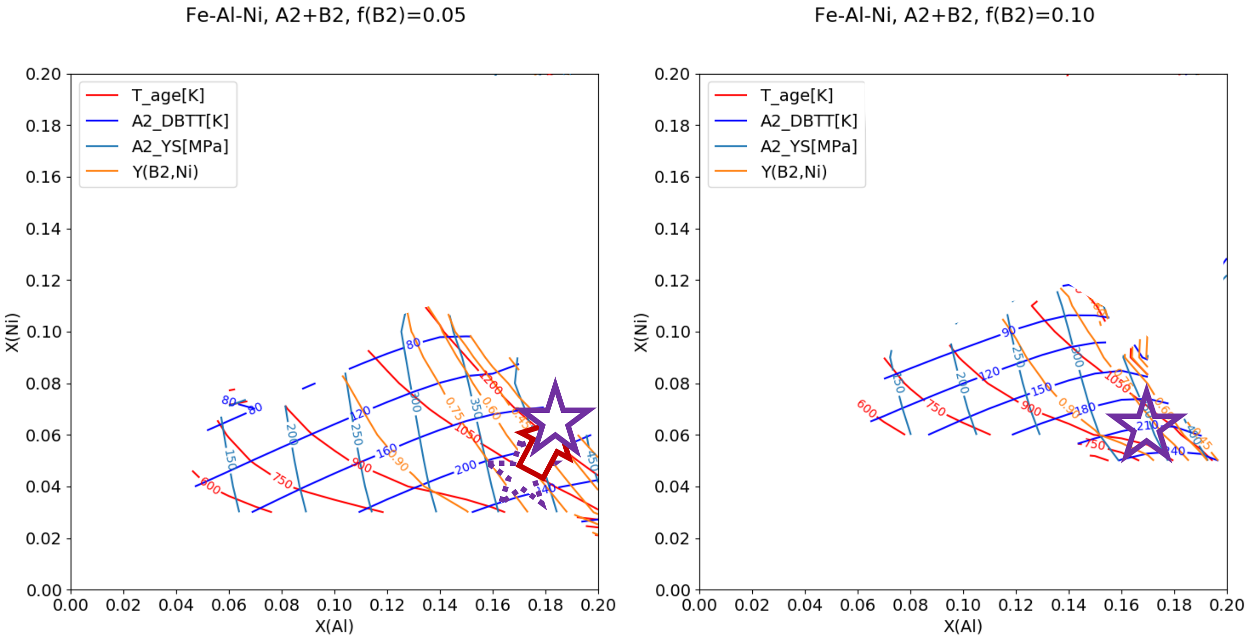
- Design: Fe-17Al-xNi-0.1Ti-0.1C (at%)

B2 fraction	15%	10%	5%
at% Ni	8	6	4
T_age[K]	900	967	995
RT density [g/cm^3]	7.08	7.05	7.02
Peak age	>10^{5}h	8760h (=1y)	

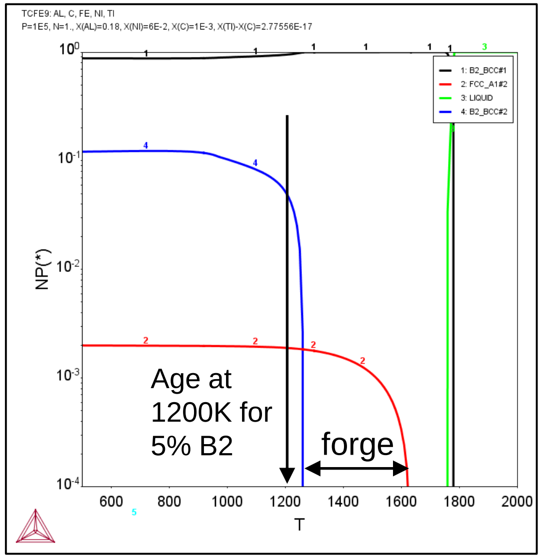
- Pros:
  - Density reduced by >10% (by Al)
  - Variety of precipitate fraction → strength, ductility combinations
- Cons:
  - Addition of Ni (6x price of Mn)
  - Peak aging time much too long for automotive applications (but can be good for lightweight structural high-temperature components)

Accelerating B2 precipitation for better processability

- Raising aging temperature is feasible for 5%-B2 design but not for 10%-B2
- New 5%-B2 design for faster B2 precipitation
  - Fe-18Al-6Ni-0.1Ti-0.1C, T_age=1200K
  - Peak age at 31min, RT density=6.97g/cm^3



New 5%-B2



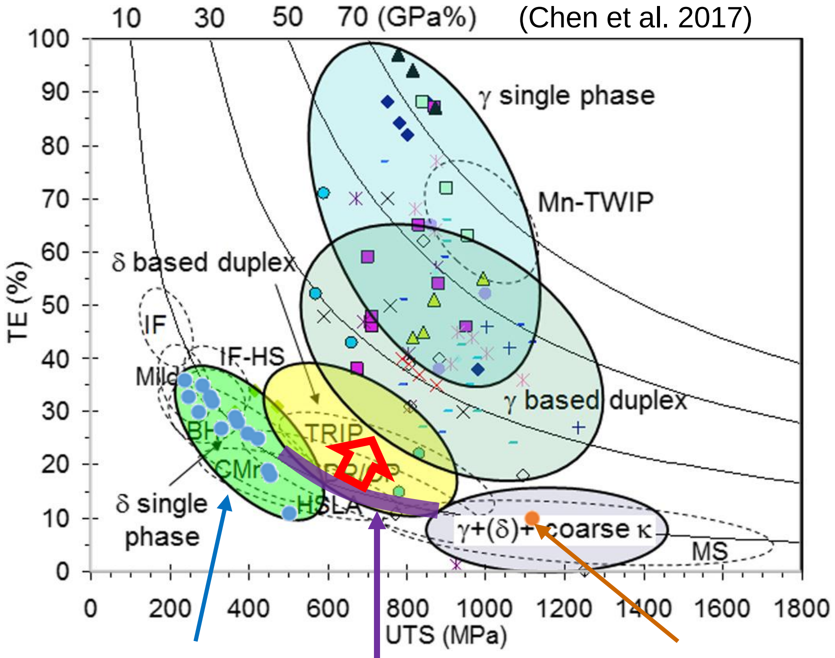
Gap analysis: fundamental research needed for a better design

- Improving TCFE9 database
  - $D0_3$ not handled
  - B2 stability may be underestimated
  - Consider thermal vacancy in B2 phase
- Predicting elongation (challenging!)

- Complex deformation mechanisms in high-Mn austenite
- Kinetics of κ-carbide precipitation in austenite
- Etc.

Technical conclusions and outlook

- ICME design is applied and is feasible
  - A2+B2+FCC carbide, Fe-Al-Ni-Ti-C system
- 5%-B2 new design has acceptable processability
  - Has better potential as heat-resistant structural steels
- Gaps are identified
  - Mechanisms not fully known
  - Basic properties (Materials Genome) not measured
  - Limitations of computational tools and databases
- Other concepts
  - High-Mn high-Al austenitic steels (2nd generation)
  - Ferrite + dispersed austenite, Fe-Mn-Al-C system (3rd generation for lightweight AHSS)



(Chen et al. 2017)

A2 binary Fe-Al
(Herrmann et al. 2003)

A2+B2 Fe-Al-Ni-Cr-Mo
(Teng et al. 2011, 2012)

Fe-Al-Ni design
(expected, this work)

Acknowledgments

- Vinnova 2018-04755 “Advanced lightweight steel: ICME-based accelerated development” (LIGHTer Small Company Project)
- Triple Steelix
- Thermo-Calc Software AB
- Dr. Weisen Zheng (Shanghai University)

References:

J.N. Hall, Evolution of Advanced High Strength Steels in Automotive Applications (2011)
AHSS Application Guidelines v6.0, WorldAutoSteel (2017)
G.B. Olson, Science 277 (1997) 1237; Acta Mater 61 (2013) 771
R. Rana et al., JOM 66 (2014) 1734
S. Chen et al., Prog Mater Sci 89 (2017) 345
M. Palm, Intermet 13 (2005) 1286
J. Herrmann et al., Acta Mater 51 (2003) 2847; 3233
Z. Teng, PhD thesis, UTK (2011); Z.K. Teng et al., MSEA 541 (2012) 22
Crystal Lattice-Structures webpage
J.H. Schneibel et al., Intermet 5 (1997) 185
Y. Tan et al., J Japan Inst Metals 57 (1993) 840; Y. Mabuchi et al., J Japan Inst Metals 62 (1998) 912
N. Cayetano-Castro et al., Adv Mater Sci Eng (2015) 485626

Thank you for your attention!

Jiayi Yan
jiayi.yan@questekeurope.com