ROYAL INSTITUTE OF TECHNOLOGY

On the development of theoretical and experimental tools for materials design of high strength steels and cemented carbides

Annika Borgenstam
Materials Science and Engineering
KTH

hero-m

Mission of competence center Hero-m 2 Innovation

To develop tools and competence for fast, intelligent, sustainable and cost efficient product development for Swedish industry. Continuous scientific breakthroughs are exploited to enable design of materials from atomistic scales to finished products.

Multi length scale engineering approach

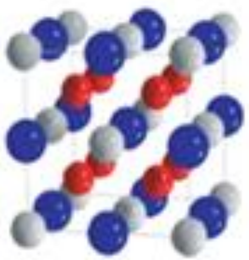
Atomic level simulation

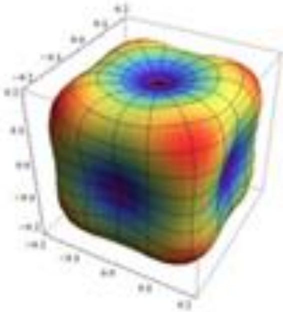
Continuum models

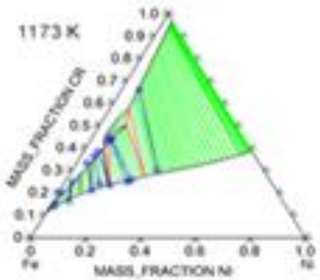
Fundamental models
Ab initio

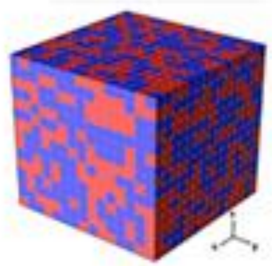
Phenomenological models
CALPHAD

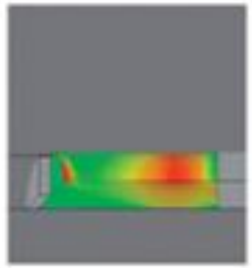
Engineering design



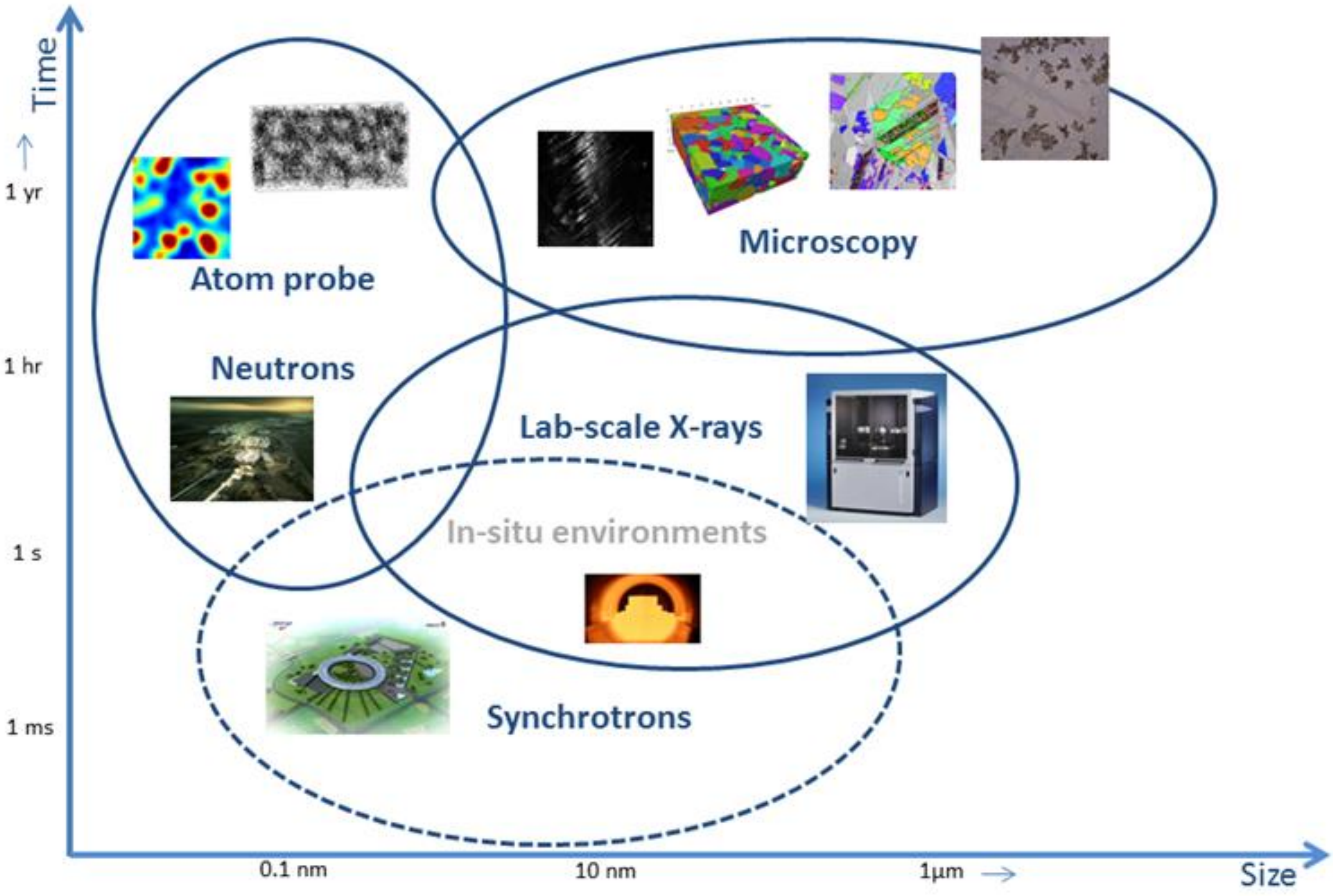








Experimental capabilities



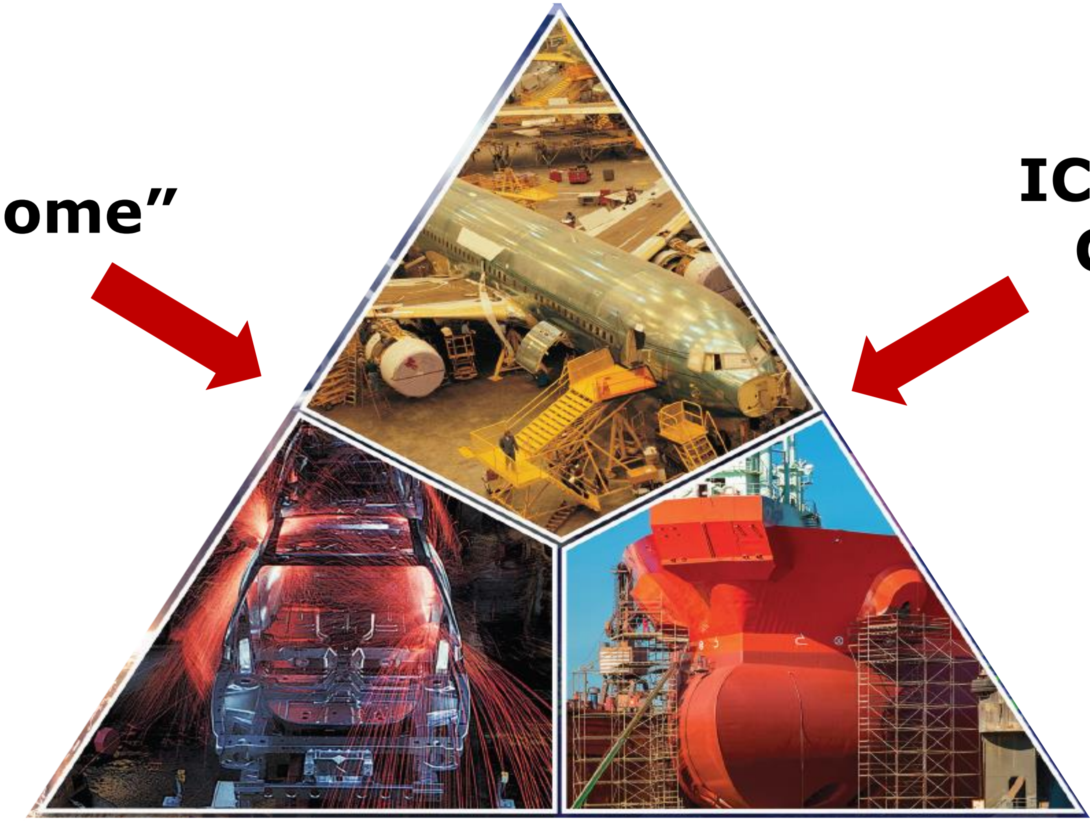
Hero-m 2 Innovation

Hero-m: 2007-2017
Hero-m 2 Innovation:2017-2022
E.g. 21 million/year in-kind+cash

The general materials design system

Development time for new materials can be decreased from 10-20 years to 3-4 years.

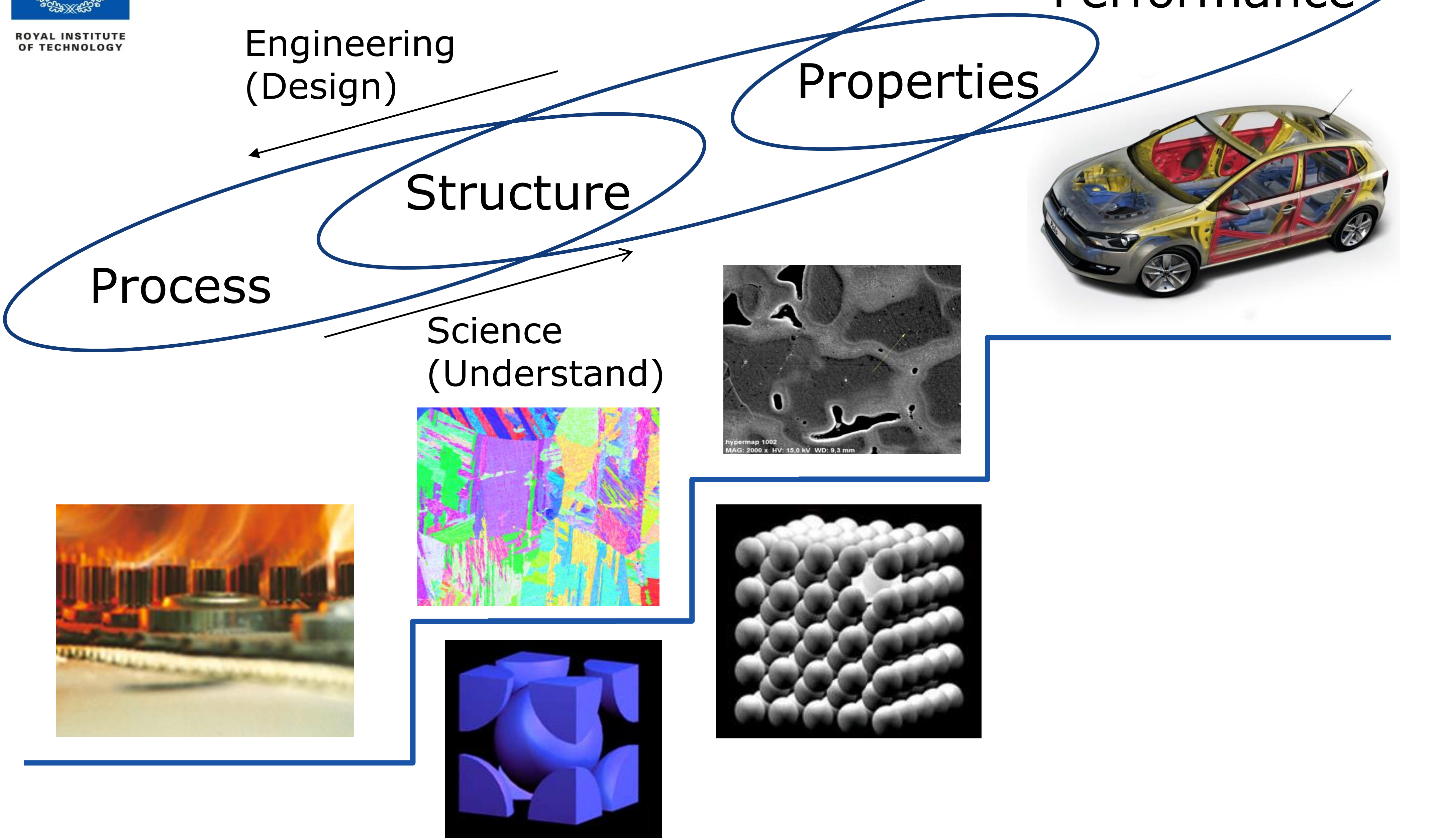
"Materials Genome" databases



ICME - Integrated Computational Materials Engineering models

Materials design method

Cohen's reciprocity



Materials Design: The needed knowledge structure

Performer

Performance

Properties

Translator

Structure

Creator

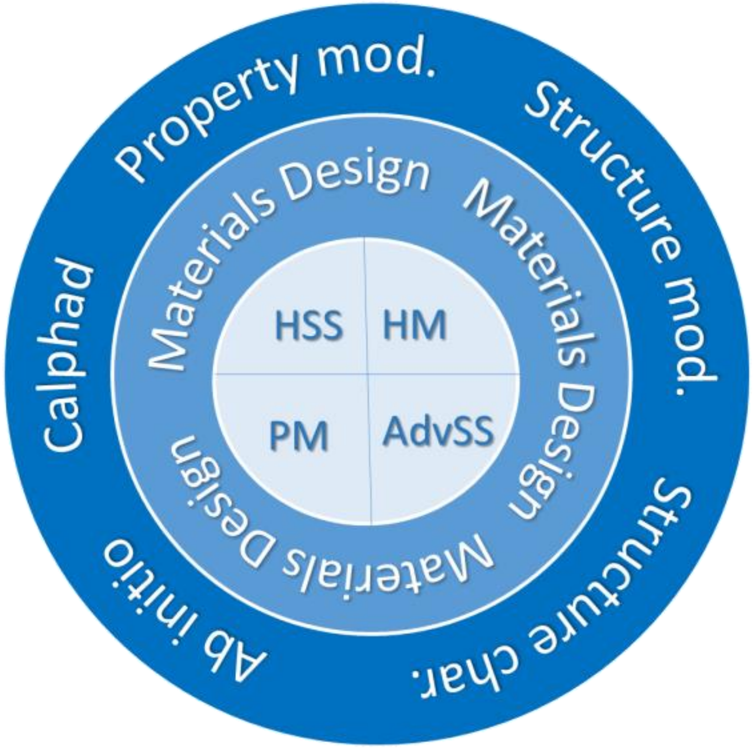
The recipe:

Composition
Processing
Heat treatment

Research programme for Hero-m 2i

Materials Design projects in four application areas

- Hard Materials (HM)
- Powder Based Materials (PM)
- High Strength Steels (HSS)
- Advanced Stainless Steels (AdvSS).



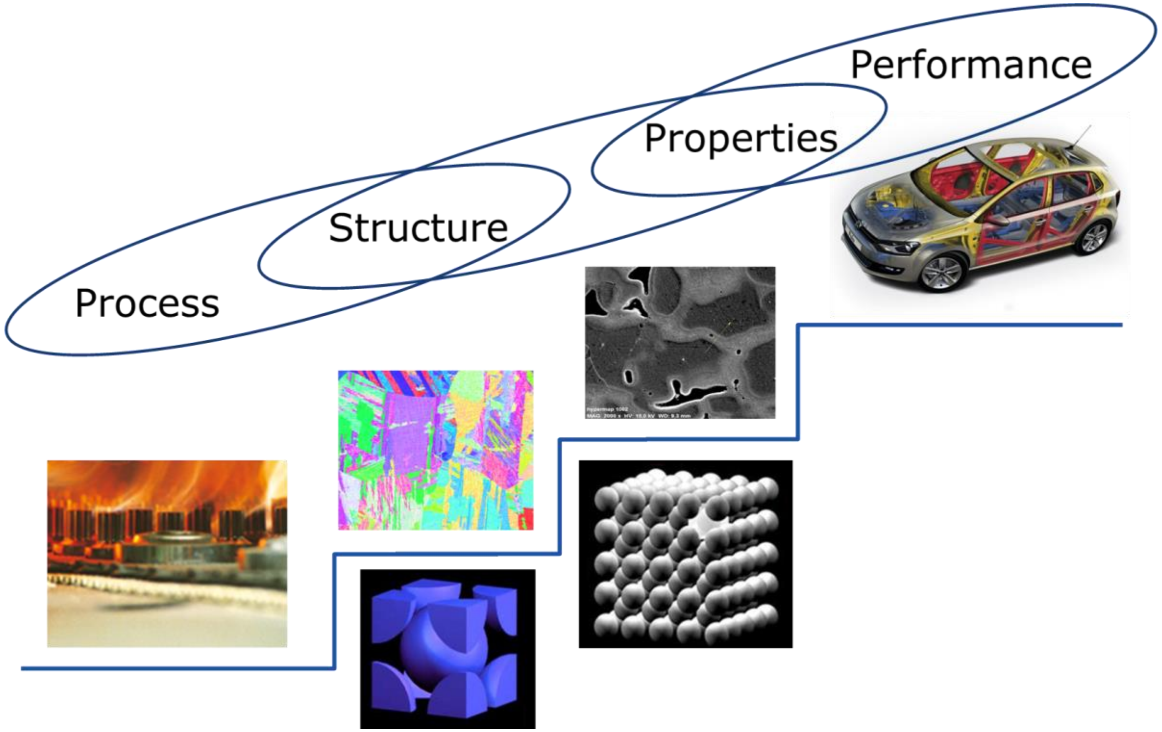
Generic projects

- Ab-Initio
- Calphad
- Structure Modelling
- Structure Characterization
- Property Modelling

Materials design projects

- Develop methods for materials design which allows an accelerated development of new materials
- Opportunity to use and test tools and models developed in Hero-m.
- To address highest priority activities for structure/property modeling.
- Educate graduate and undergraduate students in Materials design.

Examples
- High strength steels
- Cemented carbide



Design of a martensitic TRIP steel

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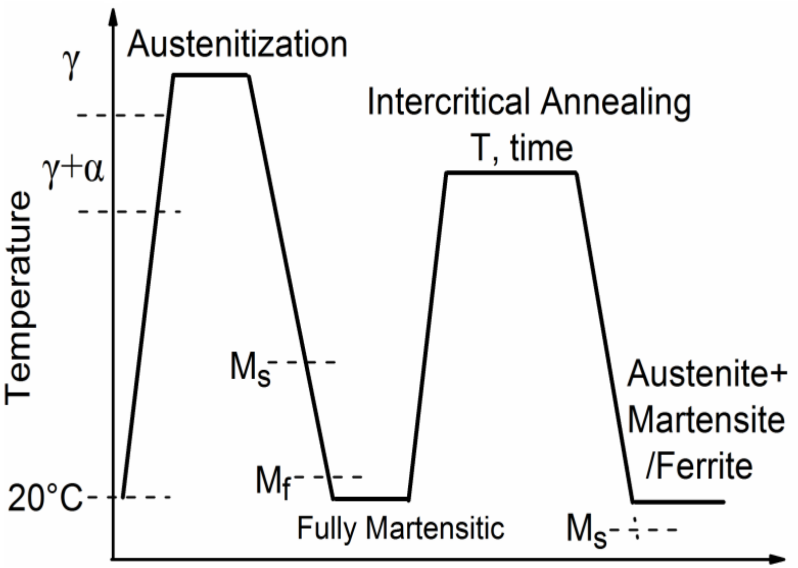
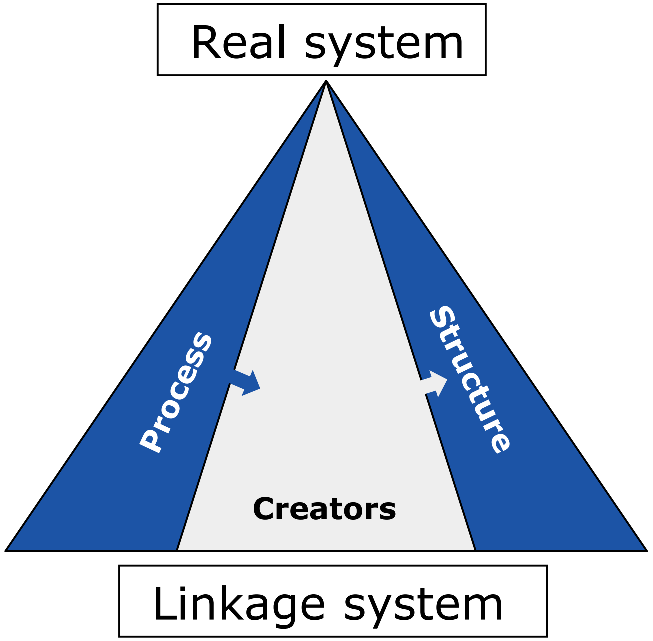
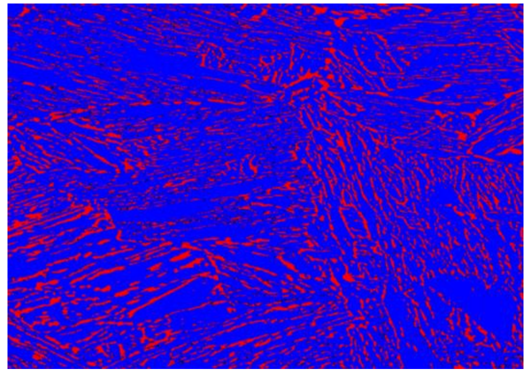
Design goal - Combination of high strength and elongation







- Austenite
- Ferrite/Martensite

- .....
- Cold rolling
- Austenitization
- Quenching
- Intercritical annealing
- Quenching

Structure

Martensitic formation under applied stress

M_s^σ

Fraction of martensite

MS Frac

Start of martensite formation

MS Calc

Formation of austenite

Formation of carbides

Thermo-Calc

DICTRA

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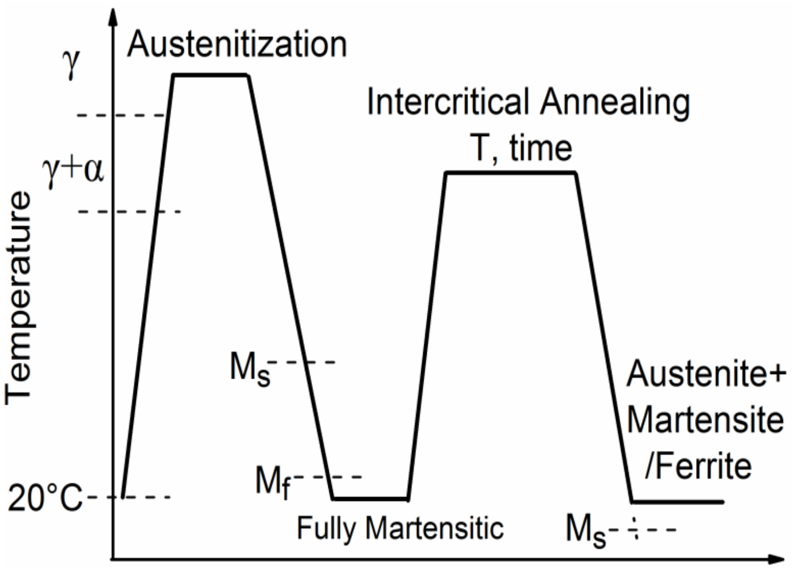
Design of a martensitic TRIP steel

Design goal - Combination of high strength and elongation



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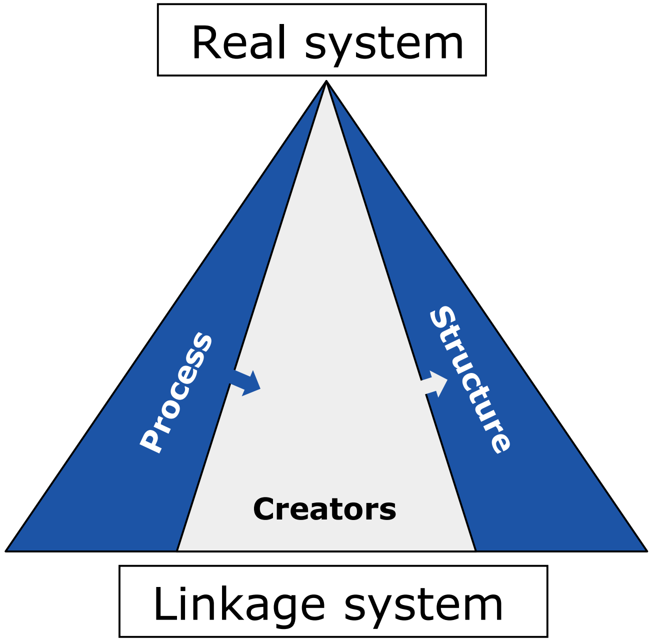
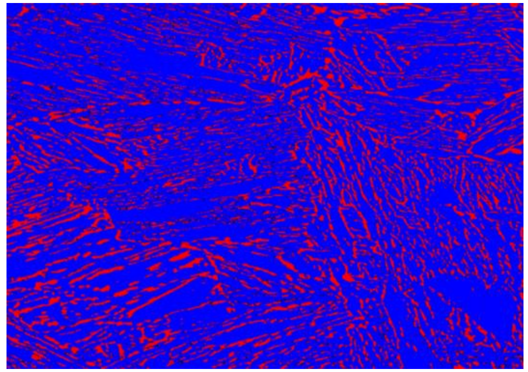




- Austenite
- Ferrite/Martensite

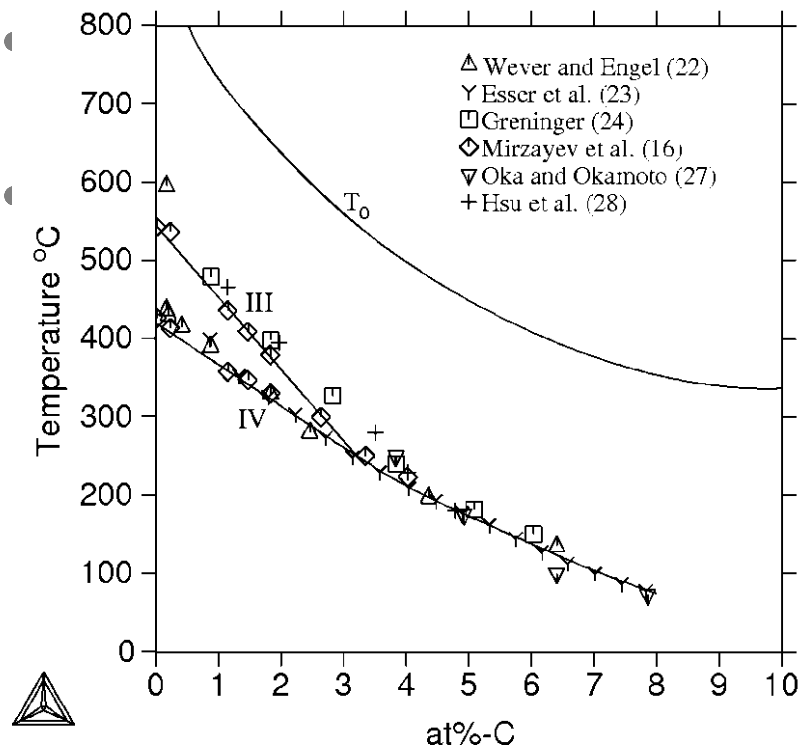
MS Calc

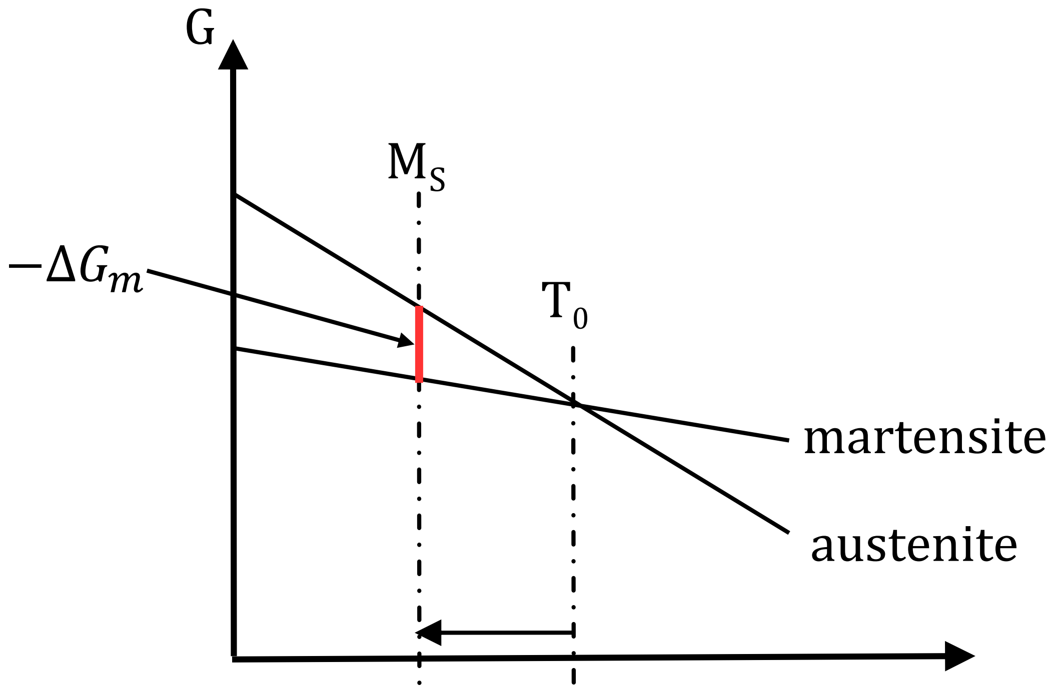
Start of martensite formation

Structure

Thermodynamics-based modeling of the martensite start temperature

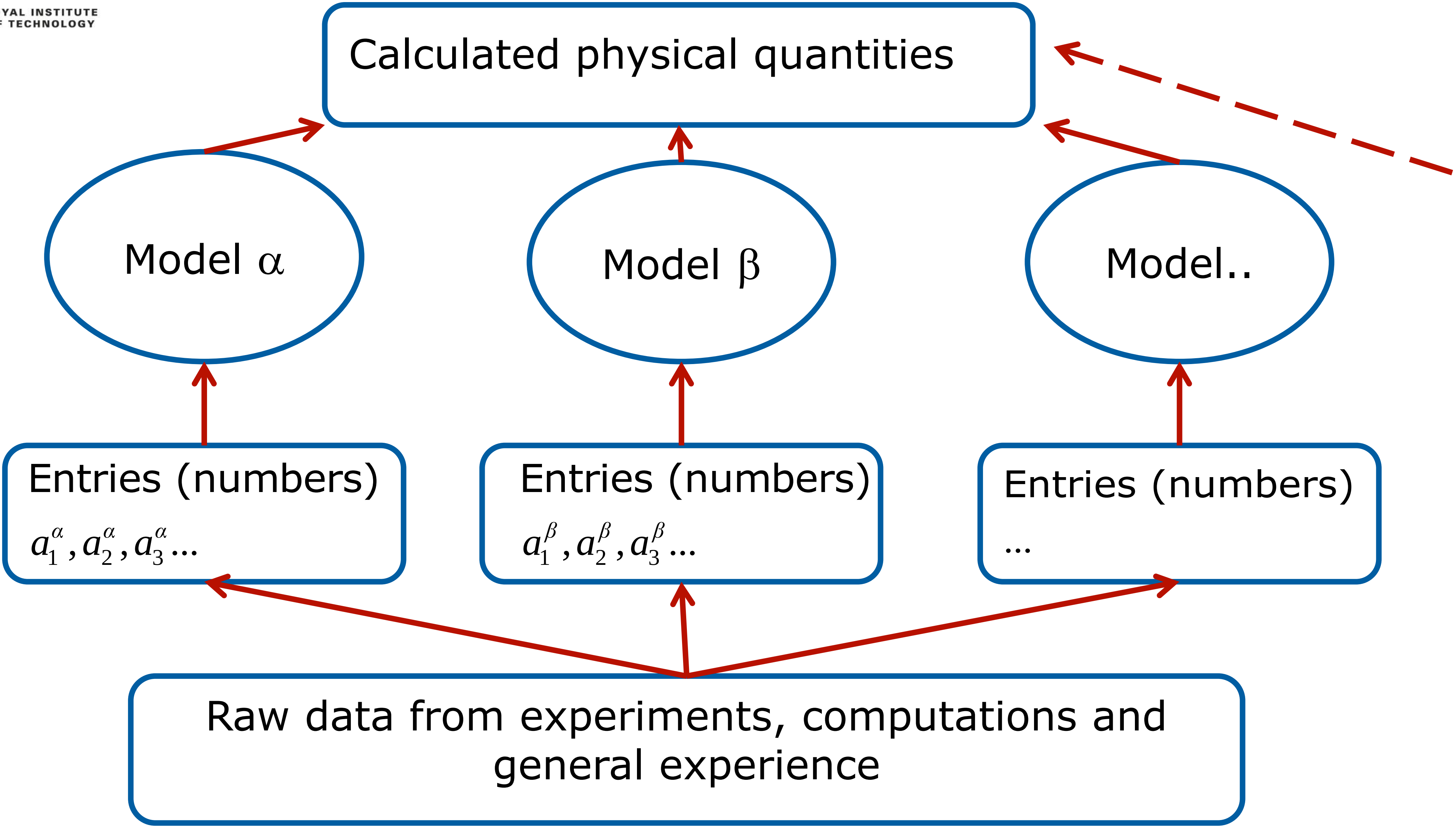
- There is a variety of models in the literature: (i) Empirical models, (ii) Neural network models and (iii) thermodynamics-based models
- Model driving force for martensitic transformation: $-\Delta G_m = G_m^{FCC} - G_m^{BCT}$





Borgenstam et al., 1997

Advanced genome databases



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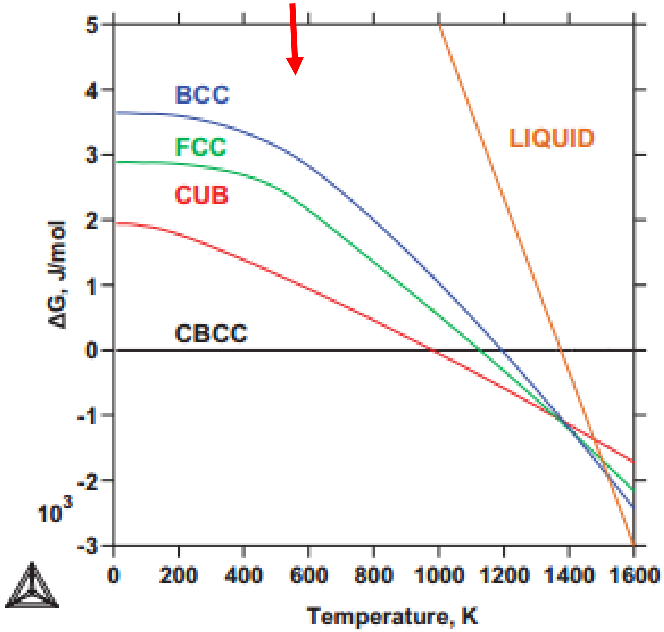
New thermodynamic descriptions

Unaries: **Cr, Ni, Mn, Co, C, Al, hcp-Fe**



- Better descriptions at low T
- More physcially based models - easier to link to ab initio
- Improve extrapolations for metastable states
- Improve description of ordering
- Improve magnetic description

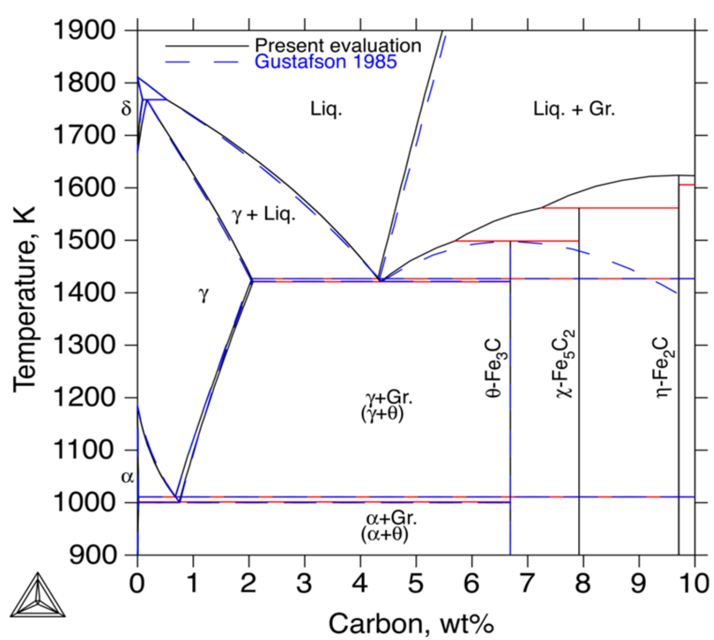
Binaries and ternaries (finished and ongoing work):

Steel: **Fe–Cr, Fe–Ni, Cr-Ni, Fe-Cr-Ni**

Fe–Mn, Mn–C, Fe-Mn–C, Fe-C

Al–Fe, Al–C, Al–Mn

Cemented carbides: **Co–Cr, Co-C, Cr–C, C-Co-Cr**



Bigdeli et al., 2016 Naghari et al., 2014

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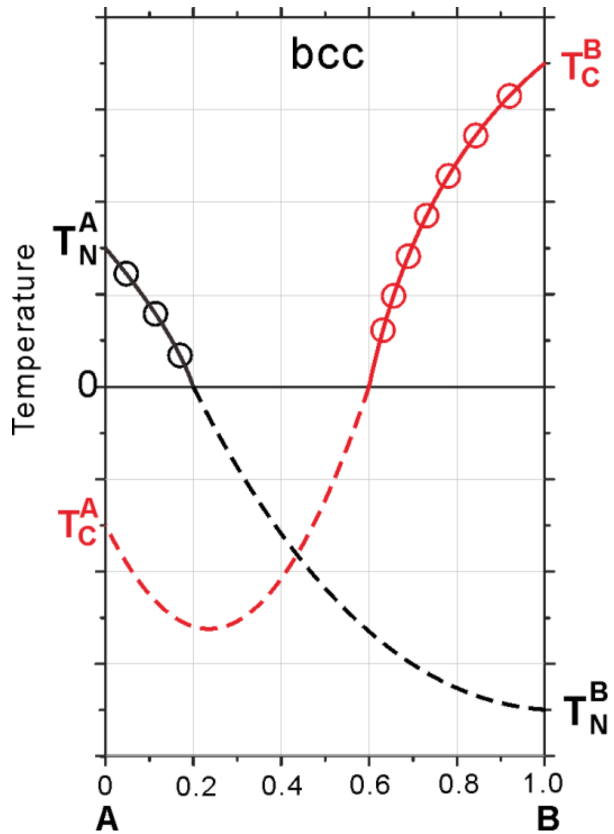
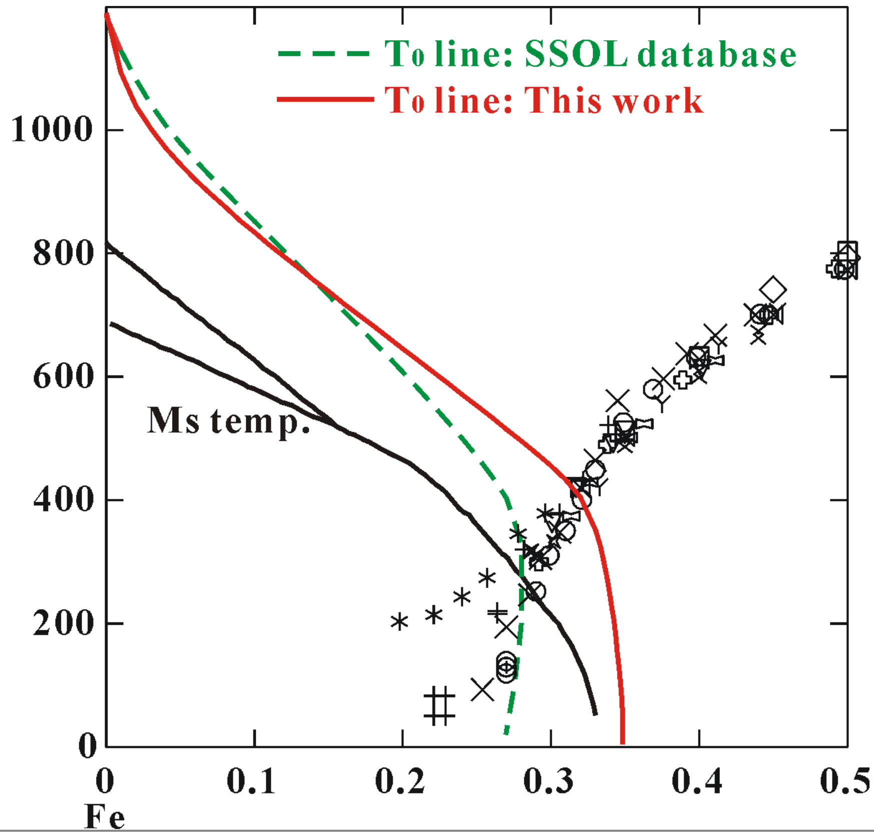
Revised magnetic model

- Use separate R-K polynomials for each magnetic state for each phase
- No contribution to Gibbs energy when T is negative
- Use effective/local magnetic moment and not mean magnetic moment.





Xiong et al., 2012

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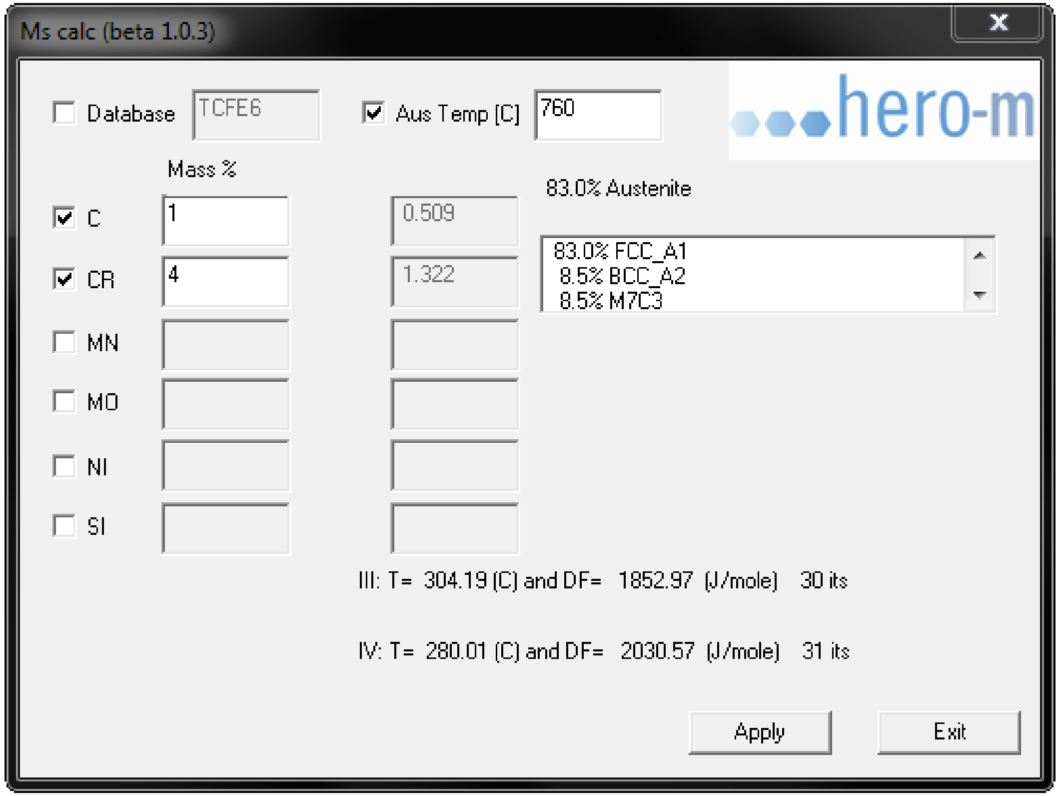
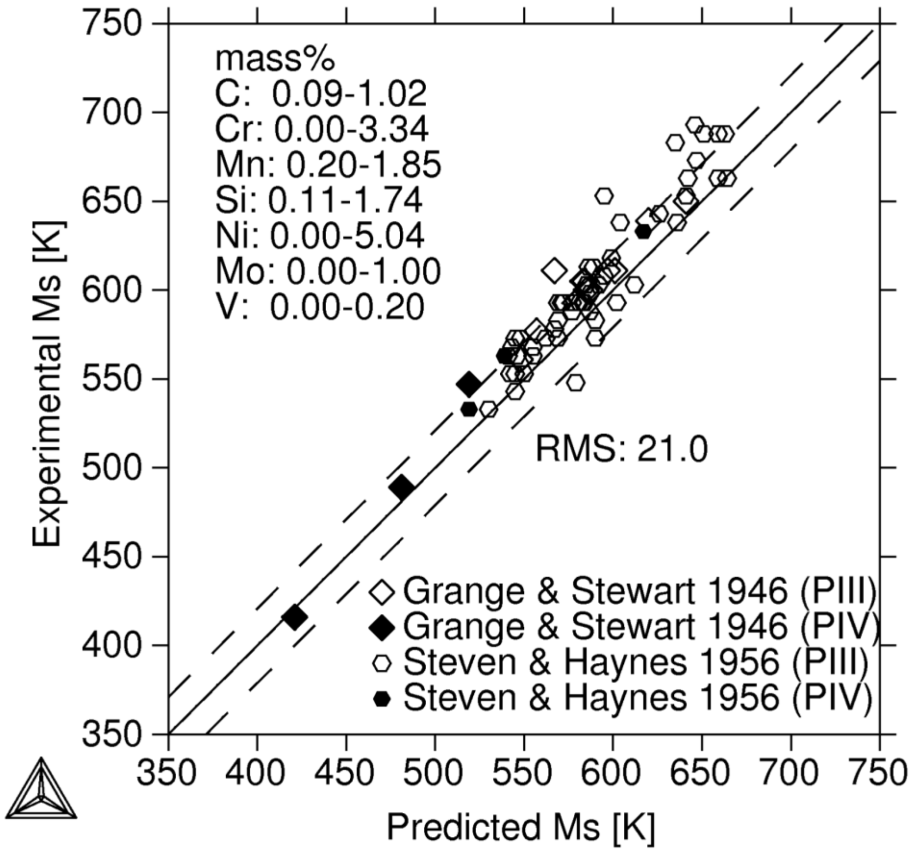
Calculation of start temperature of martensitic structure

$$\Delta G_{m(Lath)}^{\gamma\rightarrow\alpha} = 3640 - 2.92M_S + 346400\frac{{x_C}^2}{(1-x_C)} - 16430x_C - 785.5x_{Cr} + 7119x_{Mn} - 4306x_{Ni} + 350600x_C\frac{x_{Cr}}{(1-x_C)}, \text{[J/mol]}$$

$$-\Delta G_{\mathrm{m}}^{\mathrm{plate}}(M_s) = 2100 - 75000\frac{x_C^2}{1-x_C} - 11500x_C - 2970x_{Cr} + 3574x_{Mn} - 5104x_{Ni} + 441700x_C\frac{x_{Cr}}{1-x_C}$$





Stormvinter et al., 2012

Effect of thin-film austenite grain size on M_s

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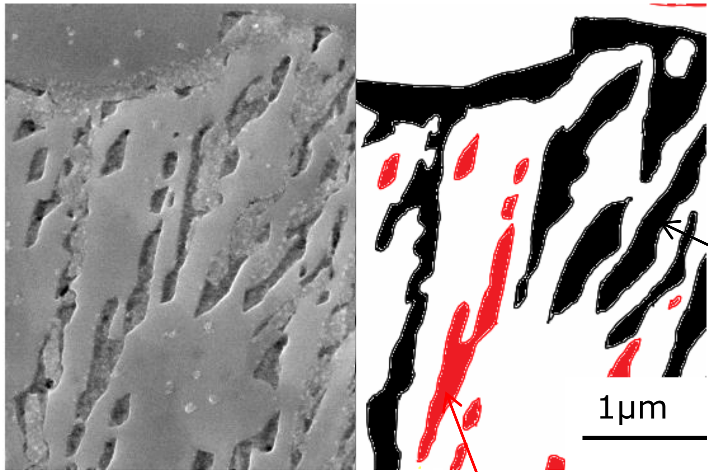
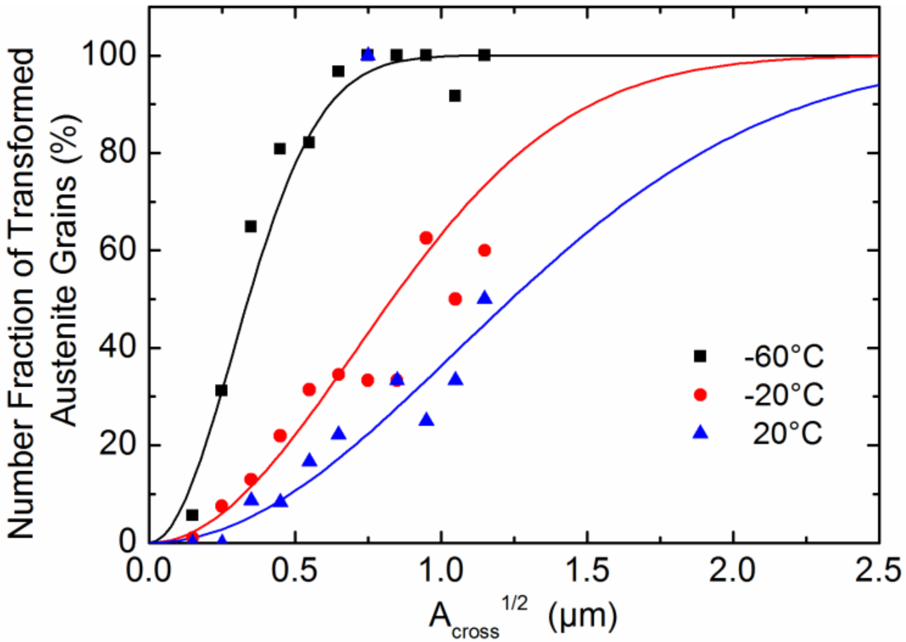
Dispersed γ:
isolated, limited autocatalysis
similar to particles



0.18C–5.08Mn
IA 680°C 5min,
Quenched to -60°C

transformed

untransformed



$$F = 1 - exp(-C\left(\Delta G^{ex}\right)^{m} A_{surf}) \rightarrow$$

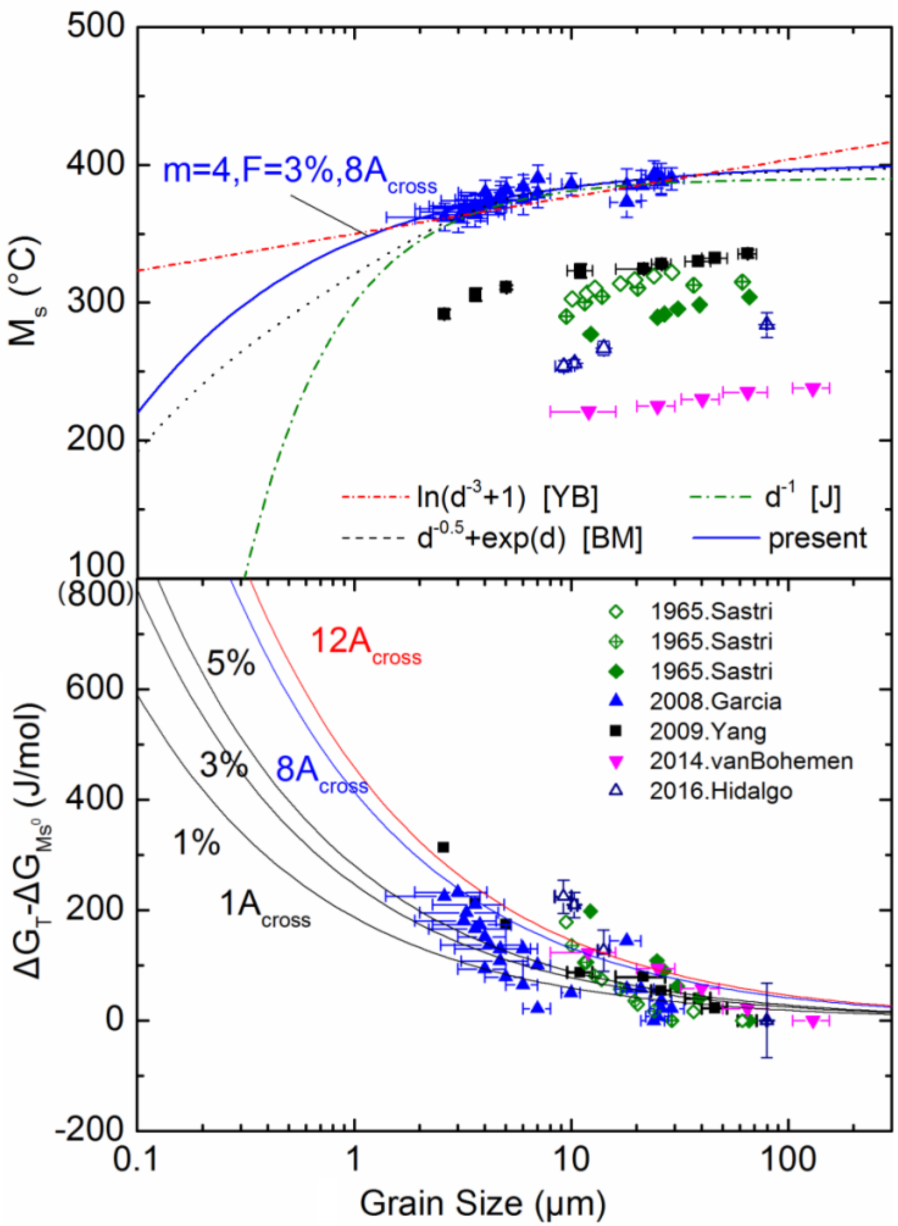
$$\Delta G^{ex} = \Delta G_{T}^{ch} - \Delta G_{M_s^0}^{ch} = -\left[-\frac{ln(1-F)}{C}\right]^{\frac{1}{m}} A_{surf}^{-\frac{1}{m}}$$

F: transformed number fraction of grains
A_{surf}: surface area

Chen et al. *Acta Metall.* 1985

Huyan et al., 2018

Effect of austenite grain size on M_s



$$\Delta G^{ex} = -\left[-\frac{\ln(1-F)}{C} \right]^{\frac{1}{m}} A_{surf}^{-\frac{1}{m}}$$

Influence of γ size (area):

$$\Delta G^{ex} = \Delta G_T^{ch} - \Delta G_{Ms}^{ch} = 415.1 A_{cross}^{-\frac{1}{4}}$$

Yang & Bhadeshia, *Scr. Mater.* 2009
Jimenez-Melero et al., *Acta Mater.* 2009
van Bohemen, Morsdorf, *Acta Mater.* 2017

Huyan et al., 2018

KTH VETENSKAP OCH KONST
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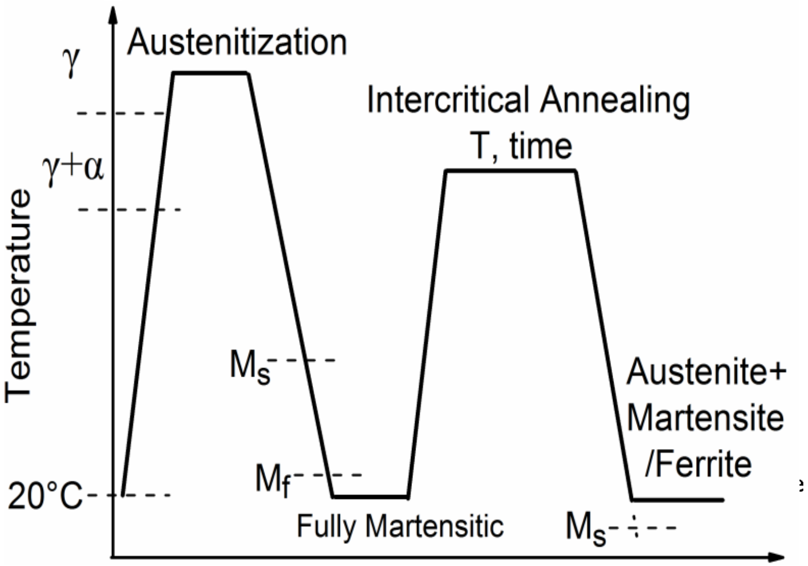
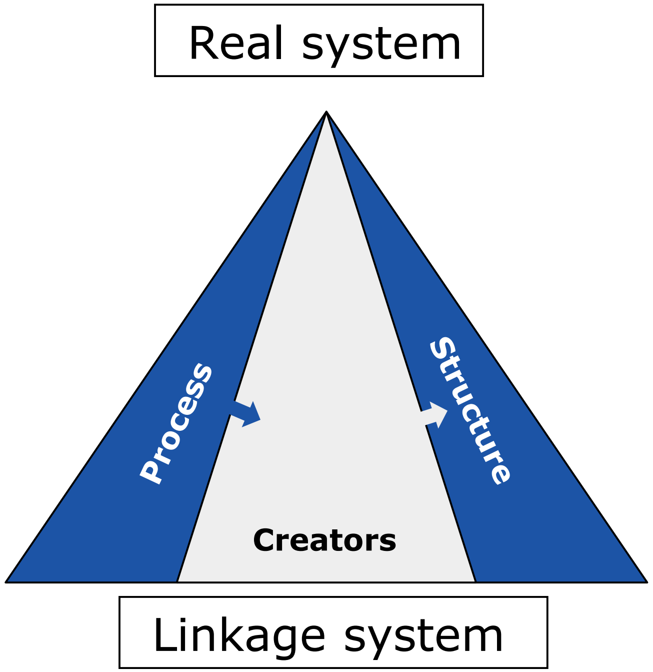
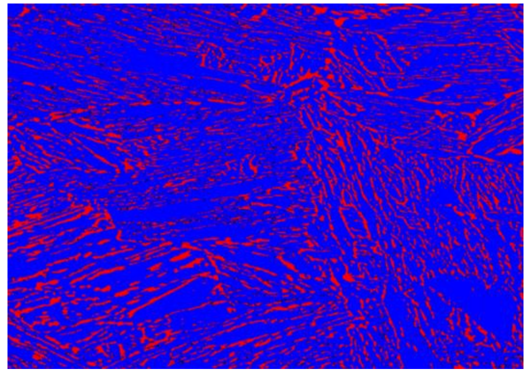
Models needed for design of a Martensitic TRIP steel



- .....
- Cold rolling
- Austenitization
- Quenching
- Intercritical annealing
- Quenching





- Austenite
- Ferrite/Martensite

Structure

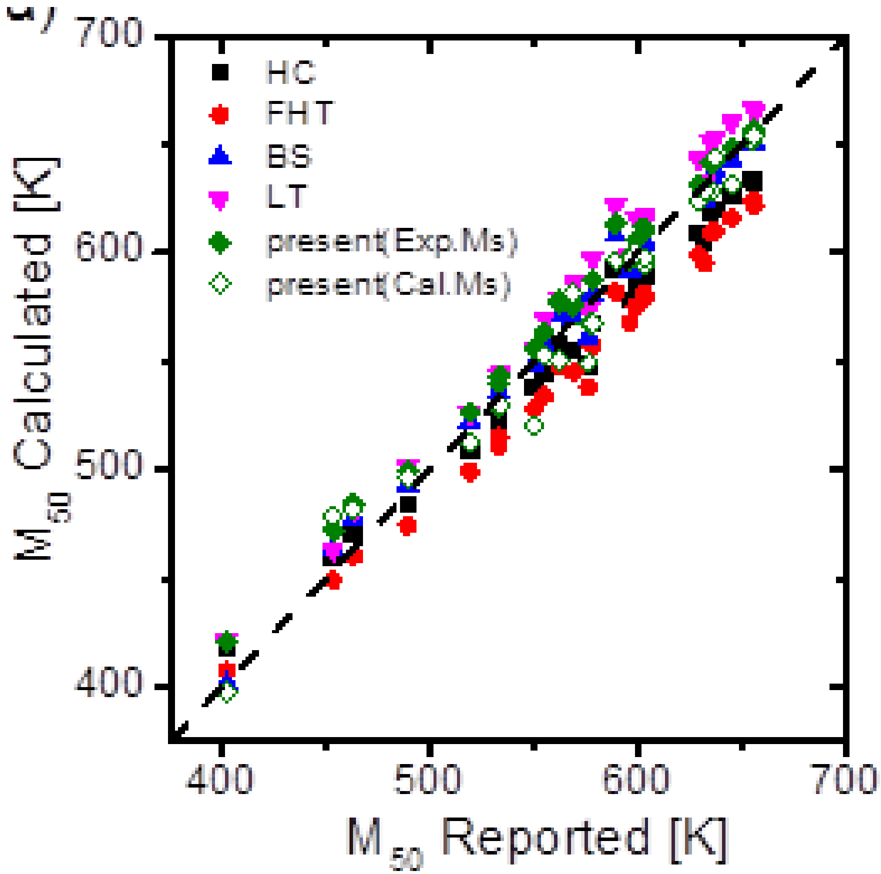
Fraction of martensite

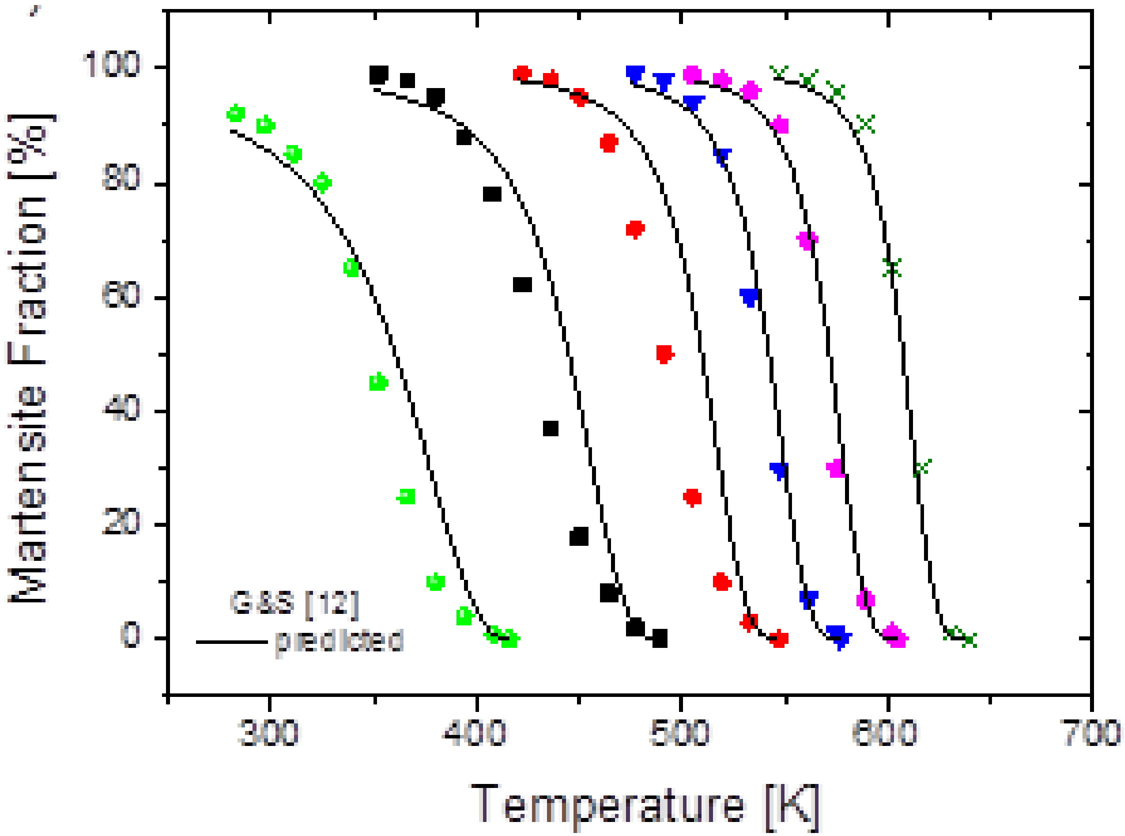
MS Frac

Fraction of martensite formed below Ms

$$f(M\%) = 100 - \frac{100}{1 + 0.05 * \left(\frac{\Delta G}{100}\right)^{b}} \qquad \Delta G = \Delta G(T) - \Delta G(\mathrm{Ms})$$

b=0.006*Ms+1.205





Huyan et al., 2014

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Martensite formation model for steels currently under development at Thermo-Calc Software

- Extend existing models to provide a semi-empirical prediction of M_s with a solid foundation in CALPHAD-thermodynamics
- Fe-based binary and some ternary systems for: Fe,Cr,Ni,Mn,C,Cu,Co,N,Mo,Al,Si,V,W,Ti,Nb
- Lath, plate and epsilon martensite
- M_s, M_f and phase fraction including effect of austenite grain size

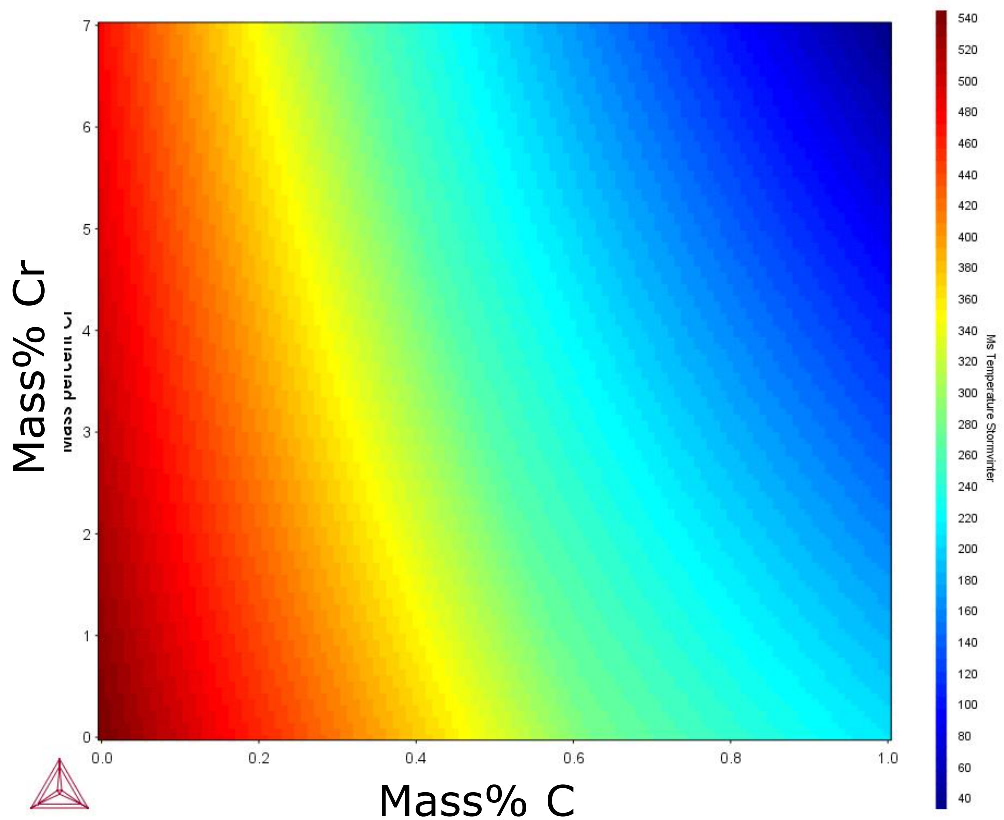
Plate Martensite:

$$\Delta G^{*\gamma\rightarrow\alpha}_{m(Plate)} = 2100 + P_{C1}x_C + P_{C2}\frac{x_C^2}{(1-x_C-x_N)} + P_{Cr}x_{Cr} + P_{Mn}x_{Mn} + P_{Ni}x_{Ni} + P_{Ni2}\frac{x_{Ni}^2}{(1-x_C-x_N)} + P_{Cr,C}x_C\frac{x_{Cr}}{(1-x_C-x_N)} + P_{co}x_{Co} + P_{Ni,Cr}x_{Ni}x_{cr} + P_{Co2}\frac{x_{Co}^2}{(1-x_C-x_N)} + P_{Ni,Co}x_{Ni}x_{Co} + P_{Al}x_{Al} + P_{Si}x_{Si}$$

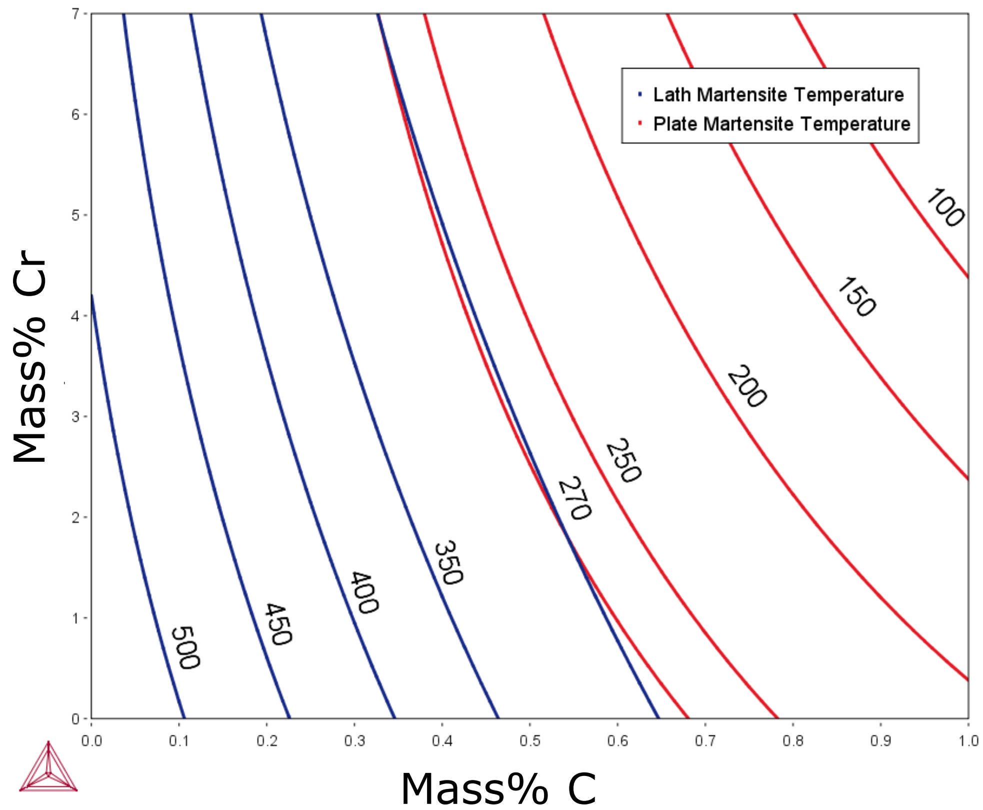
Lath Martensite:

$$\Delta G^{*\gamma\rightarrow\alpha}_{m(Lath)} = 3640 - 2.92M_s + L_Cx_C + L_{C2}\frac{x_C^2}{(1-x_C-x_N)} + L_{Cr}x_{Cr} + L_{Mn}x_{Mn} + L_{Ni1}x_{Ni} + L_{Ni2}\frac{x_{Ni}^2}{(1-x_C-x_N)} + L_{Cr,C}x_C\frac{x_{Cr}}{(1-x_C-x_N)} + L_{Co}x_{Co} + L_Nx_N + L_{Co2}\frac{x_{Co}^2}{(1-x_C-x_N)} + L_{Mo}x_{Mo} + L_{Ni,Co}x_{Ni}x_{Co} + L_{Ni,Cr}x_{Ni}x_{Cr} + L_{Ni,C}x_C\frac{x_{Ni}}{(1-x_C-x_N)} + L_{Si}x_{Si}$$

Thermo-Calc property models- Results from M_s model



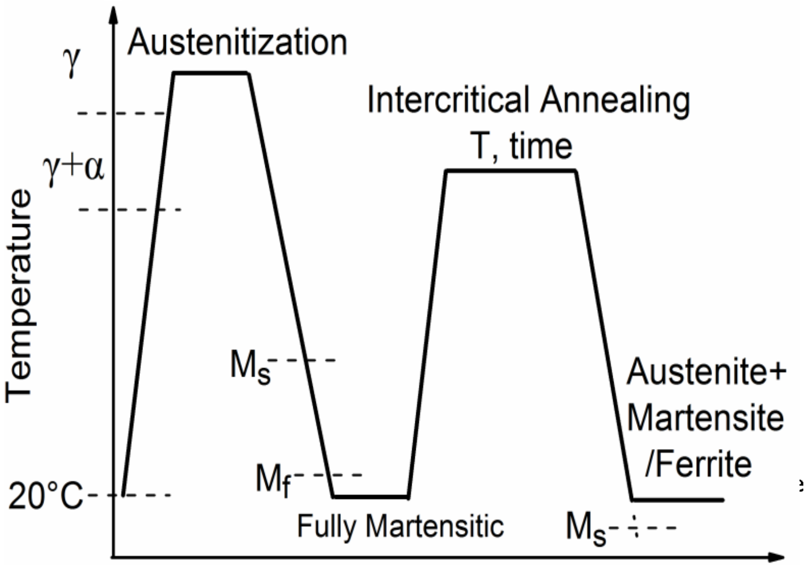
Heat map of M_s

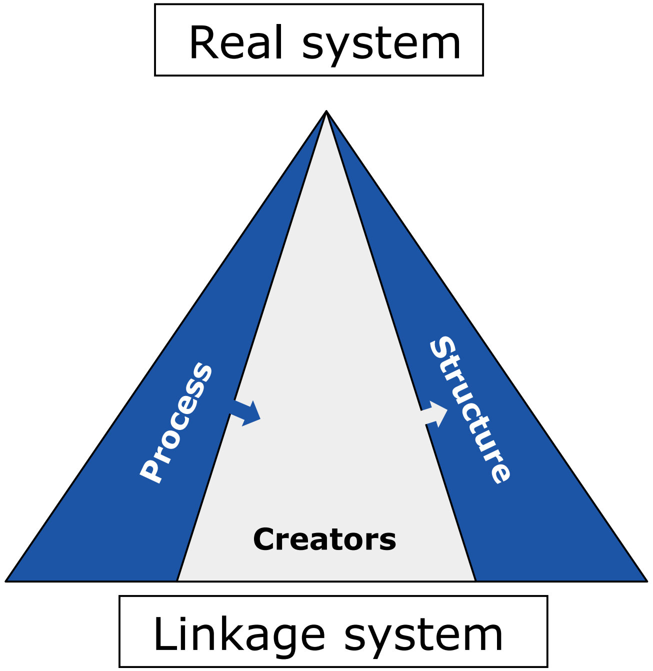


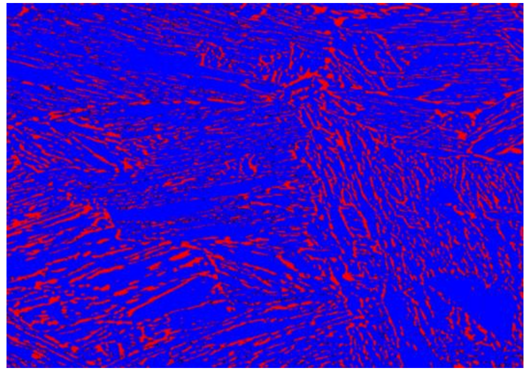
Contour plot of M_s- Lath, Plate

Jeppsson et al., 2017

Models needed for design of a Martensitic TRIP steel







- Austenite
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- .....
- Cold rolling
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- Intercritical annealing
- Quenching

Structure

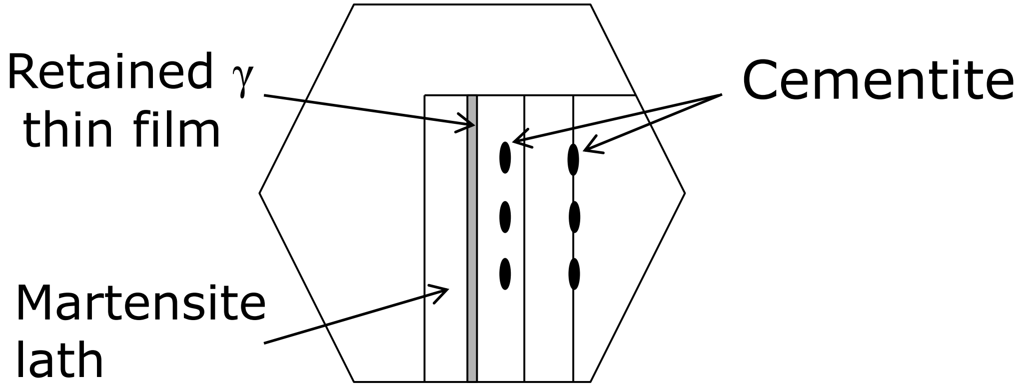
Formation of austenite

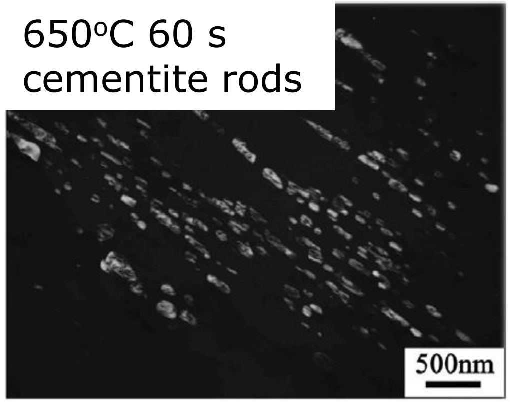
Formation of carbides

Thermo-Calc

DICTRA

Modelling of austenite growth during intercritical annealing of martensite

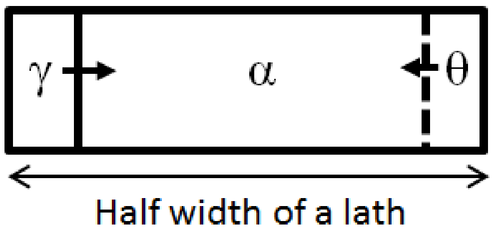




Fe-0.2C-4.72Mn (wt%)
Luo et al. *Acta Mater.* **59** (2011) 4002

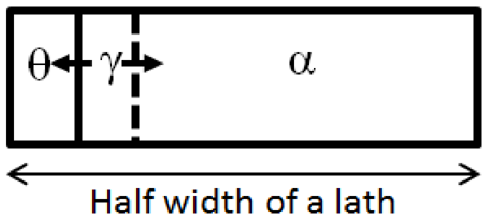
DICTRA:

Set-up A - γα[iθ]



Growth of retained γ thin films

Set-up B - θ[iγ]α



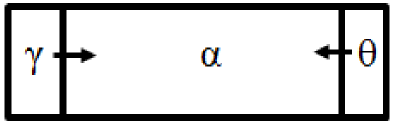
Nucleation of γ at θ/α

Only influence of cementite on austenite formation is considered, not aiming for exact cementite formation and dissolution

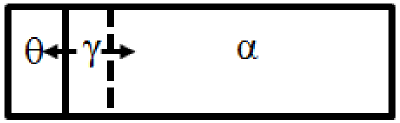
Huyan et al., 2017

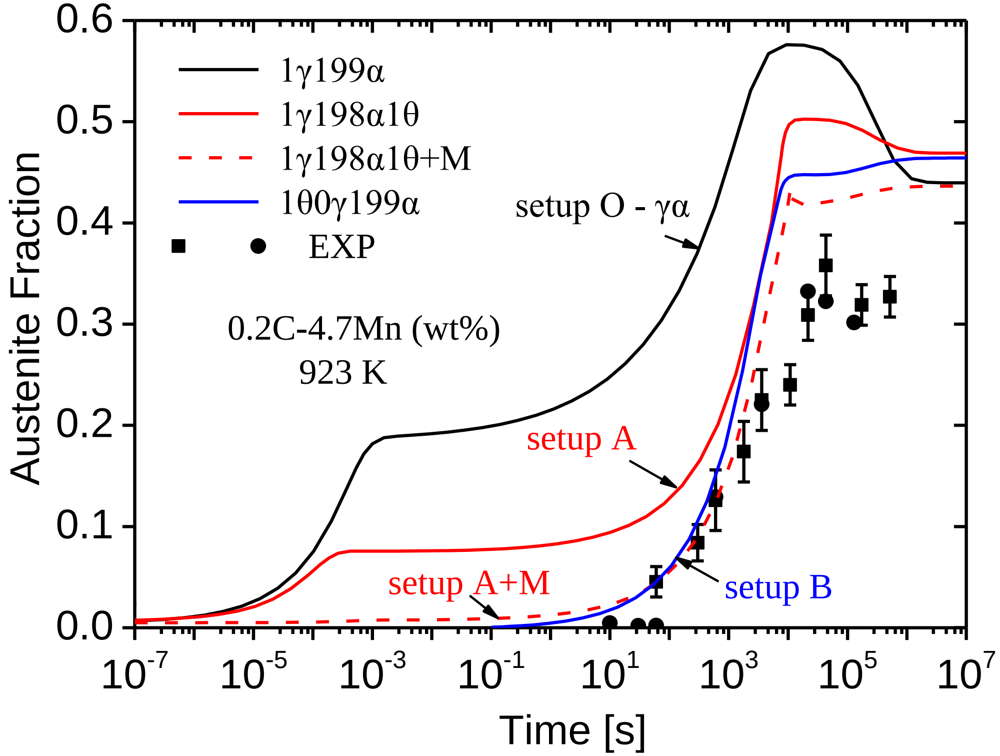
Modelling of austenite growth during intercritical annealing of martensite

Setup A - γαθ

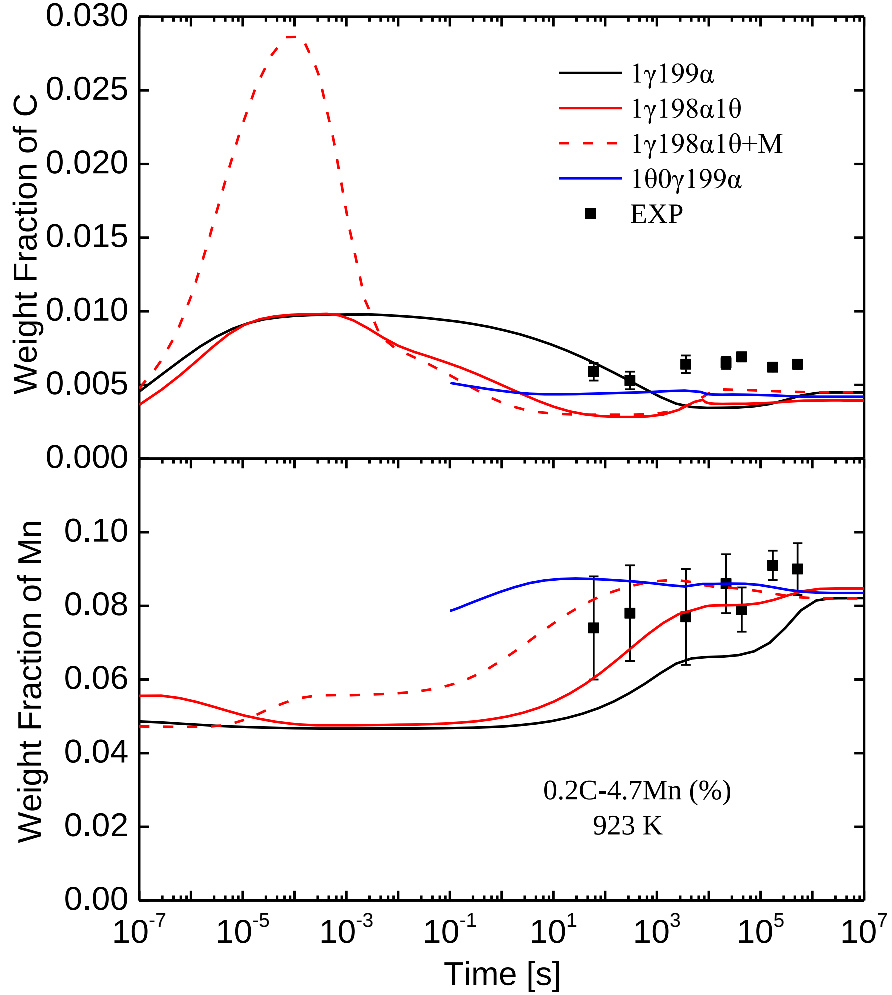


Setup B - θγα





Fraction of γ as function of time

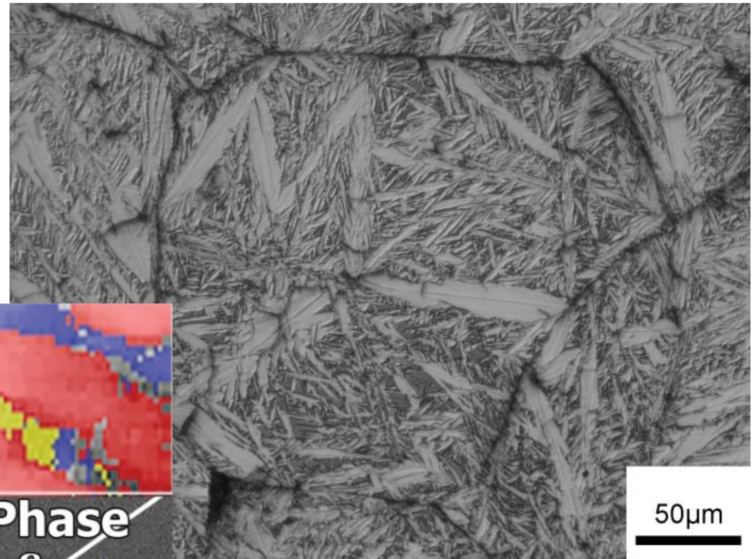


Change in C and Mn content in γ with time

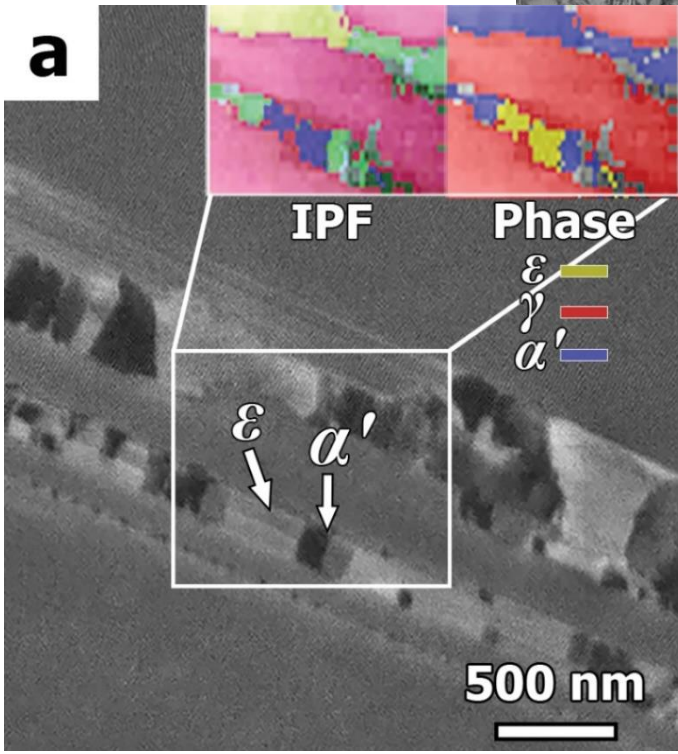
Huyan et al., 2017

Microstructure design tools

- Equilibrium structures and driving forces for non equilibrium (thermodynamics)
  - Stresses (external and internal)
  - Interfaces
- Phase field
- Prisma
- DICTRA

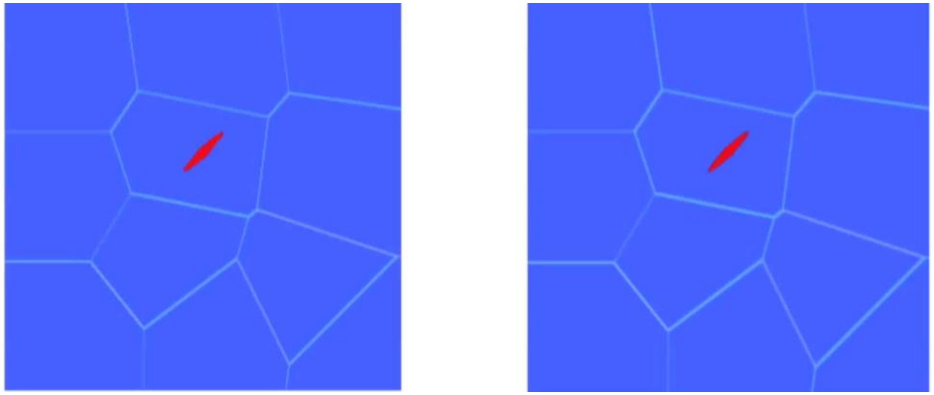


Stormvinter et al.

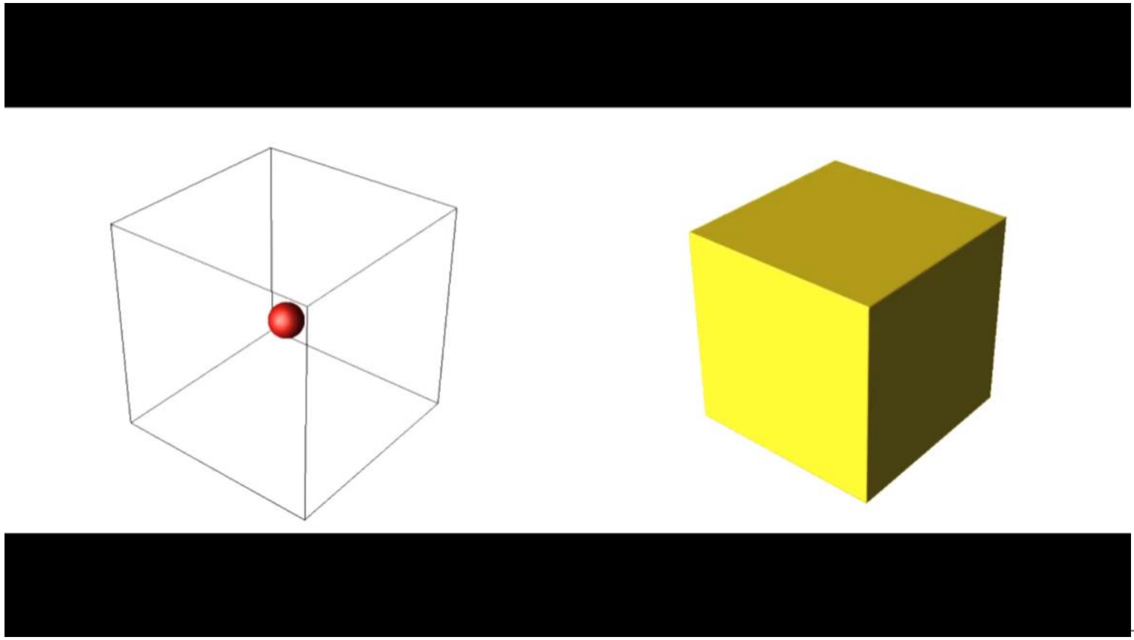


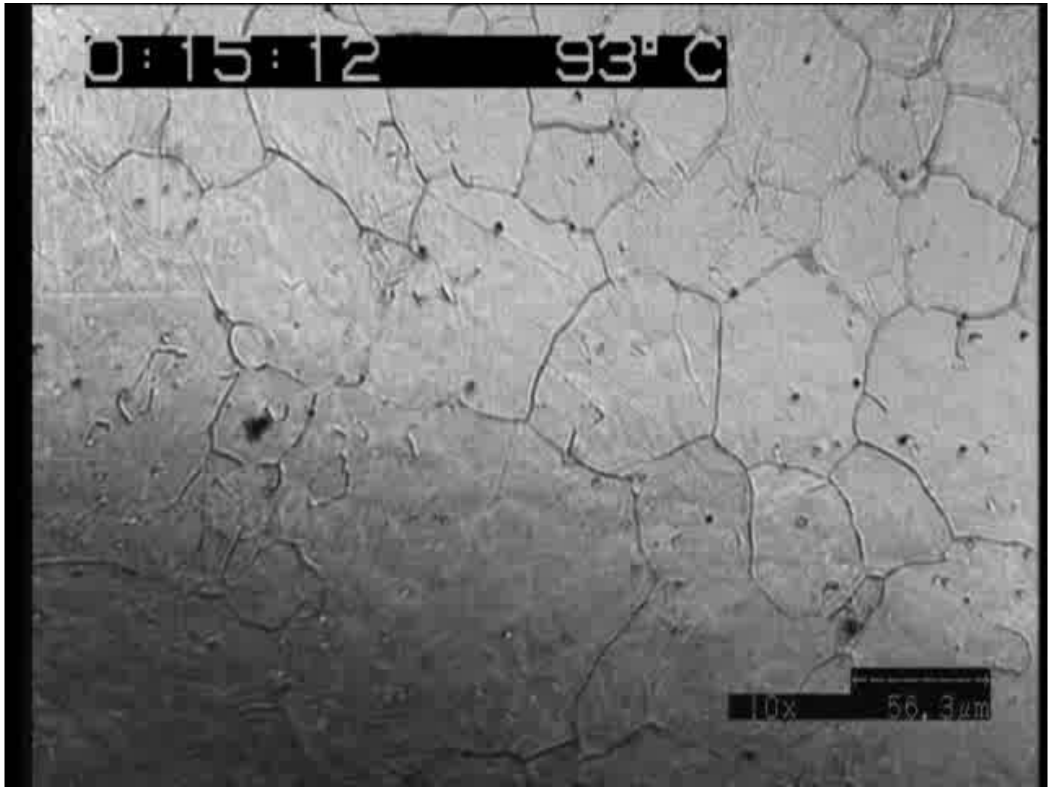
Ye et al.

Phase-field simulations of martensite compared to experiments



Malik et al.





Kolmskog et al.

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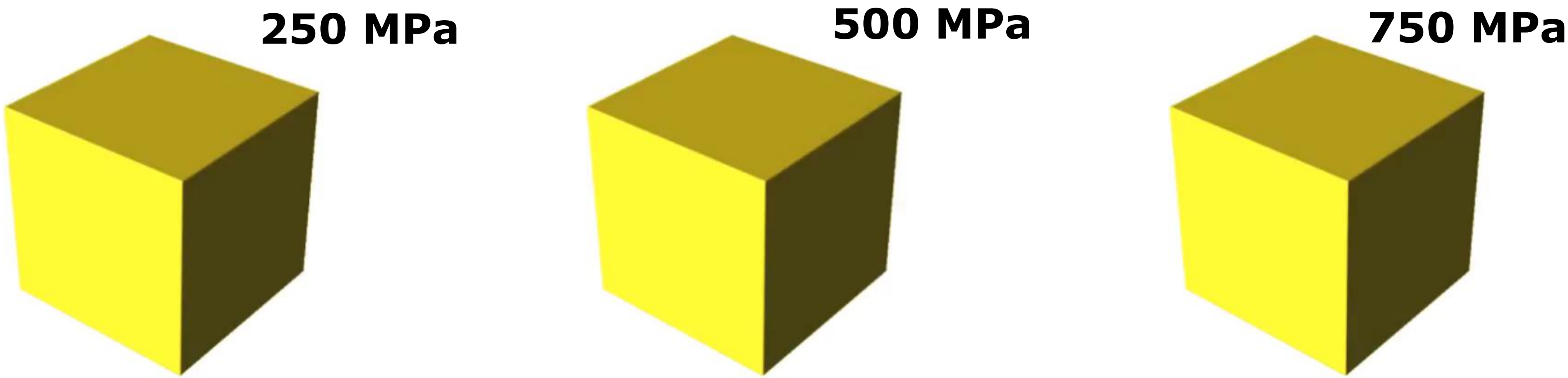
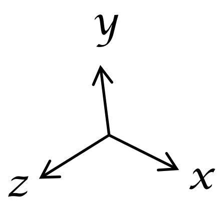
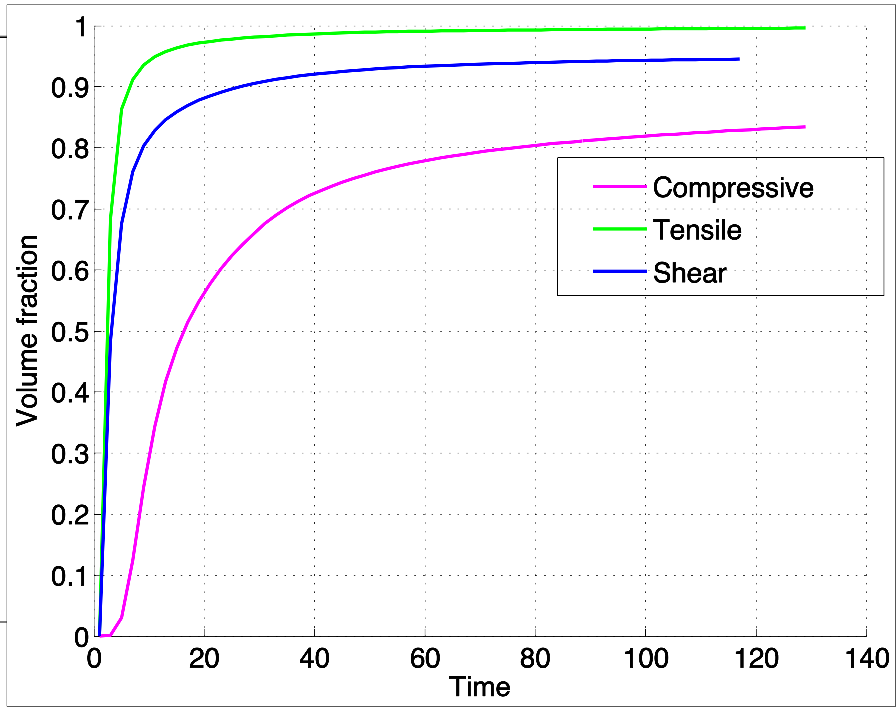
Effect of Tensile Loading- 3D





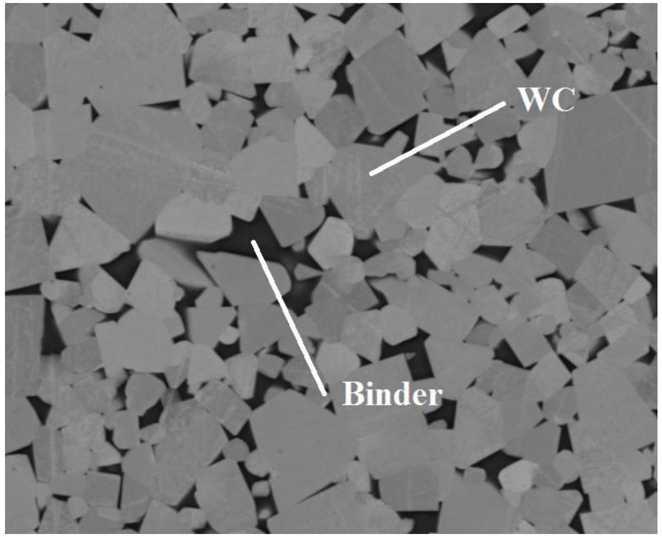
- Austenite
- Martensite-V1
- Martensite-V2
- Martensite-V3



Malik et al., 2013

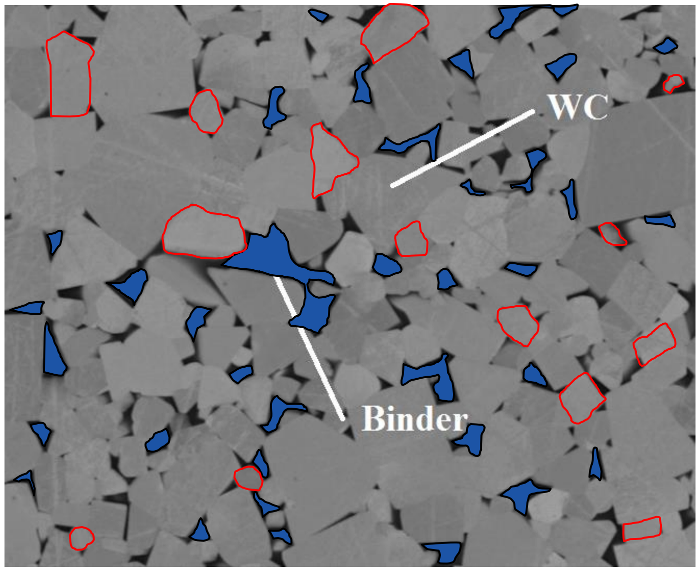
hero-m

Cemented carbides

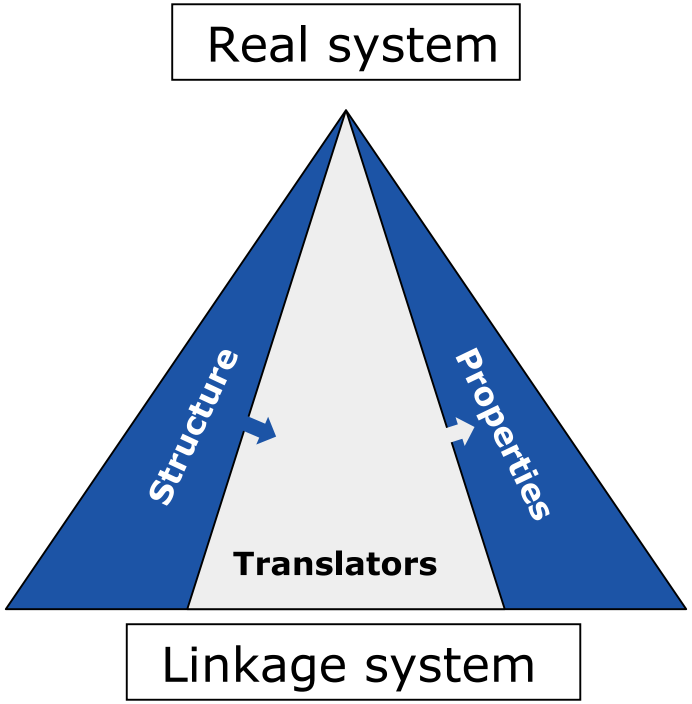


- Used for rock drilling and metal cutting applications
- WC + metallic binder (usually Co)
- Co is toxic, longtime exposure may cause serious health problems.
- Co may become banned in EU.
- Expensive and uncertain raw material supply
- Substitute Co
- Using materials design to tailor properties for metal cutting and rock drilling applications

Models needed for design of alternative binders in cemented carbides



- Binder volume fraction
- WC grain size
- Binder & overall composition



Toughness

Thermo-Calc

Solid solution hardening

DICTRA

Grain Growth model → Hall-Petch

Hardness

TC-PRISMA → Precipitation hardening

Martensite formation ← MS Calc

Work hardening

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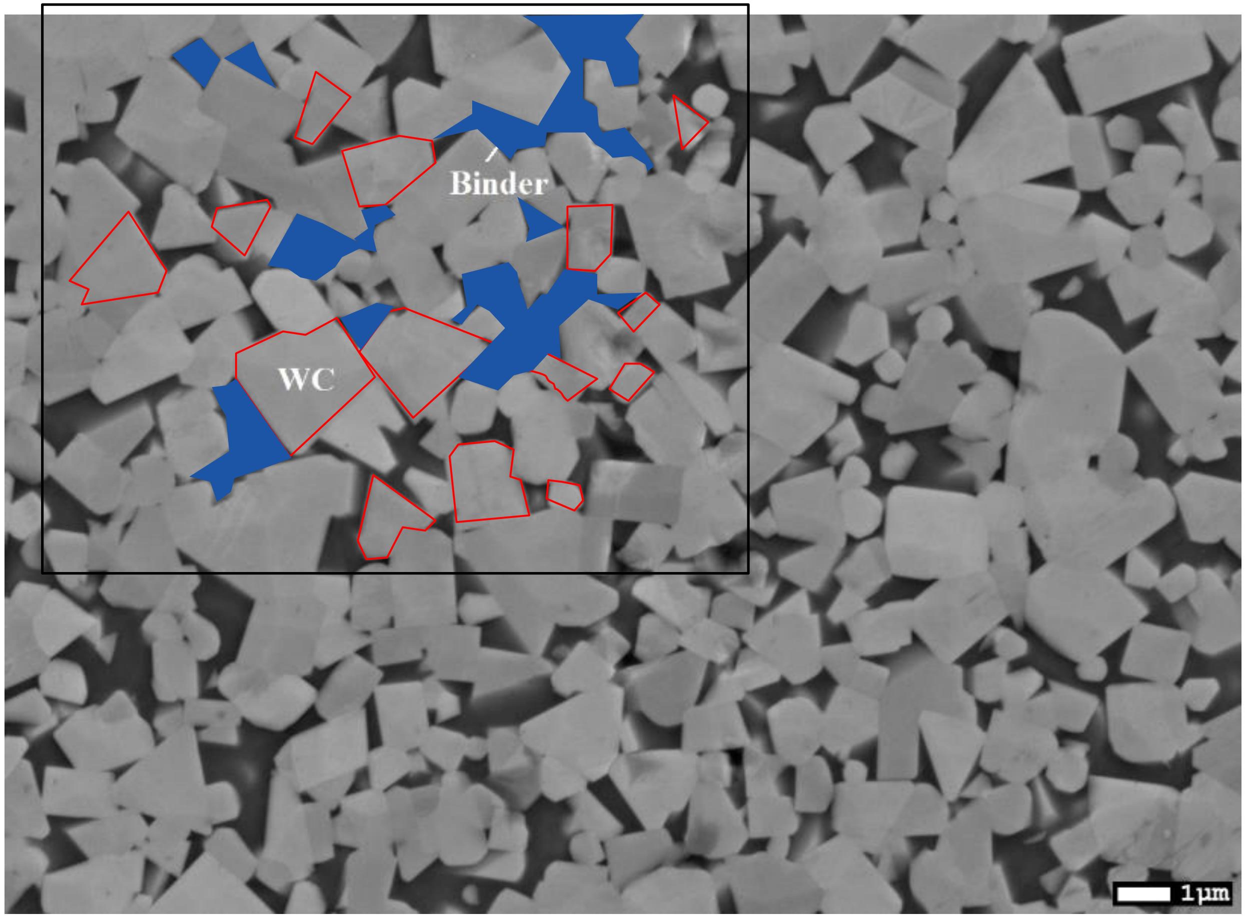
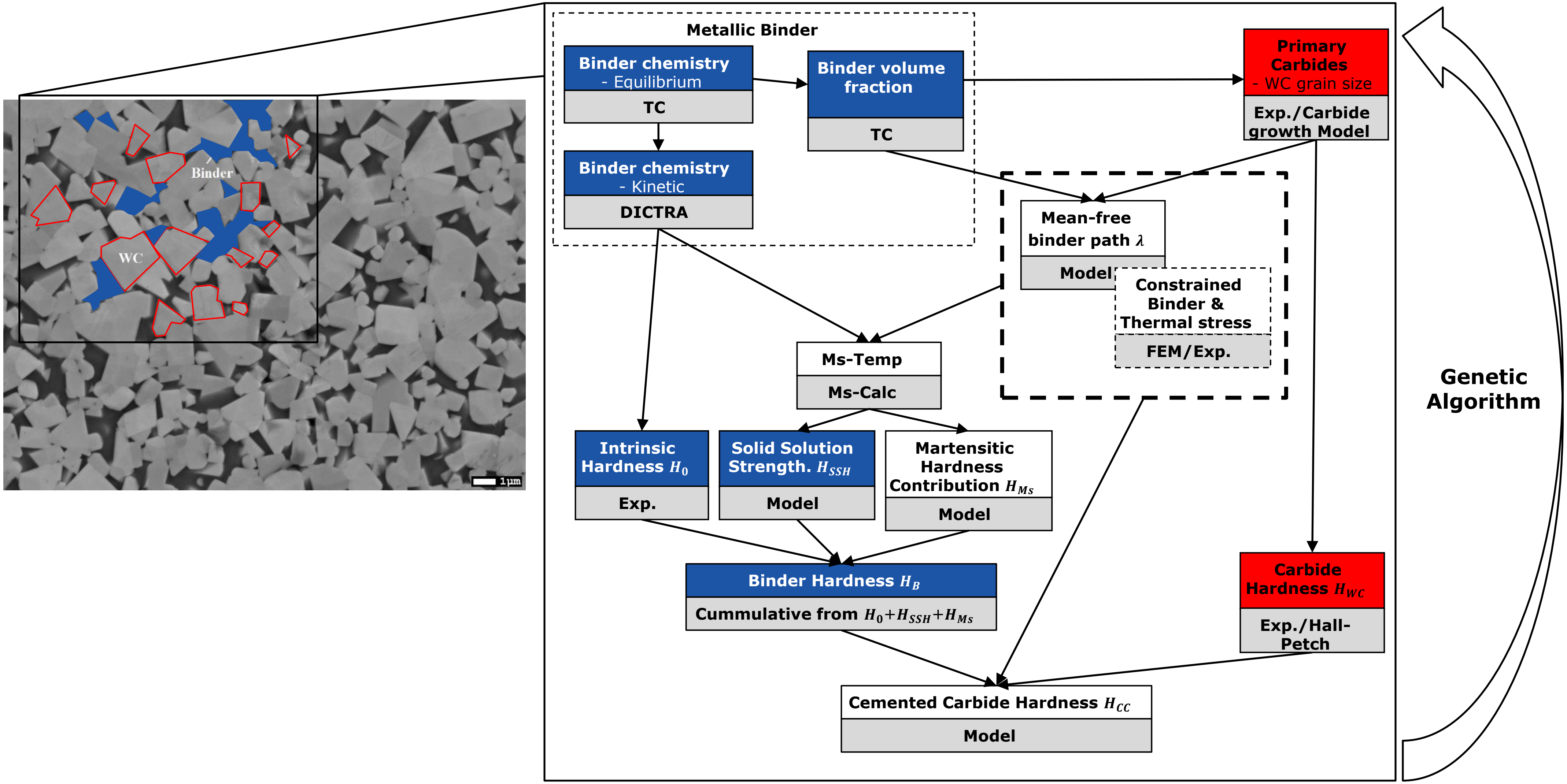
Designing cemented carbides with respect to hardness



- What is the hardness of such composite material?

- Parameters:
  - Hardness of the binder
  - Hardness of the carbides
  - Constrained effects
  - Size of the non-spherical carbides
  - Binder chemistry
  - Diffusivities
  - Sintering time
  - Sintering temperature
  - …

ICME framework for designing cemented carbides with respect to hardness



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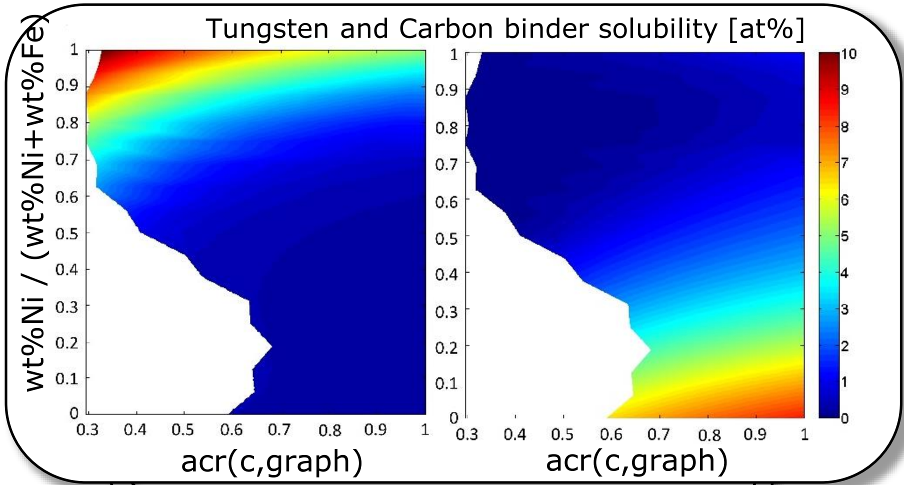
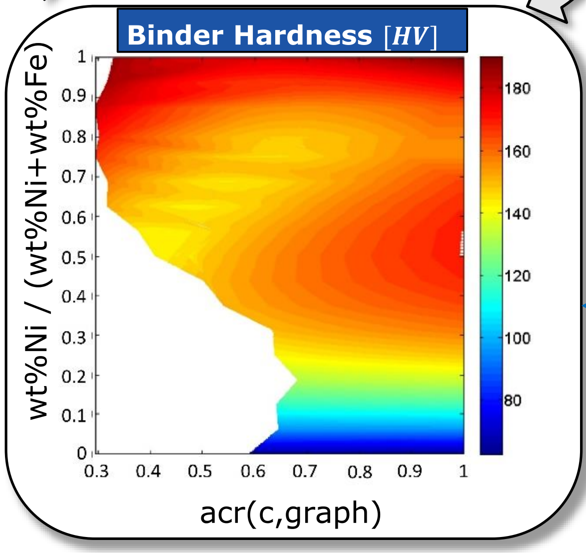
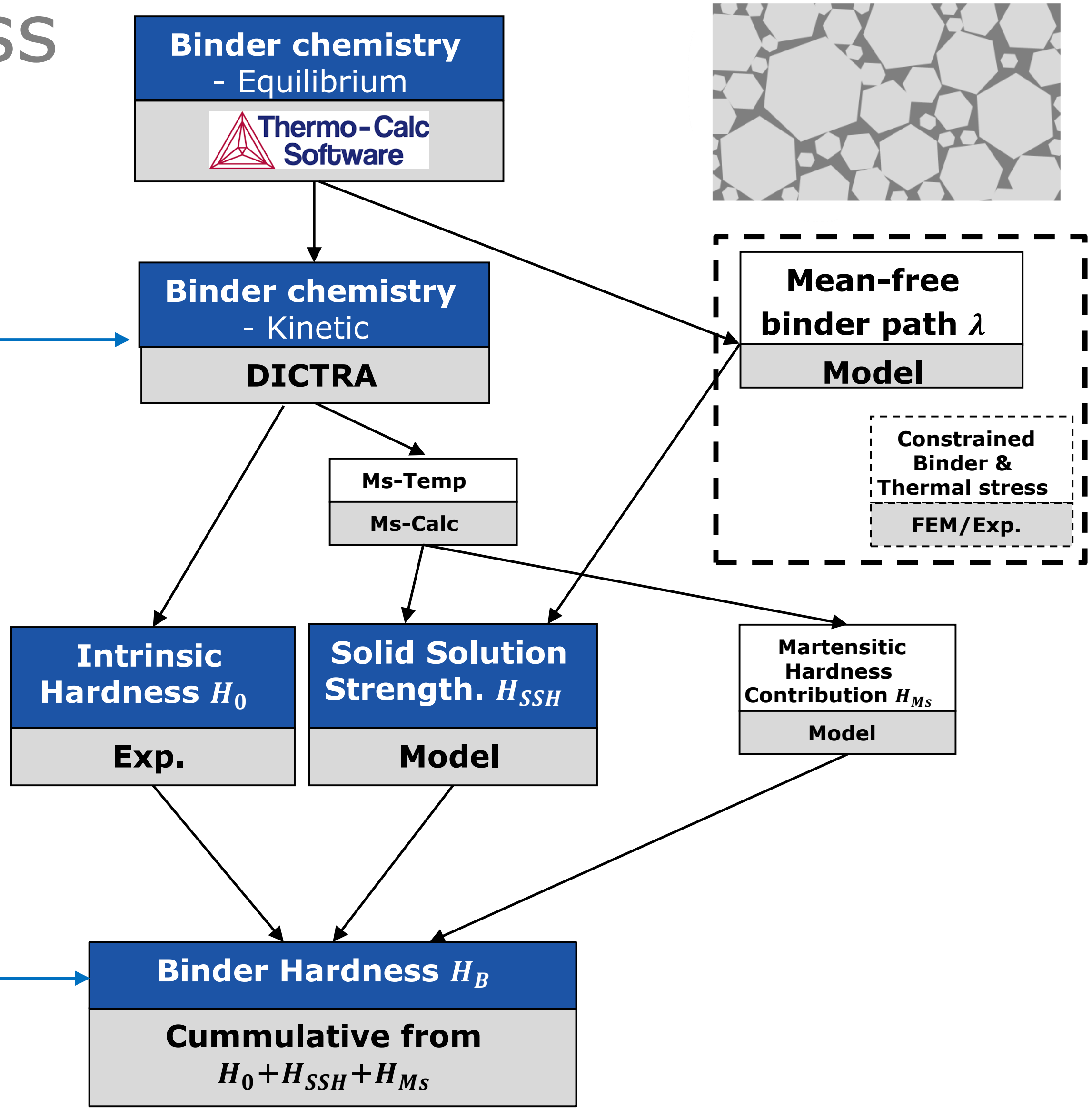
Binder Hardness







Walbrühl et al., 2017

Modelling of solid solution strengthening in multicomponent alloys, H_{SSH}

E.g. solution hardening (use the ”compound energy formalism”). For

Formula unit: $(M_1M_2...)(C,N,Va)_b$

Yield stress

$$\sigma_y = \sum_{ij} y_i^{'} y_j^{''} \sigma_{yij}^{\circ} + \Delta\sigma_y^{SSH}$$

$$\Delta\sigma_y^{SSH} = \sum_{ij}\sum_{k} \left(y_i^{'} y_j^{'}\right)^n y_k^{''} A_{ijk} + \sum_{i}\sum_{k\ell} y_i^{'} \left(y_k^{''} y_\ell^{''}\right)^m A_{ik\ell}$$

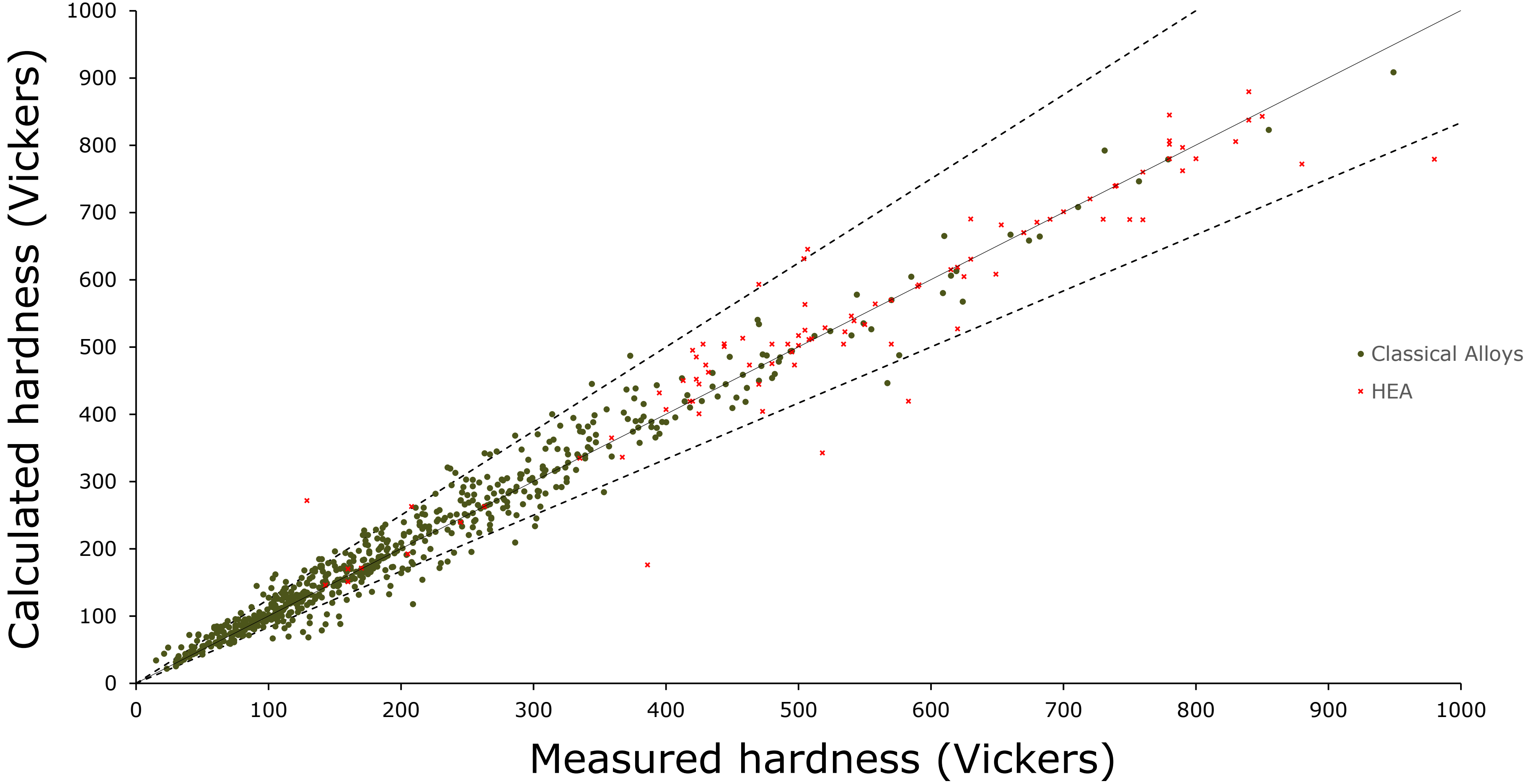
In classical models

$n = m = 2/3$

and the A parameters represent a combination of mismatch in lattice parameter and elastic constants. Here they are taken as adjustable parameters!

Walbrühl et al., 2017

Modelling of solid solution strengthening in multicomponent alloys, H_{SSH}



Walbrühl et al., 2017

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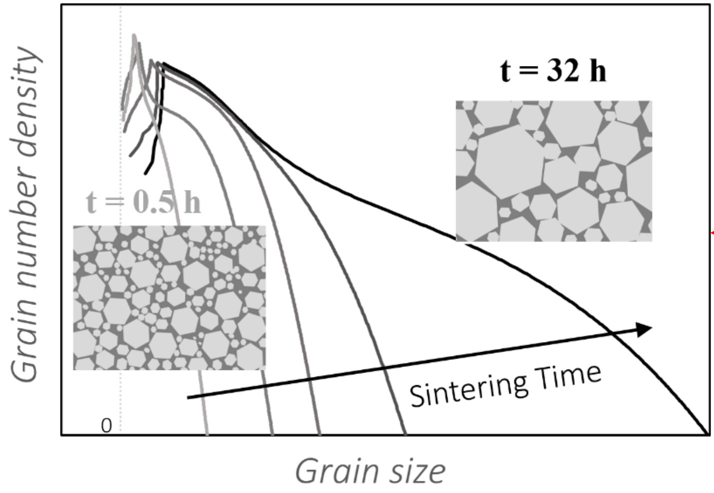
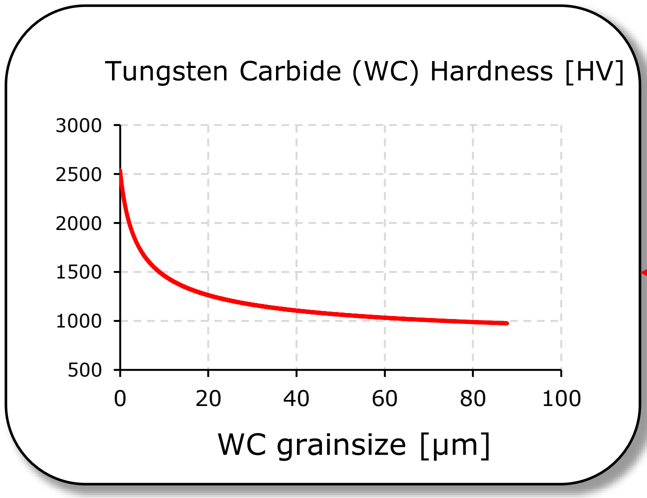
Carbide hardness





Binder chemistry
- Equilibrium

Thermo-Calc Software

Primary Carbides
- WC grain size

Exp./Mean-field Kampmann-Wagner approach

Carbide Hardness
H_{WC}

Exp./Hall-Petch

Bonvalet et al., 2018

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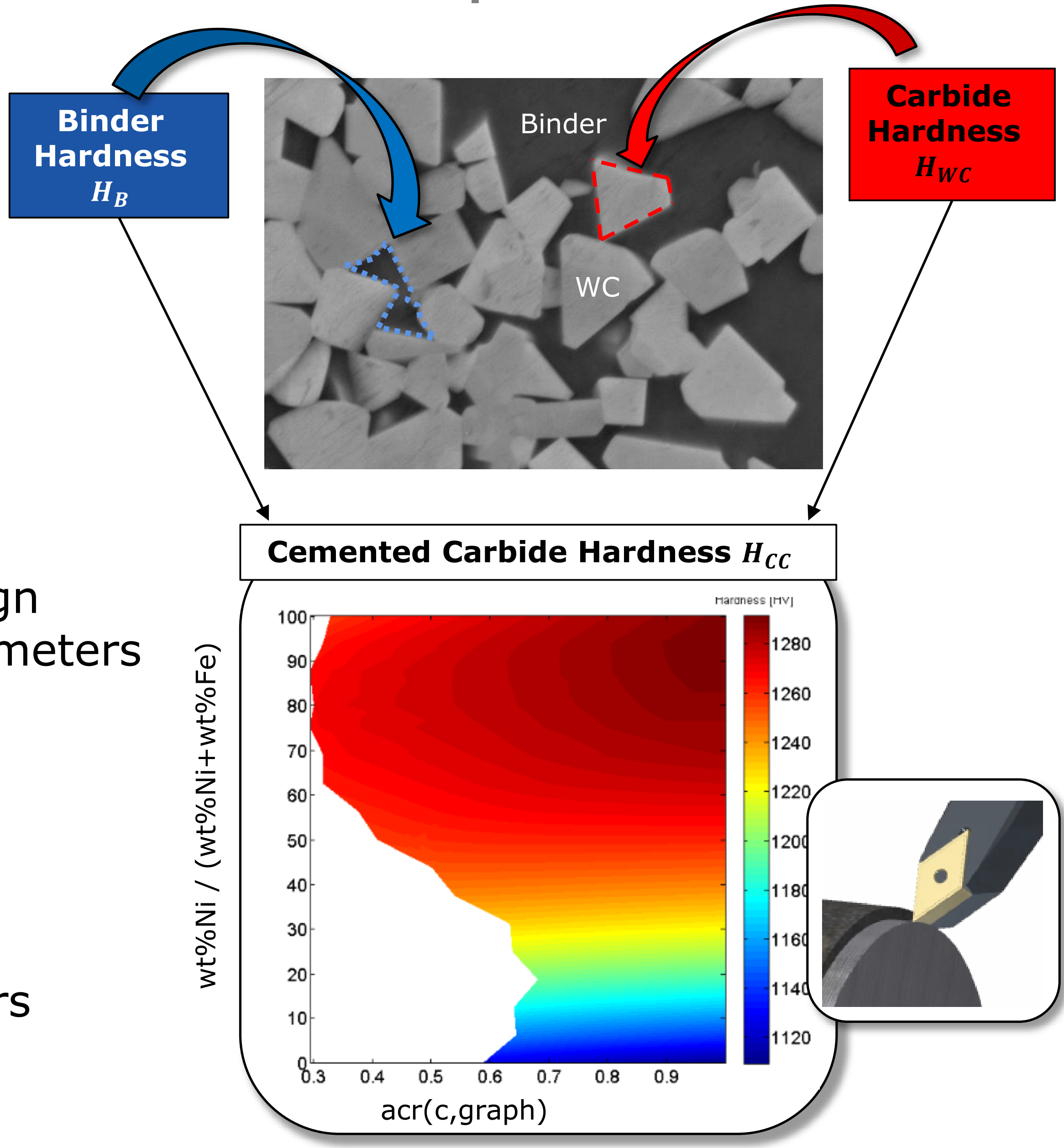
Composite hardness and its optimization



- All the models are integrated in a common platform (Python)
- Input:
  - Kinetic and thermodynamic databases (TC)
  - Compositions
  - Sintering time and temperature
  - Initial grain size distribution (before sintering)

  } Design parameters (Compositions; Sintering time and temperature; Initial grain size distribution)
- Output:
  - The composite hardness
- The optimization of the design parameters is performed through a genetic algorithm scheme

Bonvalet et al., 2018

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Thank you for your attention!

Researchers involved: Dr Manon Bonvalet, Prof Gustav Amberg, Ass Prof Peter Hedström, Fei Huyan, Dr Lars Höglund, Dr Pavel Korzhavyi, Dr Hemanth Kumar, Dr Amer Malik, Reza Naraghi, Prof Malin Selleby, Dr Albin Stormvinter, Dr Peter Kolmskog, Dr Ye Tian, Dr Johan Jeppsson, Dr Wei Xiong, Dr Jiayi Yan, David Linder, Dr Martin Wahlbrühl and Prof John Ågren