# Materials design from nano to macro based on ICME in Hero-m


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# Aims of Hero-m
## (Hierarchic Engineering of Industrial Materials)

To **create** the Engineering tools for the industrial materials of tomorrow.

- Hierarchic approach
- In collaboration with industry

To **apply** the new tools for important material problems.

- Existing materials
- New materials

# Multi length scale engineering approach

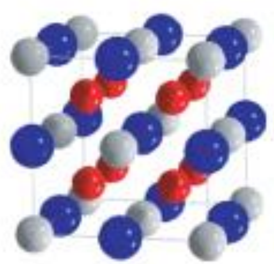
Atomic level simulation

Continuum models

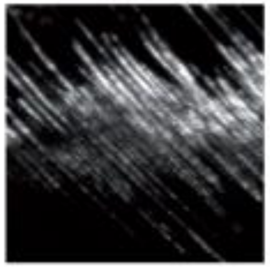
Fundamental models

Phenomenological models

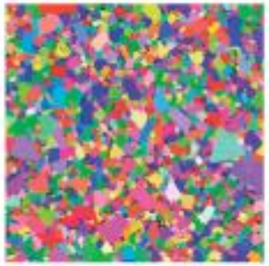
Engineering design



Ab-initio



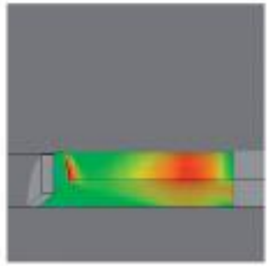
TEM



SEM

LOM

Phase field



FEM

# Projects divided in classes of materials

New materials
- Bulk glassy steels

Advanced stainless steels
- Spinodal decomposition
- Sigma-phase

High-strength steels
- Martensite formation and tempering
- Bainite formation

Cemented carbides
- Spinodal decomposition
- Cobalt-free carbide-based hard materials

Sintered steels
- Alloy element redistribution

Materials by design
- Demonstrator- Martensitic TRIP-steel

Harriet

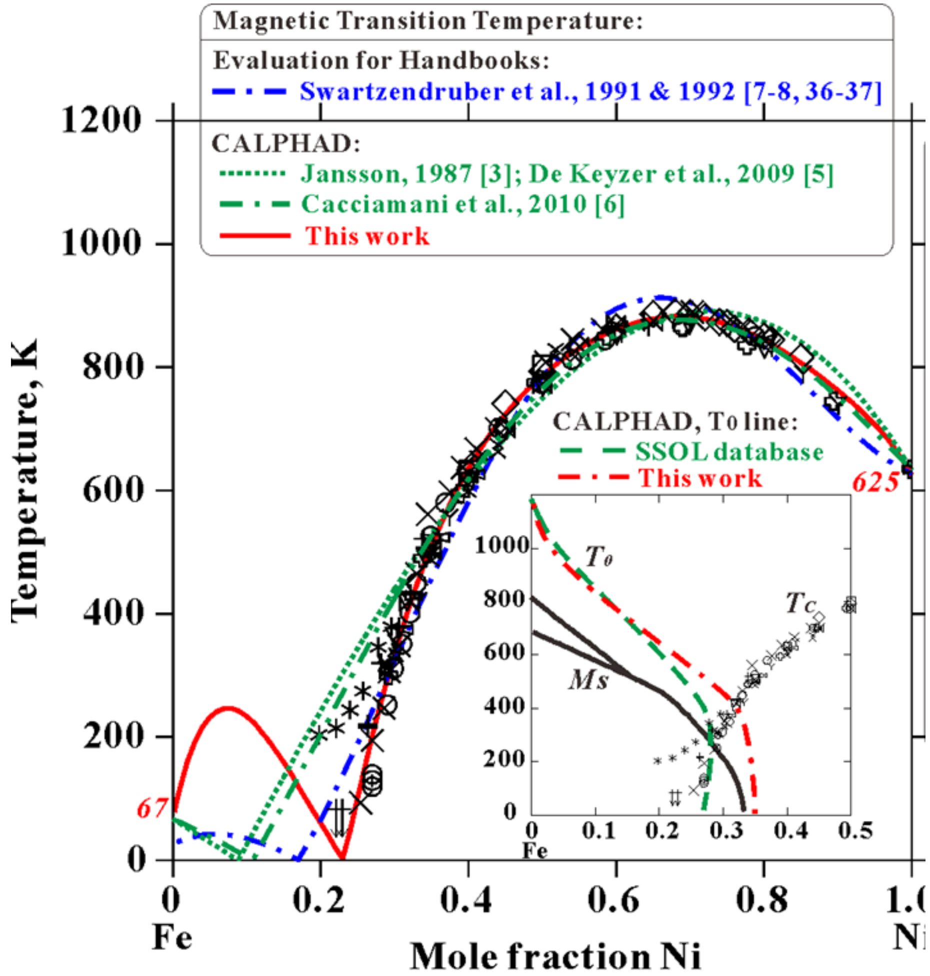
# Generic projects

Calphad
- needs from the applied projects e.g. regarding systems

Ab initio
- needs from the applied projects e.g. surface energies

Mechanical properties
- Combination of methods from atomic bonds via dislocations and cracks to constitutive equations

XRD
- X-ray diffraction using synchrotron radiation and neutrons



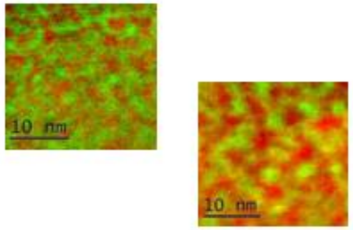

Xiong et al.

ROYAL INSTITUTE OF TECHNOLOGY

# Spinodal decomposition in Fe-Cr alloys

## Hierarchic modeling approach

supplemented by experimental characterization

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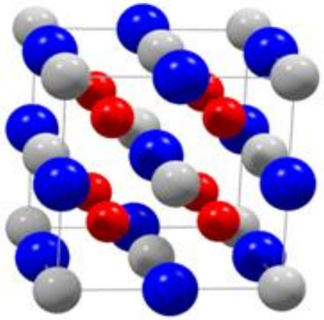
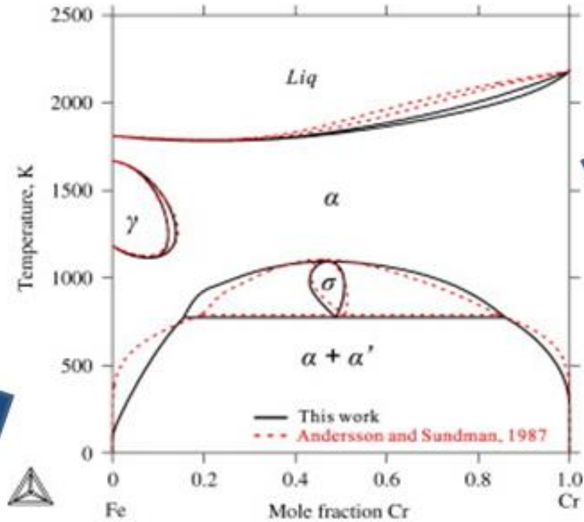
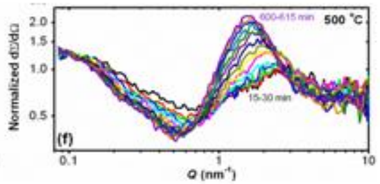


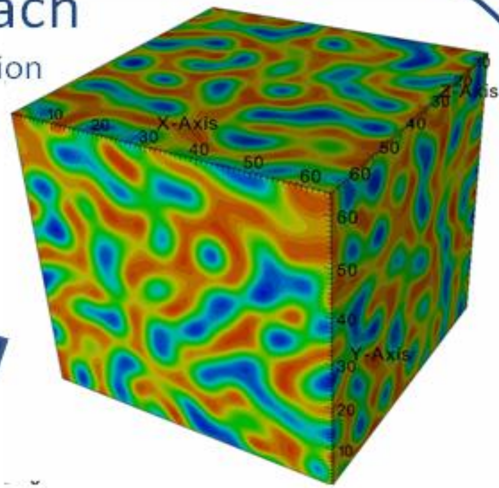
First-principles calculations
Thermodynamics
Kinetics
Elastic constants



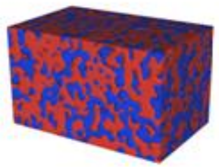

Calphad-type modeling
Thermodynamics
Kinetics

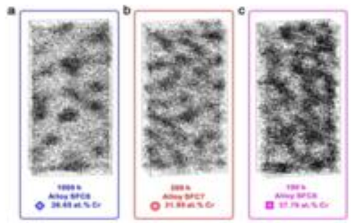



SANS




Phase-field modeling
Structural evolution





APT

hero-m

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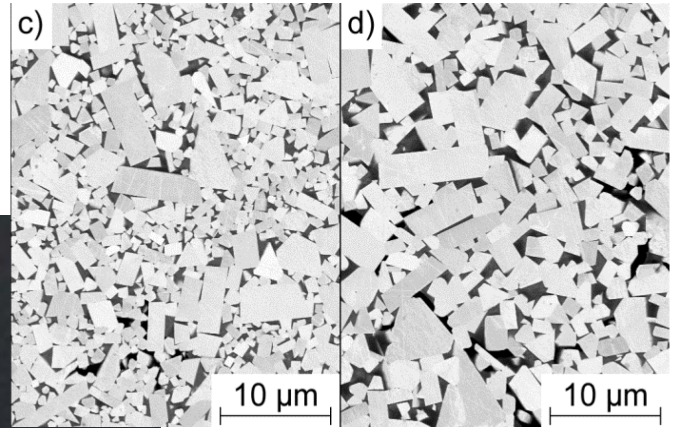
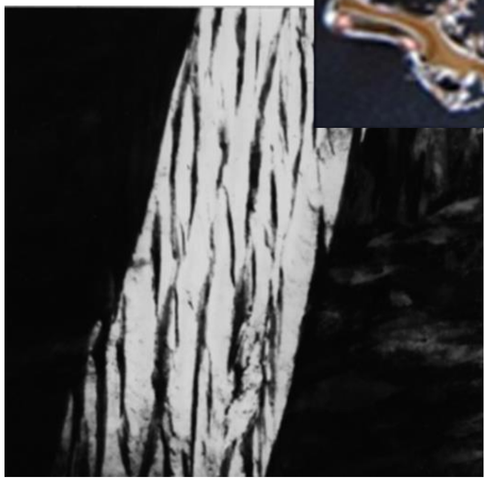
# Hero-m 2 Innovation


Atlas Copco
OVAKO
SSAB
Höganäs
SANDVIK
swerea | KIMAB
OUTOKUMPU
SECO
UDDEHOLM
VINNOVA
Thermo-Calc Software
QuesTek INNOVATIONS LLC

# What type of materials are being designed within Hero-m?

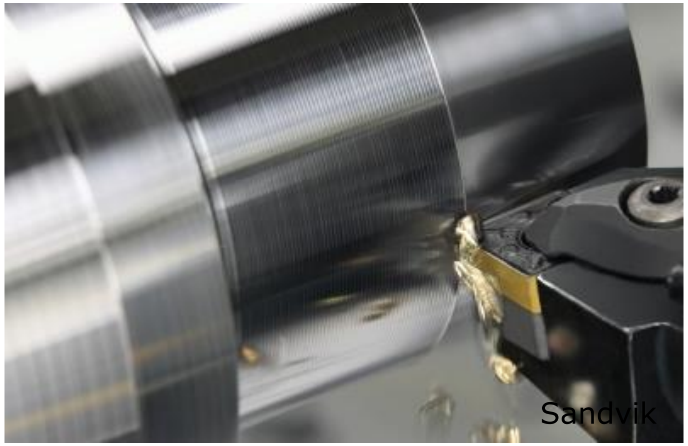
- New cobolt free cemented carbide
- BMG, bulk metallic glasses
- Martensitic TRIP steel



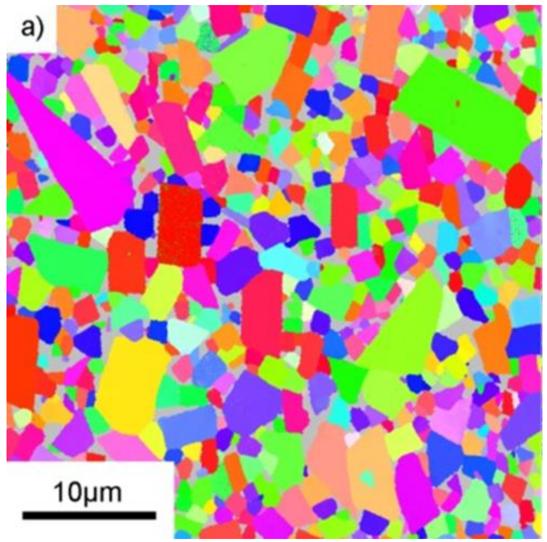



# Cemented carbides

- WC + metallic binder (usually Co)
- Co is toxic, longtime exposure may cause serious health problems.
- Co may become banned in EU.
- Substitute Co in tools for rock drilling and cutting.








Borg et al.

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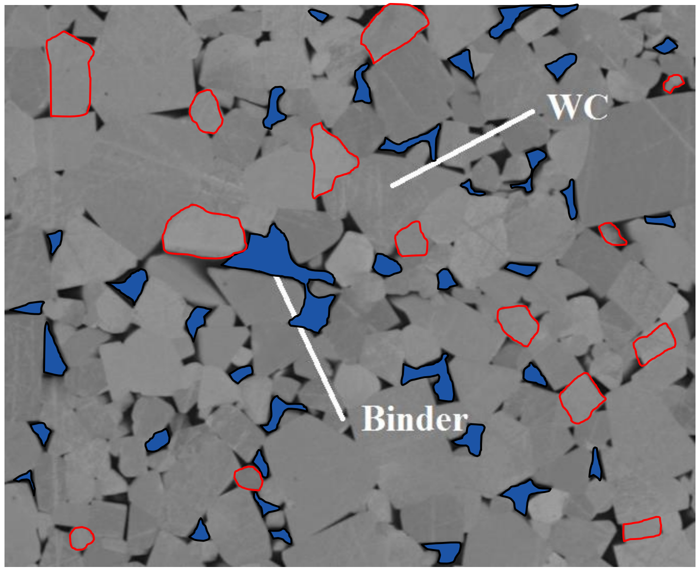
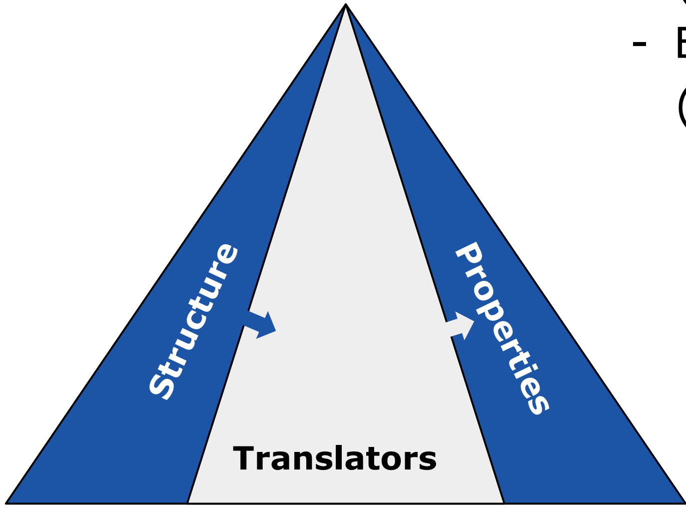
# Thus we need a set of models

- Cemented Carbide hardness:
  - Carbide hardness (WC & Cubic Carbides)
  - Binder hardness (Cobalt, Iron, Nickel ...)




Real system




Linkage system

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

**Toughness**

**Hardness**

**Grain Growth model** → Hall-Petch

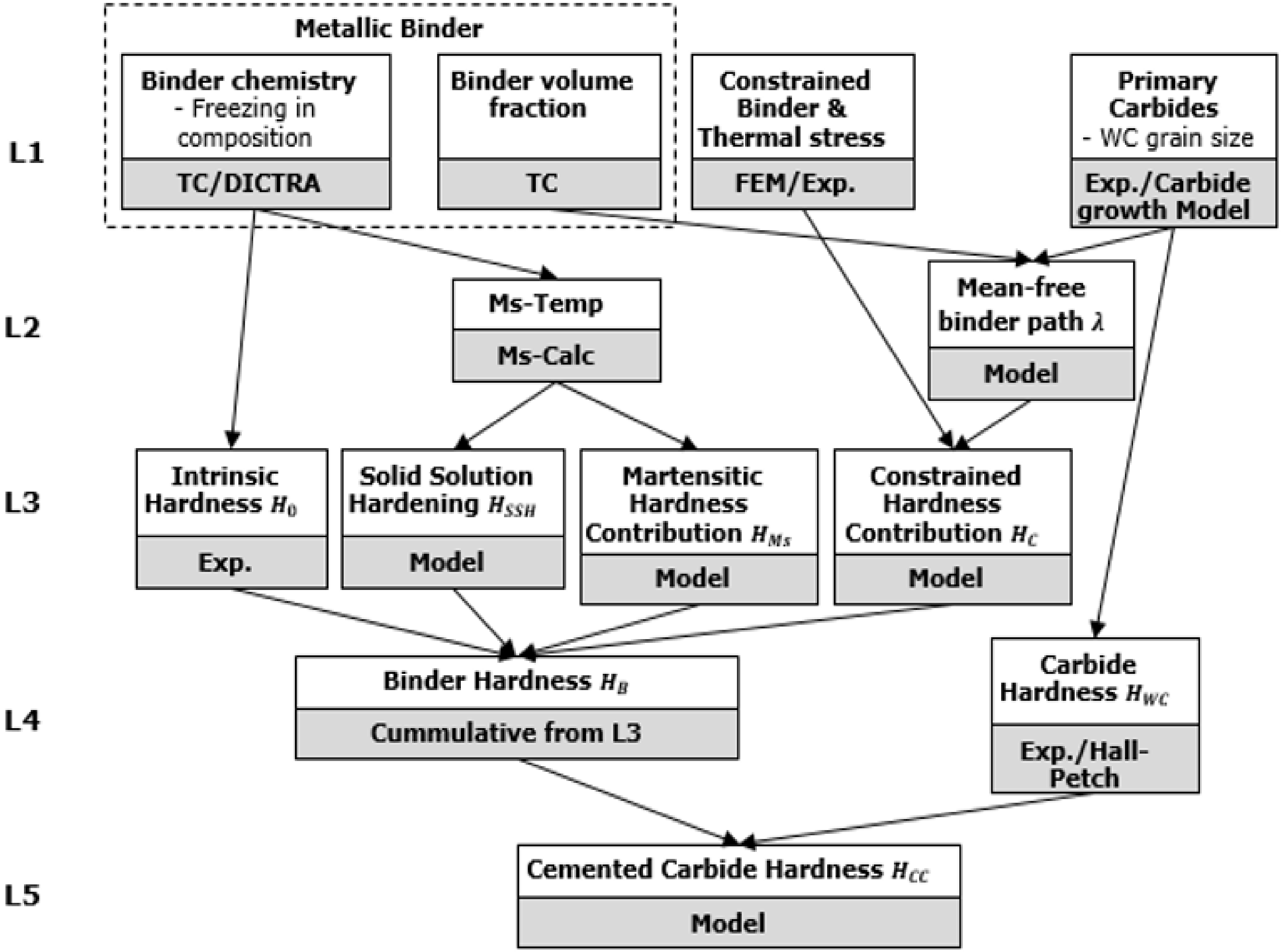
Thermo-Calc, DICTRA → Solid solution hardening

TC-PRISMA → Precipitation hardening

Martensite formation ← **MS Calc**

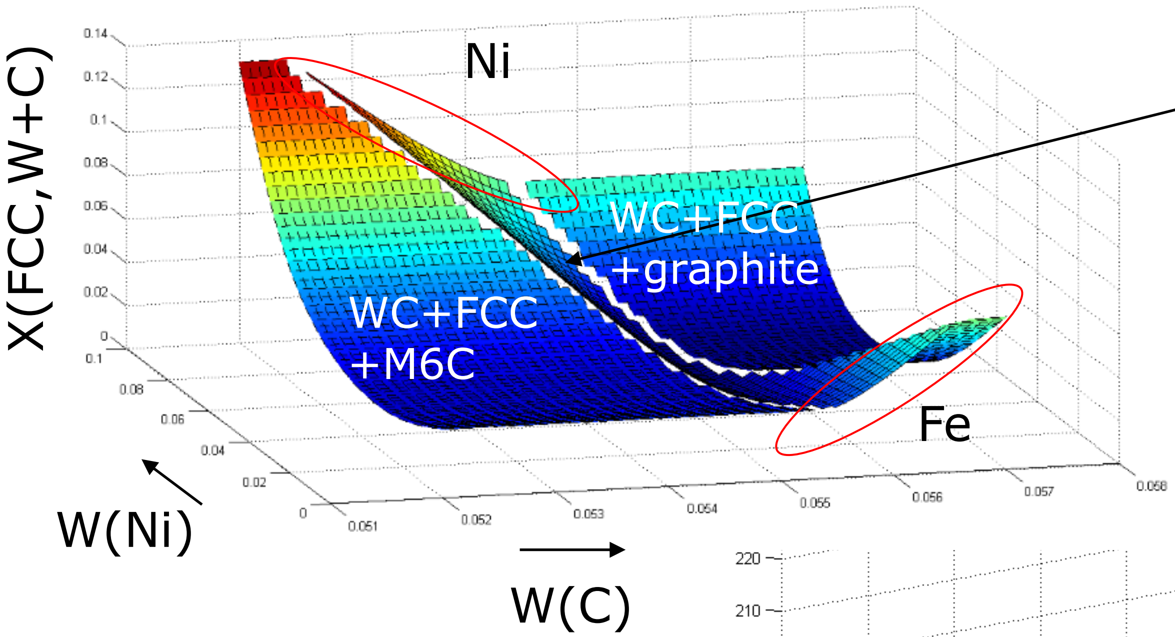
Work hardening

# Hardness modelling



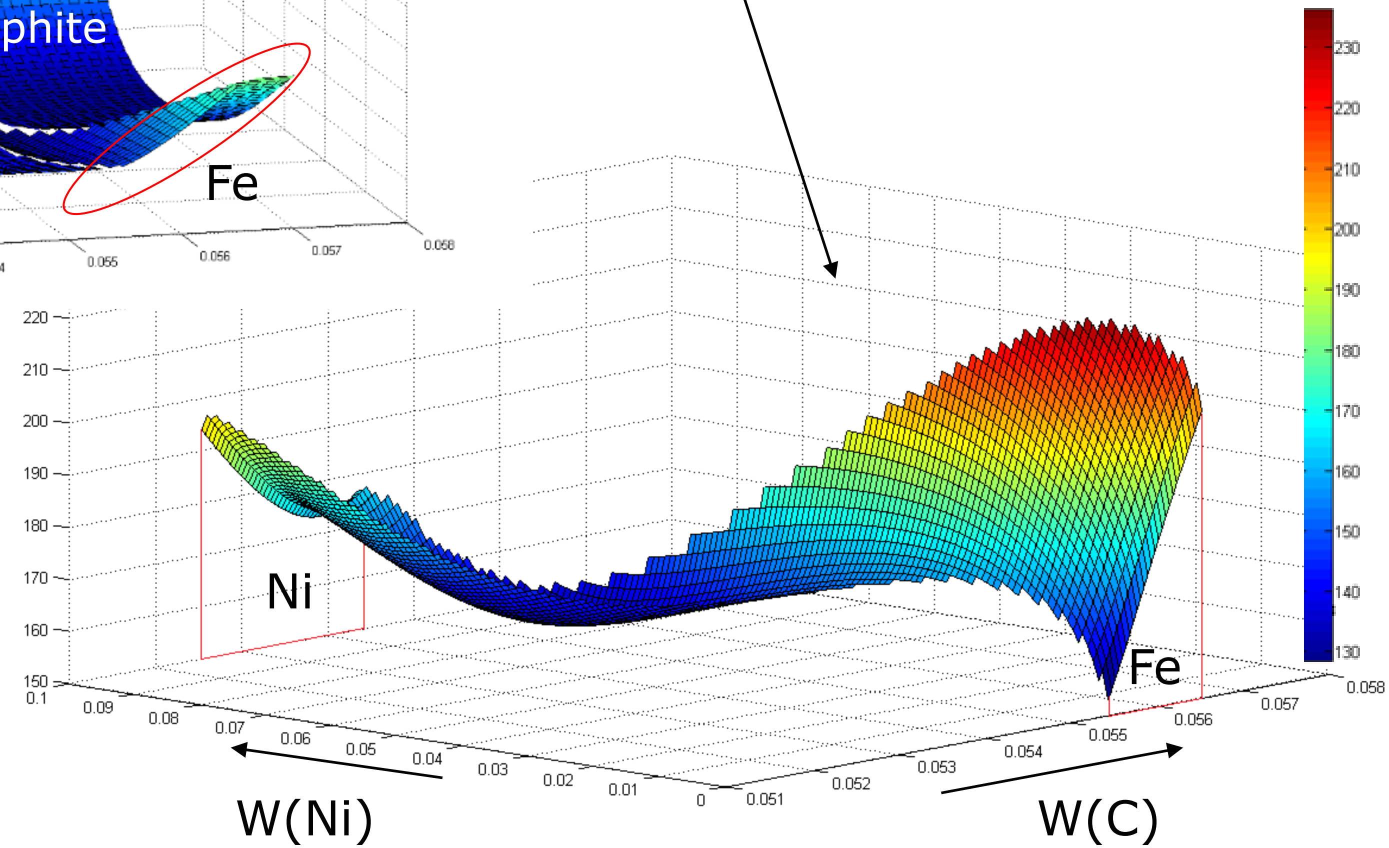
# Solubility and binder hardness

Solubility




Two-phase region
WC + FCC binder

Hardness in
W-C-Fe-Ni system




Binder hardness

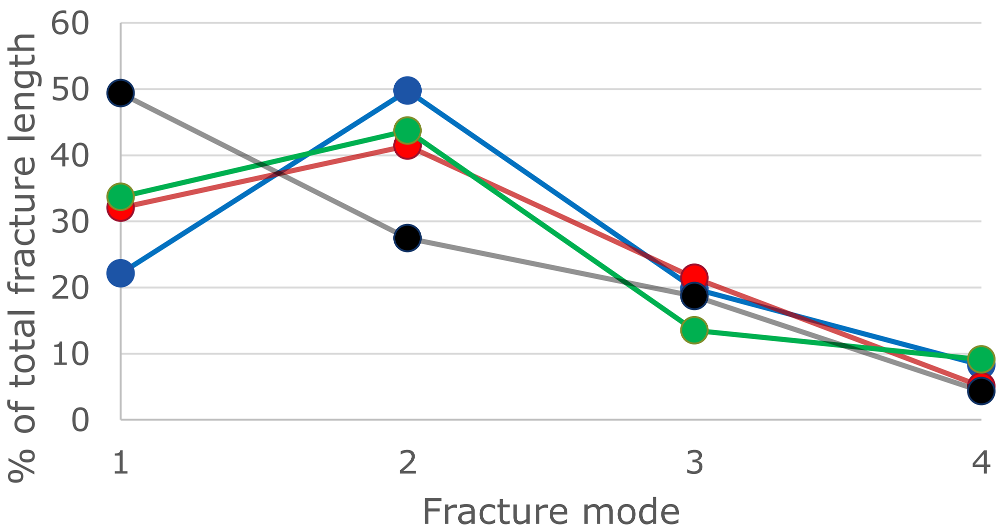
Walbrühl et al.

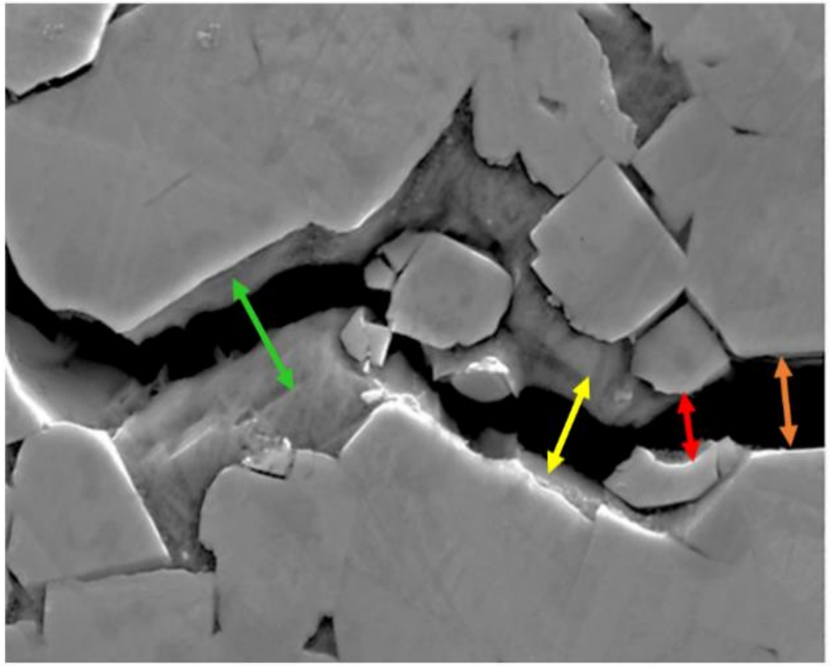
# Fracture toughness

Modeling of fracture toughness:

- Model based on energy release rate
- Measurements of fracture modes
- Simulation of binder rupture with respect to binder mean free path using FEM

Fracture modes 20 vol.% binder

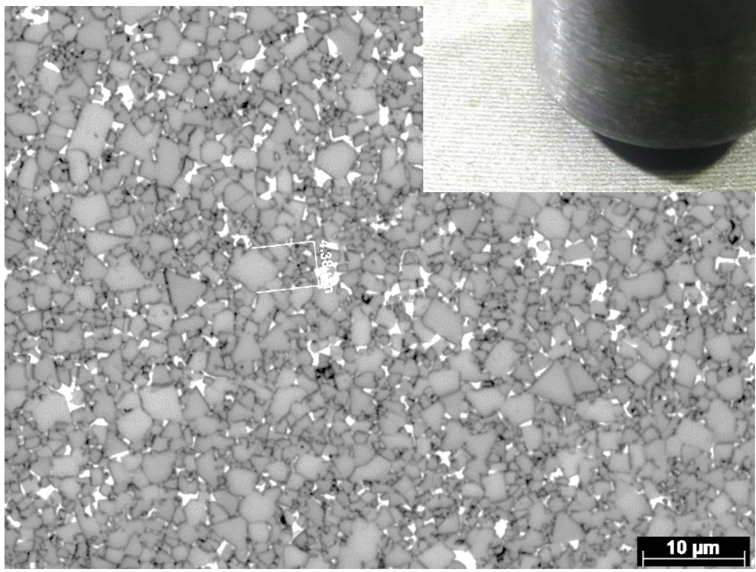


1: WC cleavage
2: WC/WC interface
3: WC/binder interface
4: Binder rupture

# Inserts after rock drilling test at Atlas Copco Secoroc, performance 20%lower than with Co

New NoCo grade, first drilling test

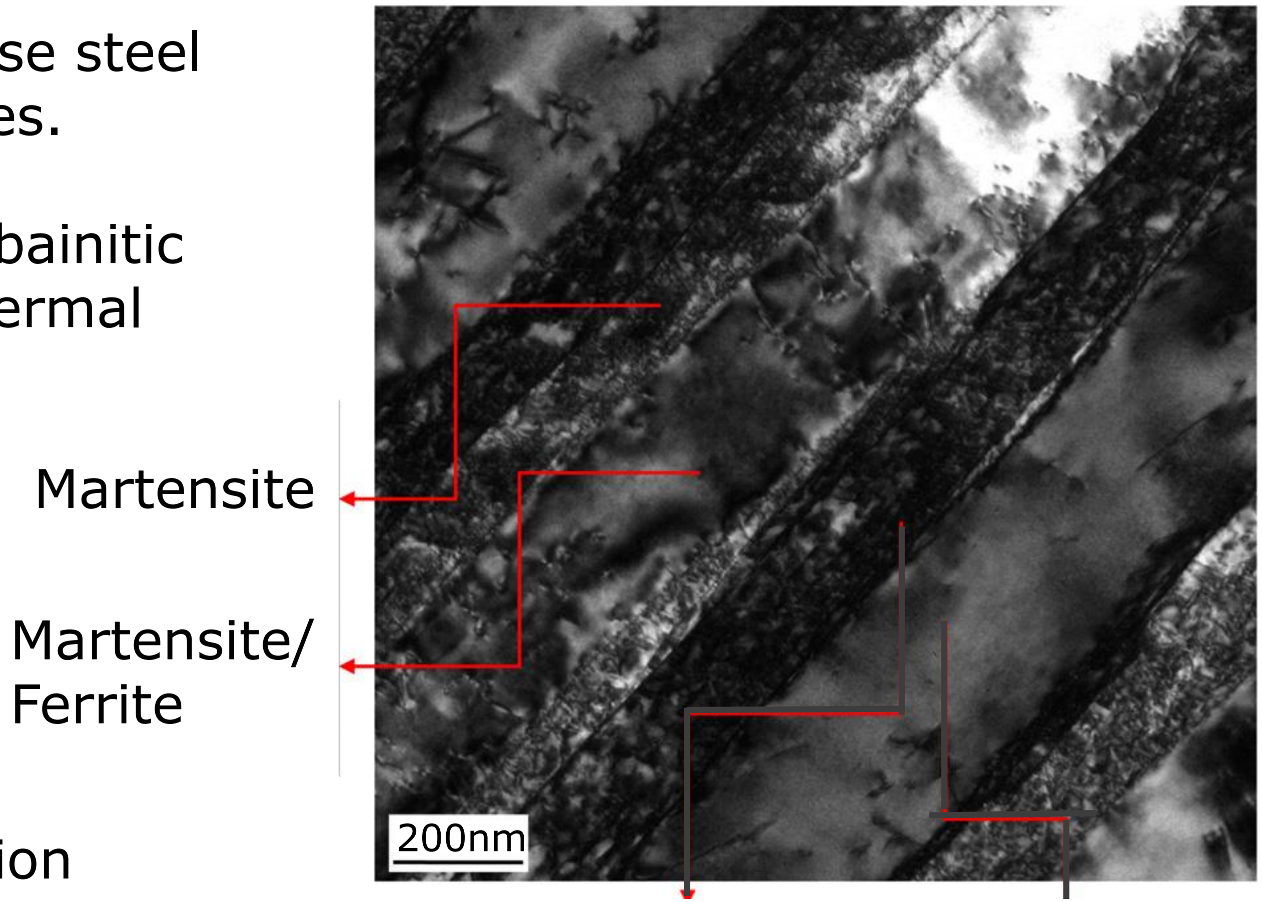



Standard Cobalt-binder grade, same test

# Martensitic TRIP-steel

Goal

- Ultra-high strength dual-phase steel strengthened by nanoparticles.
- Microstructure similar to nanostructured carbide free bainitic steels but without long isothermal heat treatments at low temperatures.



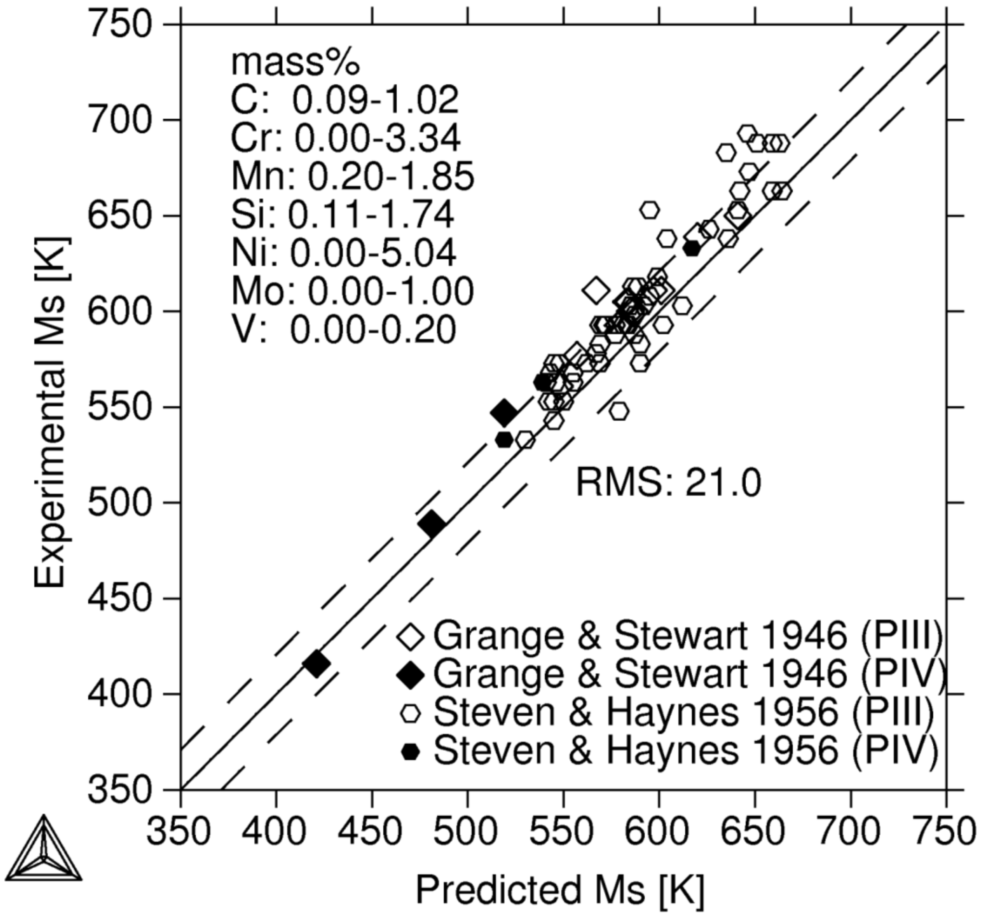

Wei et al, Acta Mater., 2013

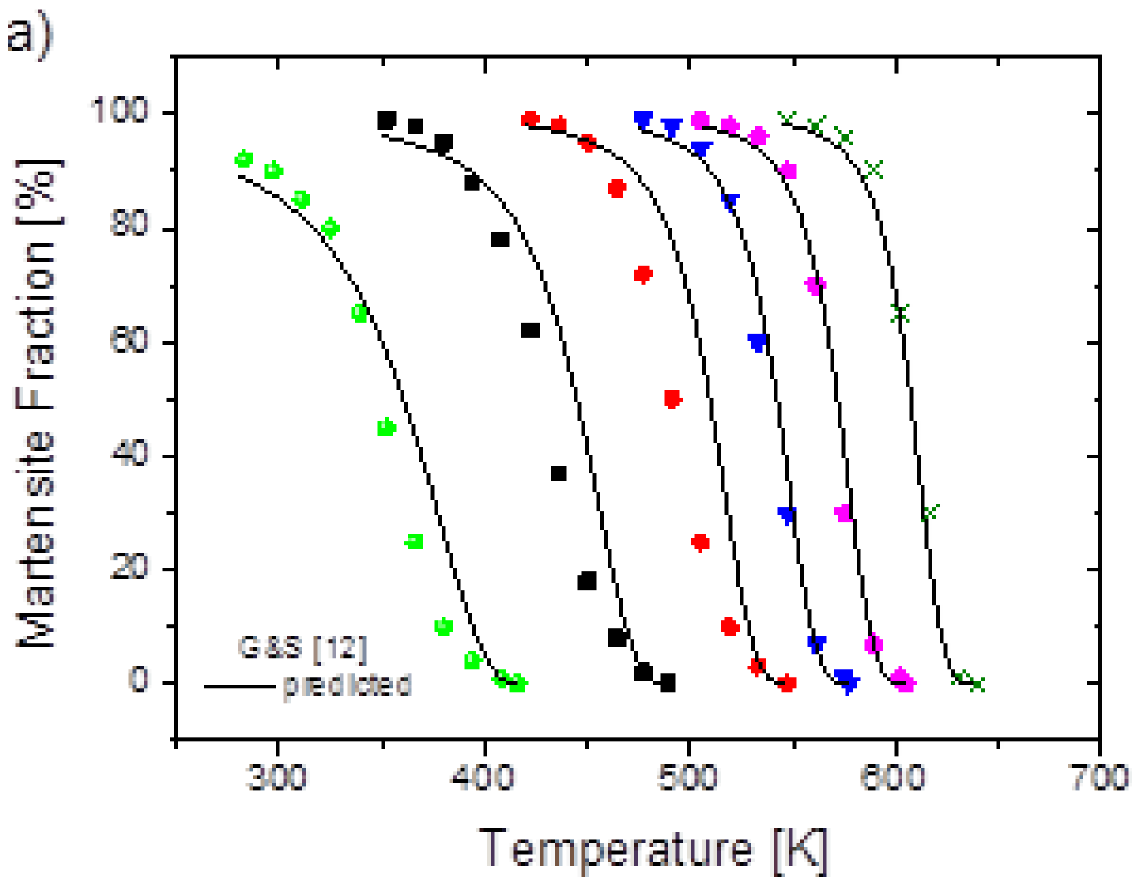
The work is done in collaboration with Professor Greg Olson at Northwestern University in US.

# We thus need a set of models

- Translators, models that predict the properties from the microstructure e.g.
  - Mechanical properties:
    - yield stress
    - strain hardening
    - elongation
    - .......
- Creators, models that predict the microstructure from processing e.g.
  - $M_s$ – martensitic start temperature
  - $M_s^\sigma$ – martensitic start temperature under applied stress
  - Fraction of martensite formed below $M_s$
  - Fraction of carbides formed upon tempering – Thermo-Calc
  - Austenitization temperature – Thermo-Calc
  - Coarsening of precipitate
  - .....

# Calculation of start temperature and fraction of martensite



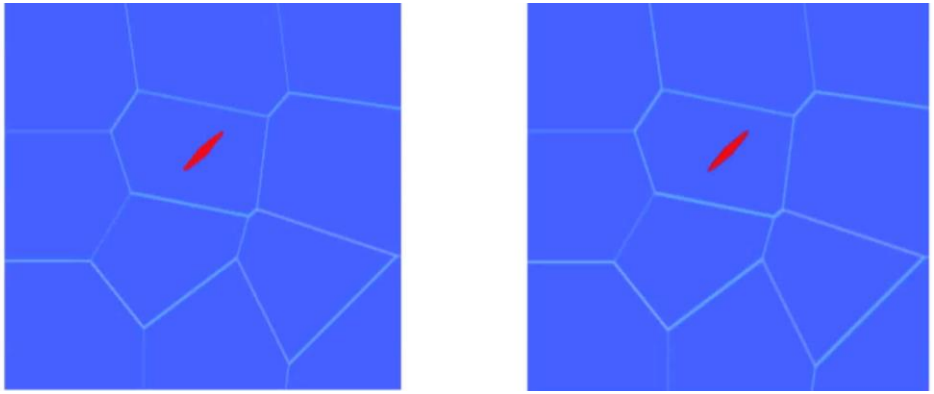




Stormvinter et al., 2012

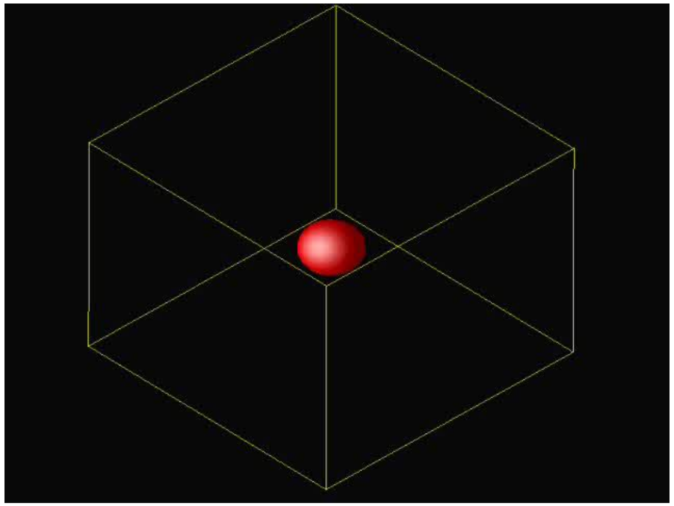
Huyan et al., 2016

# Microstructure design tools

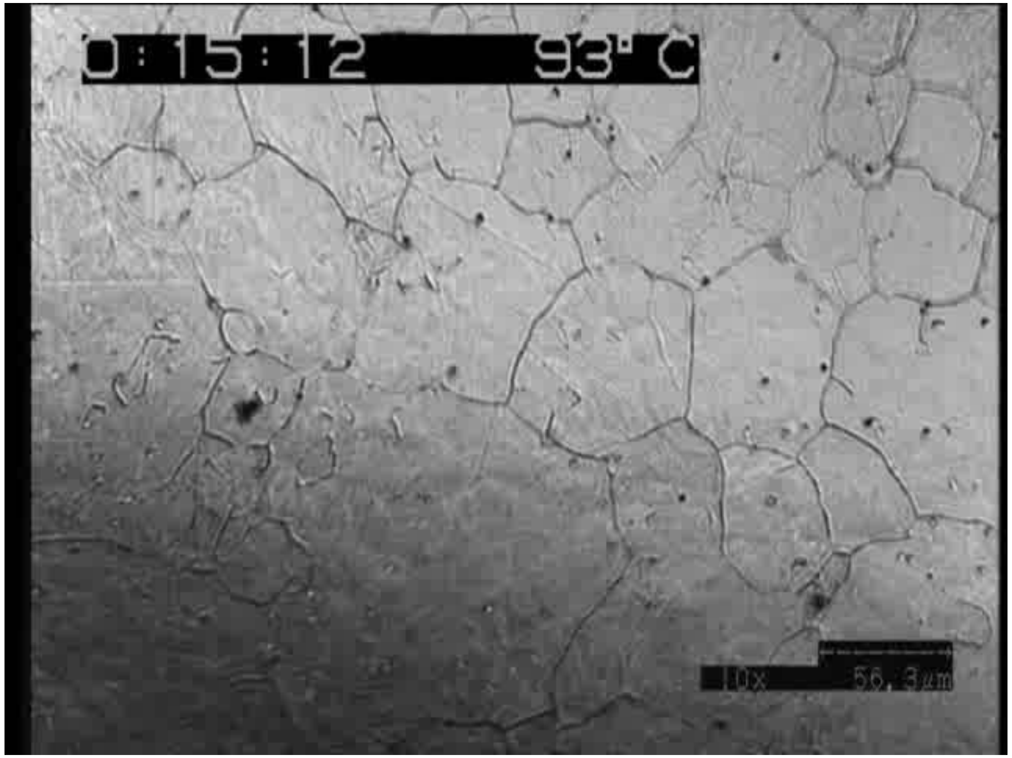
- Phase field
- Equilibrium structures and driving forces for non equilibrium (thermodynamics)
  - Stresses (external and internal)
  - Interfaces
- Prisma
- DICTRA



Malik et al.

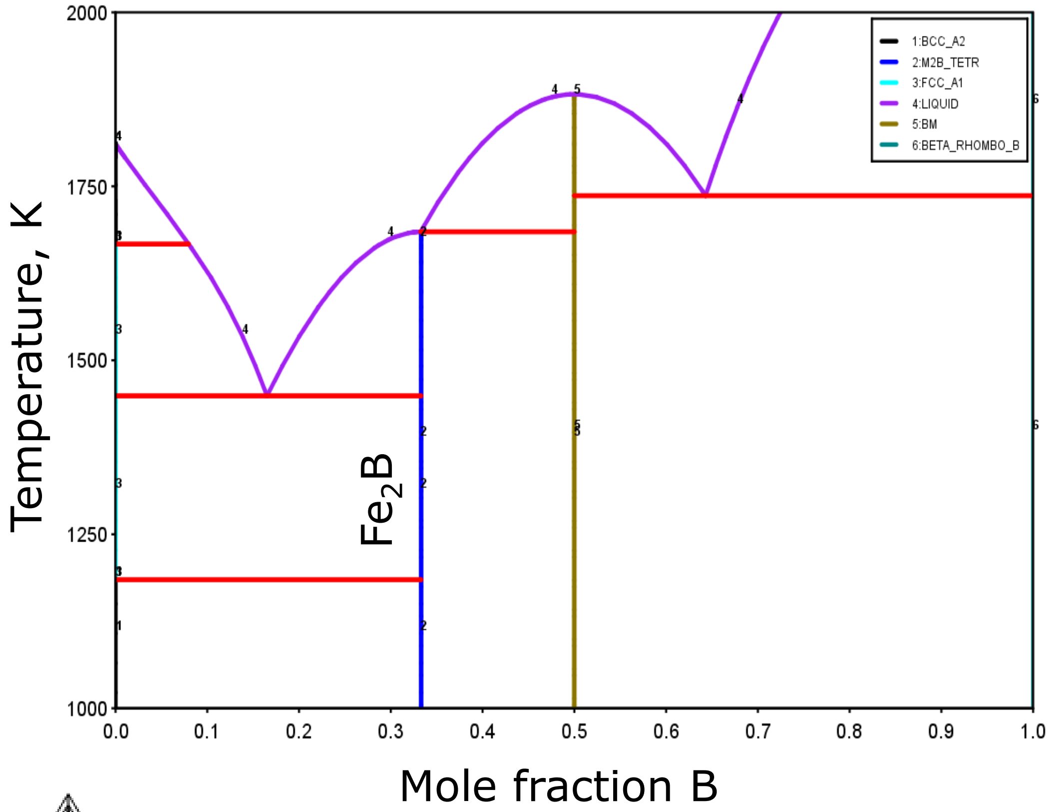


Yeddu et al.

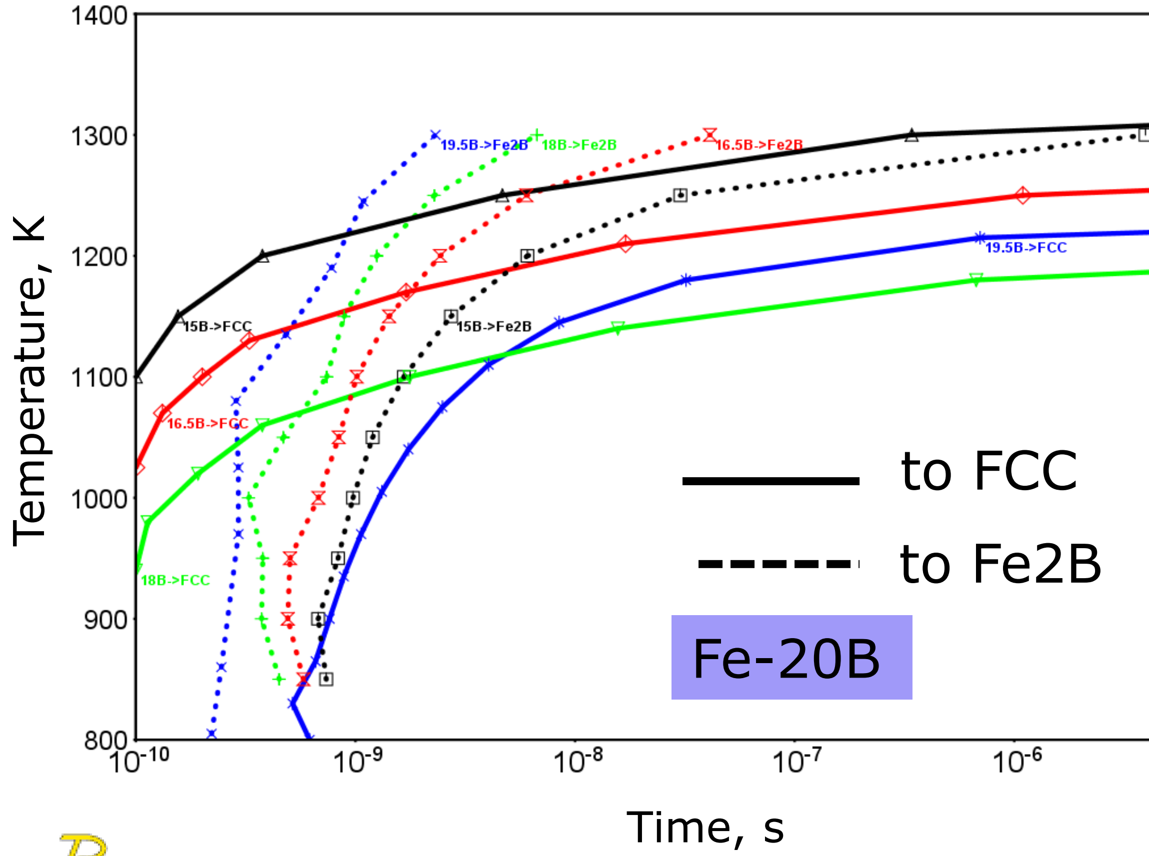



Kolmskog et al.

# Design of Fe-based bulk metallic glasses

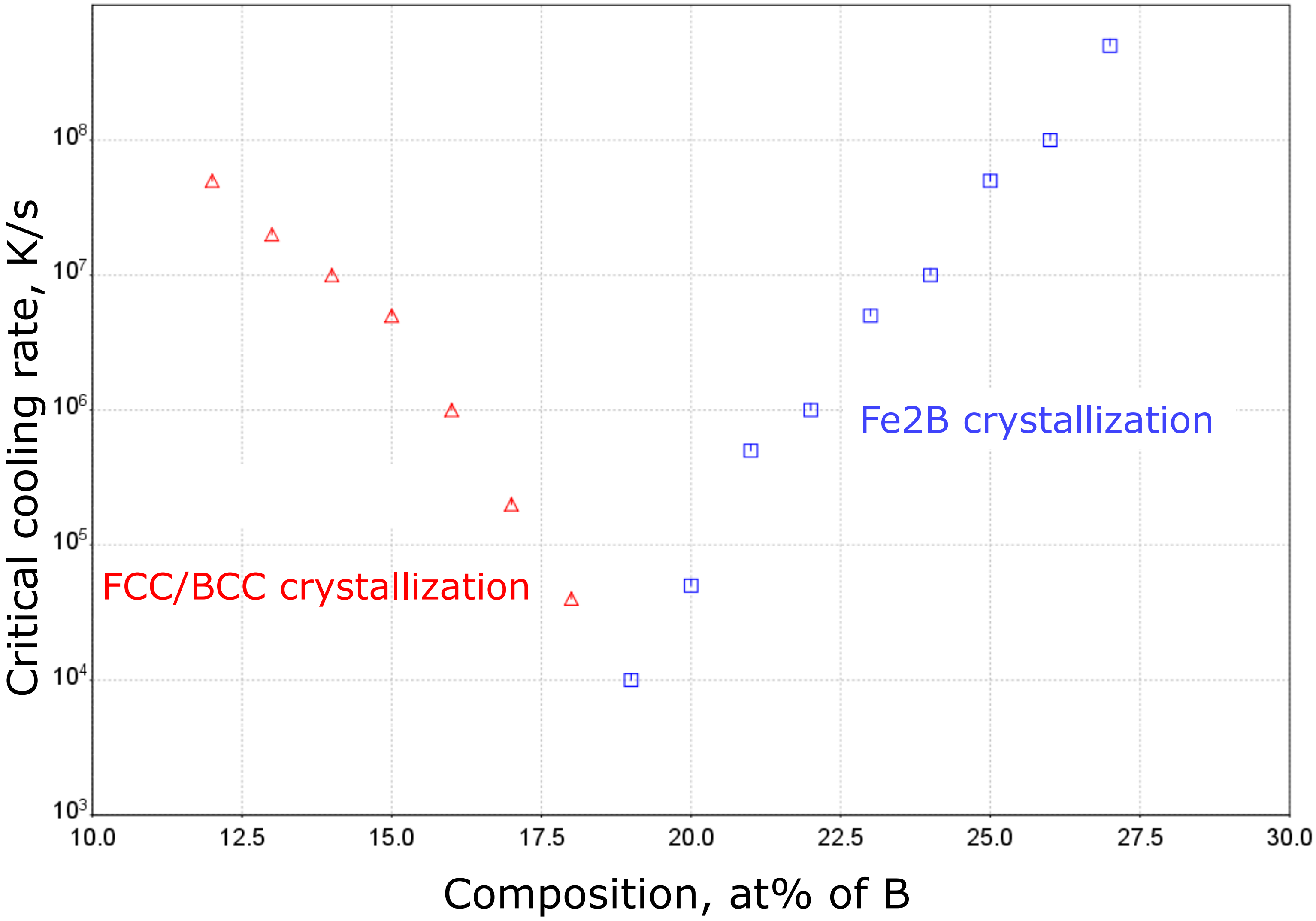



Fe-B




Mao et al.

# Optimal glass forming range based on calculated critical cooling rate (Fe-B)




Mao et al.

Thank you for your attention!

**Researchers involved:** Prof Gustav Amberg, Thomas Barkar, Ass Prof Peter Hedström, Prof Em. Mats Hillert, Fei Huyan, Dr Lars Höglund, Dr Pavel Korzhavyi, Dr Hemanth Kumar, Lindsay Leach, Dr Amer Malik, Dr Abdul Malik, Dr Huahai Mao, Reza Naraghi, Ass Prof Joakim Odqvist, Prof Greg Olson, Prof Malin Selleby, Dr Albin Stormvinter, Dr Peter kolmskog, Dr Ida Borgh, Dr Wei Xiong, Dr Jiayi Yan, David Linder, Martin Wahlbrühl and Prof John Ågren