Thermo-Calc Software

Further Developments of CALPHAD Based Tools for Accelerating Alloy Design

Paul Mason, Adam Hope, Kevin Wu, Qing Chen,
Johan Bratberg, Anders Engstrom

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ICME becomes mainstream

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THE WALL STREET JOURNAL. WSJ

CIO JOURNAL

More Manufacturers Bet on Simulation Software

Tool allows auto makers and others to assess how changes to a line will affect production

Angus Loten, Wall Street Journal, February 20, 2020

Highlighted growth in the use of simulation software within industry which allows manufacturers to test new or re-engineered product lines before starting them.

Citing a report from ABI Research, within the next five years an estimated 110,000 companies world wide are expected to use some kind of simulation software at an annual cost of more than $2.5Bn.

*But the accuracy of these simulations depends on the quality of the input data, which includes the **materials** data.*

Everyone is talking about data

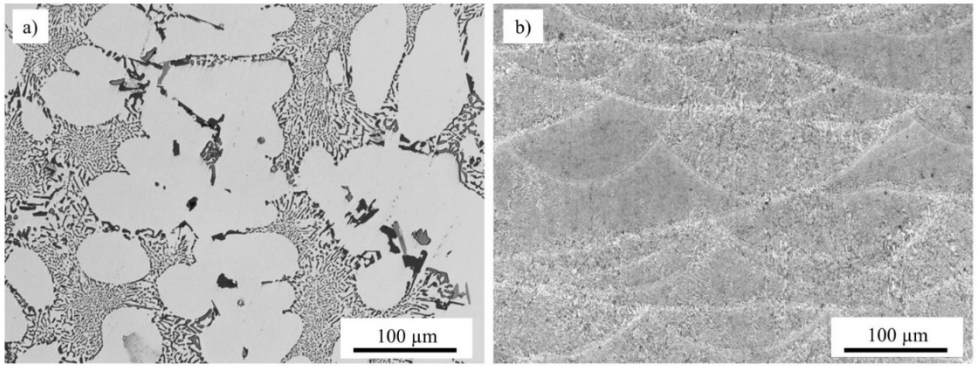
"Data is the new oil. It's valuable, but if unrefined it cannot really be used. It has to be changed into gas, plastic, chemicals, etc to create a valuable entity that drives profitable activity; so must data be broken down, analyzed for it to have value."

Clive Humby, UK Mathematician, 2006

Properties and Performance depend on…

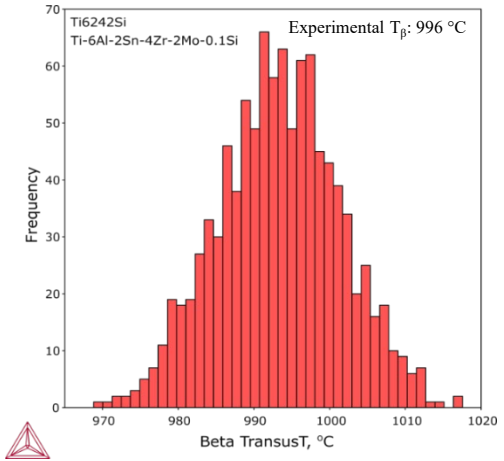
Processing:

AlSi10Mg alloy - gravity casting (a) and AM (b)

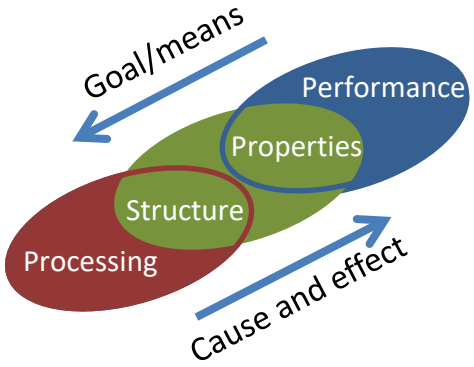


Fabio Boiocchi, Metalworking World Magazine (2019)

Chemistry:

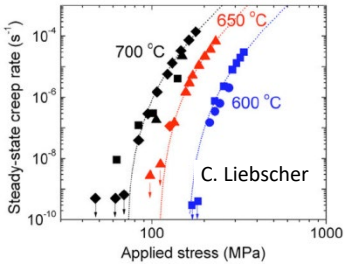


The needed knowledge structure



Performance

Properties



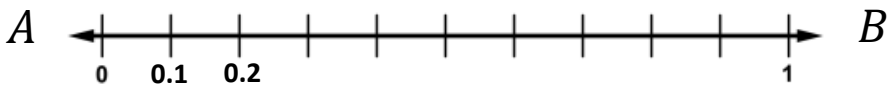
To describe these links we need <u>models</u>, but all models need <u>data</u>. A lot of which is often not known.

Structure

<u>The recipe:</u>

Composition / Processing

New alloy design – composition dependence



Many potential combinations!

n = # elements = 2 (i.e. A and B)

k = # steps = 10 => **11 combinations**

k = # steps = 100 => **101 combinations**

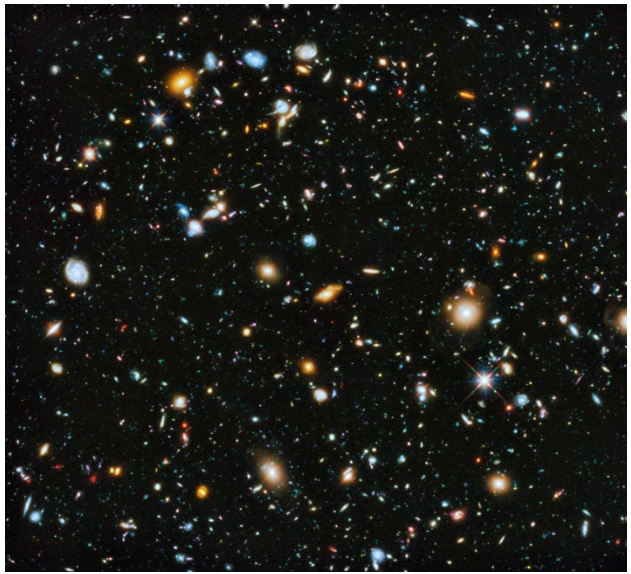
<u>For an alloy with 10 elements:</u>
n=10 and k=100 (i.e. steps of 1%) => $\mathbf{10^{12}}$

<u>Taking all elements in our Ni-database:</u>
n=30 and k=100 (i.e. steps of 1%) => $\mathbf{10^{27}}$

Our universe has existed for $< 10^{18}$ *seconds*

Unlimited design space!

…and only an infinitesimally small fraction of that possible composition space has been explored.



The materials data challenge: Small amounts of data in a big data world

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Traditional data sources:

Experiments

- Costly
- Time Consuming
- Need more experiments for each new material or novel process.

Handbooks

- A typical handbook contains data for < 1000 alloys
- And far from all properties of interest
- Data lacking for new alloy design / materials discovery
- Data not always applicable to new processes (e.g. additive)

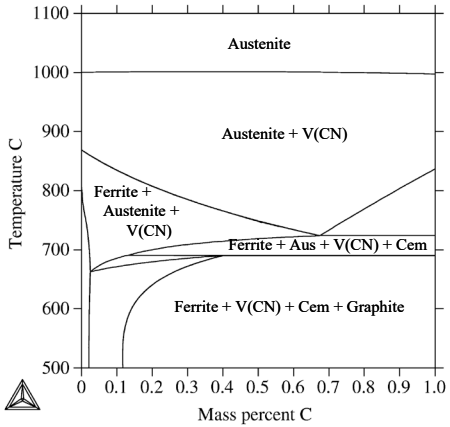
Alternative: data can be simulated or estimated

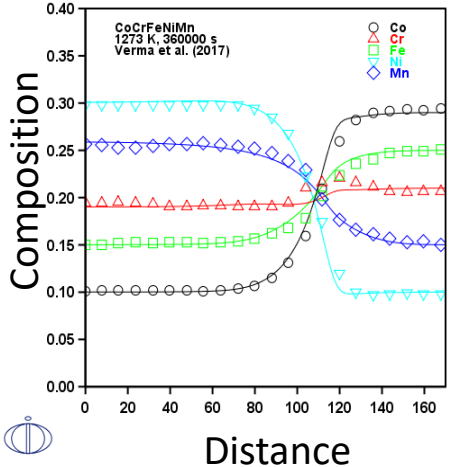
- Mechanistic models
- Phenomenological models
- Machine Learning
- Ab Initio/Molecular dynamics
- Regression analysis

Thermo-Calc Software

CALculation of PHAse Diagrams

- A phase-based approach which captures the composition and temperature dependence of properties in a self consistent framework.
- Databases are developed through the fitting of binary and ternary systems and extrapolated to multicomponent systems.
- Applicable to “real” engineering materials.
- Extendable far beyond traditional thermochemistry.





$$G(p,T) = H - TS$$

Gibbs Free Energy

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$$

Ficks Laws of Diffusion

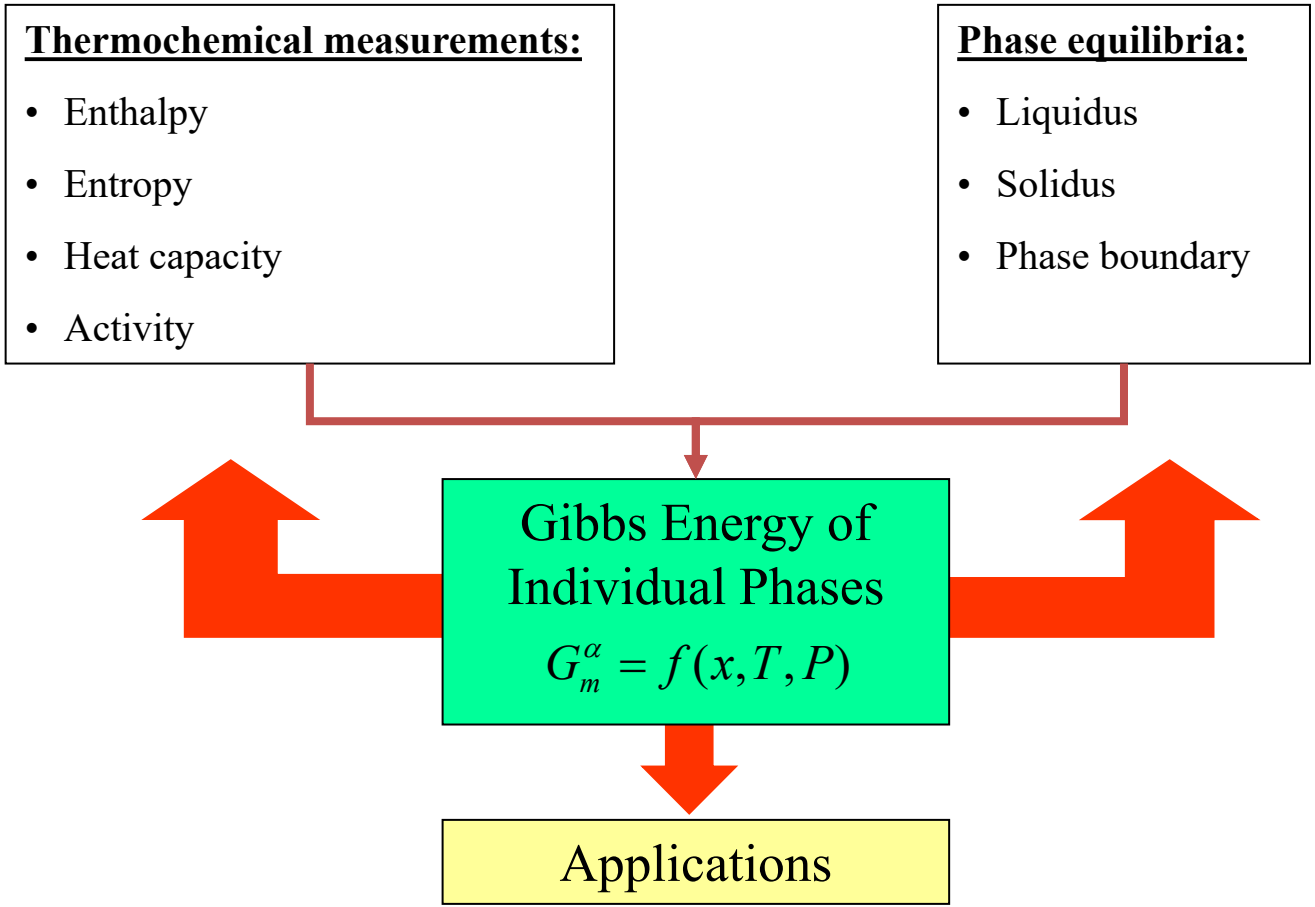
$$\Delta G = \frac{4}{3}\pi r^3 \Delta g + 4\pi r^2 \sigma$$

Classical Nucleation Theory

CALPHAD (2)

Thermo-Calc Software

Thermodynamic Databases (*The CALPHAD approach)*



Databases based on binary and ternary systems

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	Al	B	C	Co	Cr	Cu	Fe	Hf	Mn	Mo	N	Nb	Ni	O	Pd	Pt	Re	Ru	Si	Ta	Ti	V	W	Y
B	x																							
C	x	x																						
Co	x	x	x																					
Cr	x	x	x	x																				
Cu	x	x	x	x	x																			
Fe	x	x	x	x	x	x																		
Hf	x	x	x	x	x	x	x																	
Mn	x	x	x	x	x	x	x	x																
Mo	x	x	x	x	x	x	x	x	x															
N	x	x		x	x	x	x		x	x														
Nb	x	x	x	x	x	x	x	x	x	x	x													
Ni	x	x	x	x	x	x	x	x	x	x	x	x												
O	x	x	x	x	x	x	x	x	x	x	x	x	x											
Pd	x	x	x	x	x	x	x	x	x	x		x	x	x										
Pt	x	x	x	x	x	x	x	x	x	x		x	x	x	x									
Re	x	x	x	x	x	x	x	x	x	x		x	x	x	x									
Ru	x	x	x	x	x	x	x	x	x	x		x	x	x	x									
Si	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x						
Ta	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x					
Ti	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x				
V	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x			
W	x	x	x	x	x	x	x	x		x	x	x	x	x	x	x	x	x	x	x	x	x		
Y	x	x	x	x	x	x	x	x	x	x		x	x	x	x	x	x	x	x	x	x	x	x	
Zr	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x

TCNI8

280 assessed binary systems in full range of composition and temperature

Al-B-Co	Al-Cr-O	Al-Nb-Ni	B-Cr-Ni	C-Cr-W	C-Ti-W	Co-O-Si	Cr-Ni-Ti	Fe-Nb-Zr	Ni-O-Si
Al-B-Cr	Al-Cr-Pt	Al-Nb-O	B-Cr-Re	C-Cr-Zr	C-Ti-Zr	Co-O-W	Cr-Ni-W	Fe-Ni-O	Ni-O-W
Al-B-Hf	Al-Cr-Ta	Al-Nb-Si	B-Fe-Nb	C-Cu-Fe	C-W-Zr	Co-Re-W	Cr-Ni-Zr	Fe-Ni-W	Ni-O-Y
Al-B-Mo	Al-Cr-Ti	Al-Ni-O	B-Hf-Nb	C-Fe-Mn	Co-Cr-Cu	Co-Ta-W	Cr-O-Si	Fe-O-Si	Ni-O-Zr
Al-B-Ni	Al-Cr-Zr	Al-Ni-Pd	B-Hf-Ni	C-Fe-O	Co-Cr-Mo	Co-Ti-W	Cr-O-Y	Fe-O-W	Ni-Re-Ta
Al-B-Re	Al-Cu-Fe	Al-Ni-Pt	B-Hf-Re	C-Hf-Mo	Co-Cr-Nb	Co-Ti-Zr	Cr-O-Zr	Fe-O-Y	Ni-Re-Ti
Al-B-Ti	Al-Cu-Mn	Al-Ni-Re	B-Hf-Ta	C-Hf-Ni	Co-Cr-Ni	Co-W-Zr	Cr-W-Zr	Fe-O-Zr	Ni-Re-W
Al-B-Zr	Al-Cu-Ni	Al-Ni-Ru	B-Mo-Nb	C-Hf-Re	Co-Cr-O	Cr-Cu-Fe	Cu-Fe-Mn	Hf-Mo-Ni	Ni-Re-Zr
Al-C-Cr	Al-Cu-Si	Al-Ni-Si	B-Mo-Ni	C-Hf-Ta	Co-Cr-Re	Cr-Cu-Nb	Cu-Fe-Mo	Hf-Nb-Si	Ni-Ru-Ti
Al-C-Hf	Al-Fe-Mn	Al-Ni-Ta	B-Mo-Re	C-Hf-Ti	Co-Cr-Ti	Cr-Cu-Ni	Cu-Fe-N	Hf-Ni-Ta	Ni-Ta-W
Al-C-Mo	Al-Fe-Mo	Al-Ni-Ti	B-Nb-Re	C-Hf-W	Co-Cr-W	Cr-Cu-Si	Cu-Fe-Nb	Hf-O-Si	Ni-W-Zr
Al-C-Ni	Al-Fe-Ni	Al-Ni-V	B-Ni-Re	C-Hf-Zr	Co-Cu-Fe	Cr-Fe-Mo	Cu-Fe-Ni	Mn-Ni-O	O-Si-Ti
Al-C-Ta	Al-Fe-O	Al-Ni-W	B-Ni-Ta	C-Mo-Ni	Co-Cu-Mn	Cr-Fe-N	Cu-Fe-Si	Mn-O-Si	O-Si-Y
Al-C-Ti	Al-Fe-Ti	Al-Ni-Zr	B-Re-Ta	C-Mo-Ta	Co-Cu-Nb	Cr-Fe-Ni	Cu-Fe-Ti	Mn-O-W	O-Si-Zr
Al-C-W	Al-Hf-Mo	Al-O-Si	B-Re-Ti	C-Mo-Ti	Co-Cu-Ni	Cr-Fe-O	Cu-Fe-V	Mn-O-Y	O-Y-Zr
Al-C-Zr	Al-Hf-Ni	Al-O-Ti	B-Re-W	C-Mo-W	Co-Cu-Ti	Cr-Fe-Si	Cu-Mn-Ni	Mn-O-Zr	Re-Ta-W
Al-Co-Cr	Al-Hf-O	Al-O-Y	B-Re-Zr	C-Mo-Zr	Co-Fe-Nb	Cr-Fe-W	Cu-Mn-Si	Mo-Nb-Ni	Re-Ta-Zr
Al-Co-Fe	Al-Hf-Re	Al-O-Zr	C-Co-Cr	C-N-Ta	Co-Fe-O	Cr-Hf-Nb	Cu-Mo-Ni	Mo-Ni-O	Re-W-Zr
Al-Co-Hf	Al-Hf-Ta	Al-Ru-Ti	C-Co-Mo	C-Nb-Re	Co-Fe-Ti	Cr-Mn-N	Cu-Ni-Si	Mo-Ni-Re	Ta-W-Zr
Al-Co-Mo	Al-Hf-Ti	Al-Ta-Ti	C-Co-Ti	C-Nb-W	Co-Hf-W	Cr-Mn-O	Cu-Ni-Ti	Mo-Ni-Ta	Ti-W-Zr
Al-Co-Ni	Al-Hf-W	B-Co-Cr	C-Co-W	C-Ni-Ti	Co-Mn-O	Cr-Mo-Ni	Cu-Ti-Zr	Mo-Ni-Ti	
Al-Co-O	Al-Hf-Zr	B-Co-Hf	C-Co-Zr	C-Ni-W	Co-Mo-Ta	Cr-Nb-Ni	Fe-Mn-N	Mo-Ni-W	
Al-Co-Ta	Al-Mn-Ni	B-Co-Mo	C-Cr-Hf	C-Ni-Zr	Co-Mo-W	Cr-Nb-Si	Fe-Mn-Ni	Mo-Re-Ta	
Al-Co-Ti	Al-Mn-O	B-Co-Ni	C-Cr-Mo	C-Re-Ta	Co-Ni-O	Cr-Ni-O	Fe-Mn-O	Nb-Ni-Ti	
Al-Co-W	Al-Mn-Si	B-Co-Re	C-Cr-Ni	C-Re-W	Co-Ni-Re	Cr-Ni-Re	Fe-Mn-Si	Nb-Ni-W	
Al-Co-Zr	Al-Mn-Ti	B-Co-Ta	C-Cr-Re	C-Ta-Ti	Co-Ni-Ru	Cr-Ni-Ru	Fe-Mo-Ni	Nb-O-Si	
Al-Cr-Hf	Al-Mo-Ni	B-Co-Ti	C-Cr-Ta	C-Ta-W	Co-Ni-Ta	Cr-Ni-Si	Fe-Mo-W	Nb-Re-Ta	
Al-Cr-Ni	Al-Mo-Re	B-Co-W	C-Cr-Ti	C-Ta-Zr	Co-Ni-W	Cr-Ni-Ta	Fe-Nb-Ni	Nb-Re-W	

272 assessed ternary systems in full range of composition and temperature

What makes a good database?

Database	Elements	Binaries	Ternaries
TCFE9 (Steel)	28	255	256
TCNI9 (Nickel)	28	350	308
TCAL6 (Aluminum)	36	260	88
TCTI2 (Titanium)	27	269	95
TCMG5 (Magnesium)	31	195	91
TCCU3 (Copper)	30	133	50
TCHEA3 (HEAs)	26	294	445

Number of possible binary systems $\frac{N * (N-1)}{2}$

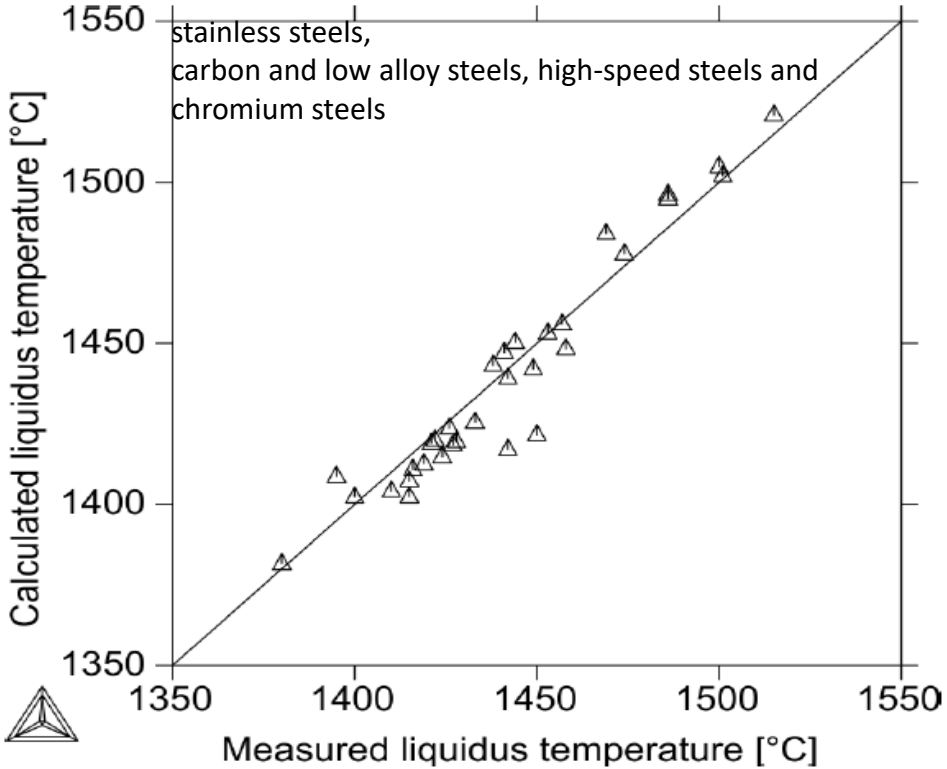
TCHEA3 = 294/325 assessed = 90%

Number of possible ternary systems $\frac{N * (N-1 * (N-2))}{6}$

TCHEA3 = 445/2600 assessed = 17%

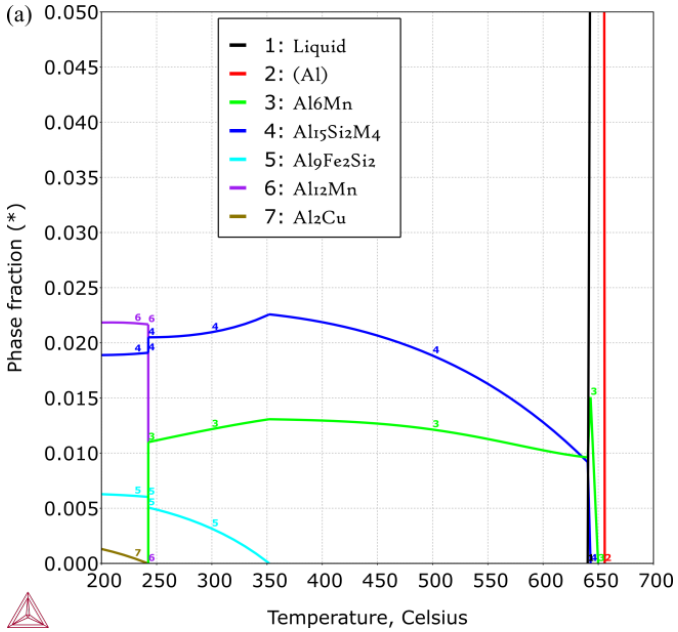
TCHEA4 = 495/2600 assessed = 19%

Validating against multi-component alloys



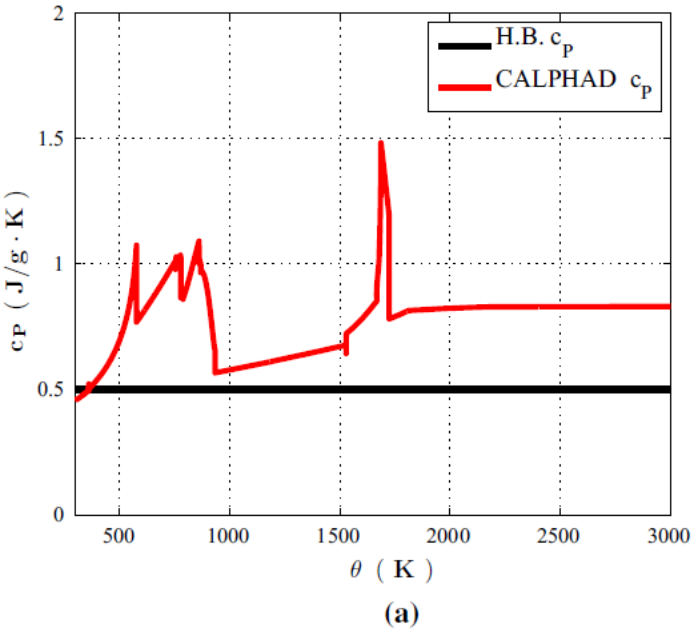
Composition/process – structure link I

- The most rudimentary assumption would be to assume full equilibrium.
- No specific consideration of the process.



Phase stability as function of Temp for alloy 3003

- Predict phase transformation temps.
- Volume fractions of phases (and composition)
- Thermodynamic properties (e.g. Cp)

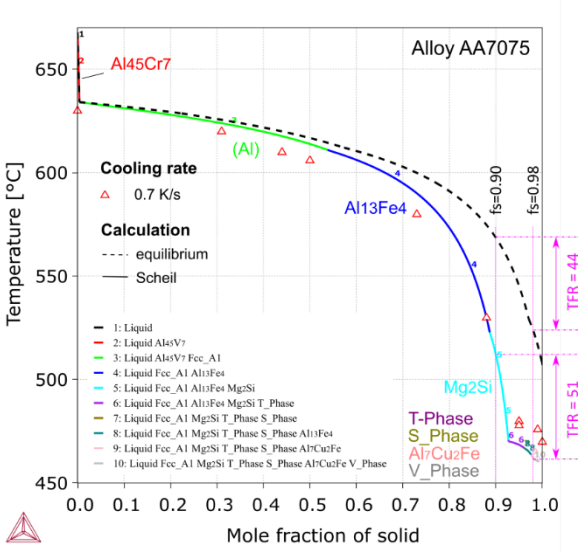


Comparison of handbook values and CALPHAD calculated values of Cp – from Smith, et al. / Computational Mechanics 57.4 (2016): 583-610.

Composition/process – structure link II

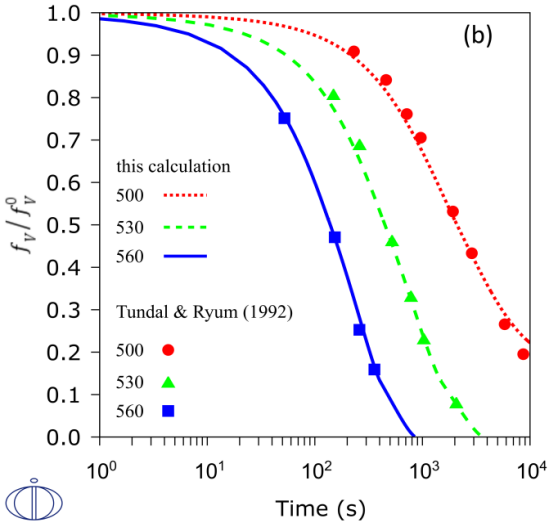
- Next step is to account for kinetics, i.e. non-equilibrium processes.
- Some consideration of the process, e.g. temperature-time evolution.

=> Allows us to predict non-equilibrium states and some geometrical aspects, e.g. precipitate size and distribution.



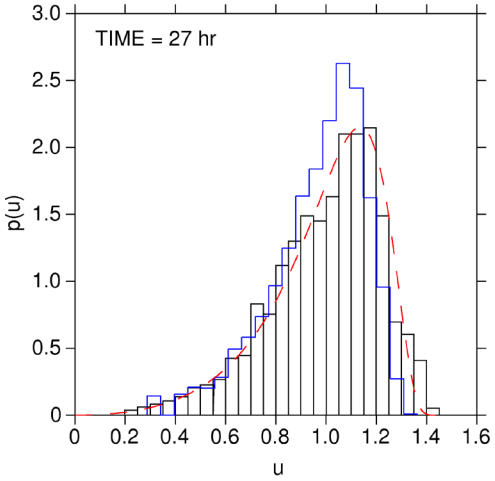
Non-eqm solidification of alloy AA7075

CASTING



Dissolution of particles

HOMOGENIZATION



Size distribution of precipitates

ANNEALING / AGING

Early example using thermodynamic calcs in alloy design

- The first systematic use of of Calphad computational tools and databases for industrial purposes. Based only on equilibrium calculations.
- In 1983 Swedish steel producer Sandvik developed a new generation of duplex stainless steels.
  - –Same price level as the conventional 18/8 steel
  - –Twice the strength
  - –Better corrosion resistance
  - –Reduced experimental costs (2 instead of 10 years)
- Most important to have 50/50 mixture of FCC-BCC.
- Avoid TCP (e.g. sigma phase)
- Same PRE-number in both phases. PRE (Pitting Resistance Equivalent) calculated empirically from phase composition.

Slide courtesy of Prof. J. Ågren, KTH

Alloy Design – Thermodynamics & kinetics

Thermo-Calc Software

Used phase equilibrium calculations to:

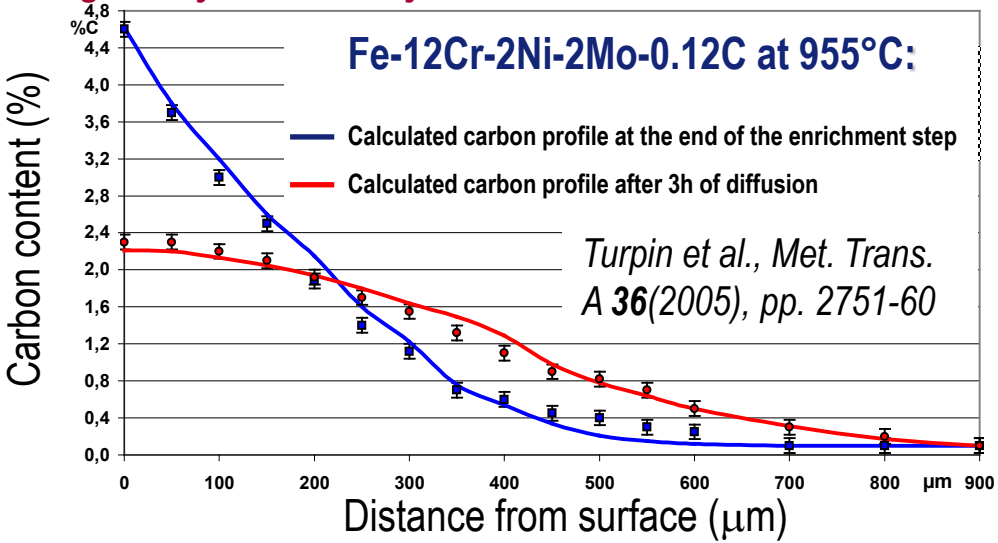
a) Optimize the amount of M23C6 and M7C3 carbides for strength

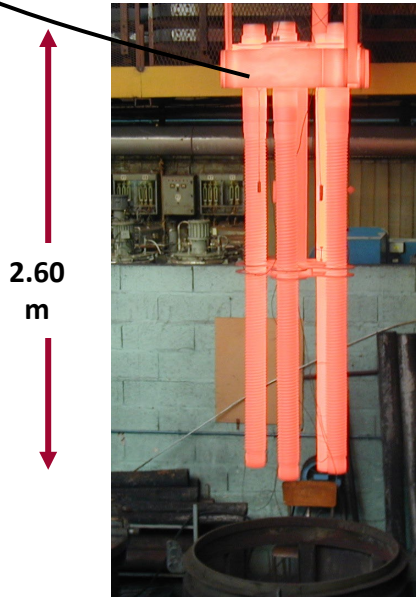
b) Avoid formation of M3C carbides which weaken the microstructure

c) Minimize Cr depletion from the matrix phase (important for corrosion resistance)

d) Balance adding carbon into the matrix phase for hardness with depleting carbon through the formation of carbides.

***Example:* Simulation of carbon evolution in high alloyed steels by Aubert & Duval, France.**





Density Calculations

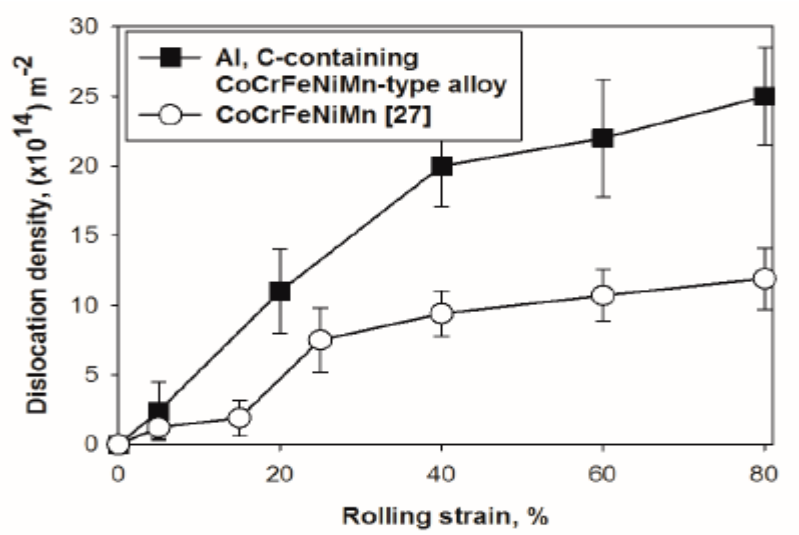
Table 1. Calculated lattice parameter and density compare with experimental data. Calculation was made at 673K.

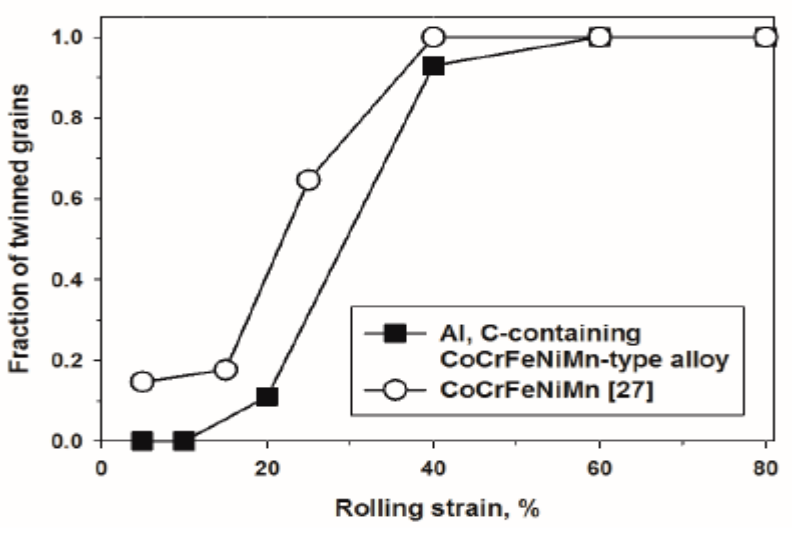
	LP Exp. (nm)	LP Cal. (nm)	Density Exp. (g/cm^3)	Density Cal. (g/cm^3)
CrFeCoNi	0.357	0.359	8.1	8.03
CrCoNi	0.357	0.359	8.2	8.08
CrFeNi	0.359	0.360	7.9	7.88
FeCoNi	0.358	0.359	8.4	8.30
MnCoNi	0.360	0.363	8.1	7.91
MnFeNi	0.362	0.365	7.9	7.81
CoNi	0.354	0.356	8.8	8.62

LP within 0.5% +/- 0.3% Density within 1.3% +/- 0.7%

Laplanche, Guillaume, et al. "Elastic moduli and thermal expansion coefficients of medium-entropy subsystems of the CrMnFeCoNi high-entropy alloy." *Journal of Alloys and Compounds* 746 (2018): 244-255.

Deformation mechanism – stacking fault energy





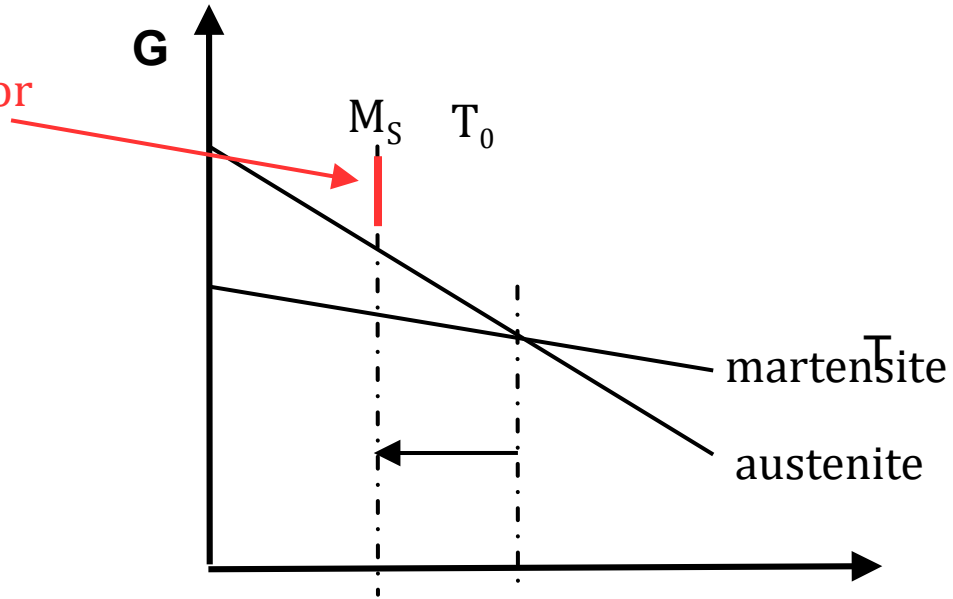
- Twinning occurs at low SFE
- Stacking fault energy $\gamma = 2\rho\Delta G^{hcp-fcc} + 2\sigma$
- Calculated $\Delta G_{hcp\text{-}fcc}$=0.98 & 0.72 kJ/mol for Al-C-containing and equiatomic HEA, respectively
- Larger **SFE** require higher stresses for twinning initiation; thus, the onset of deformation in Al, C-containing alloy was generally associated with slip promoting a more intensive increase in dislocation density.

Klimova, Stepanov, Shaysultanov, Chernichenko, Yurchenko, Sanin, Zherebtsov; *Materials*. 11 (2018) 53.

Modeling Martensite transformations

- γ→α diffusionless transformation by shear
- Martensite start temperature M_S is the temperature where the available driving force overcomes the barrier to switch the lattice to Martensite phase

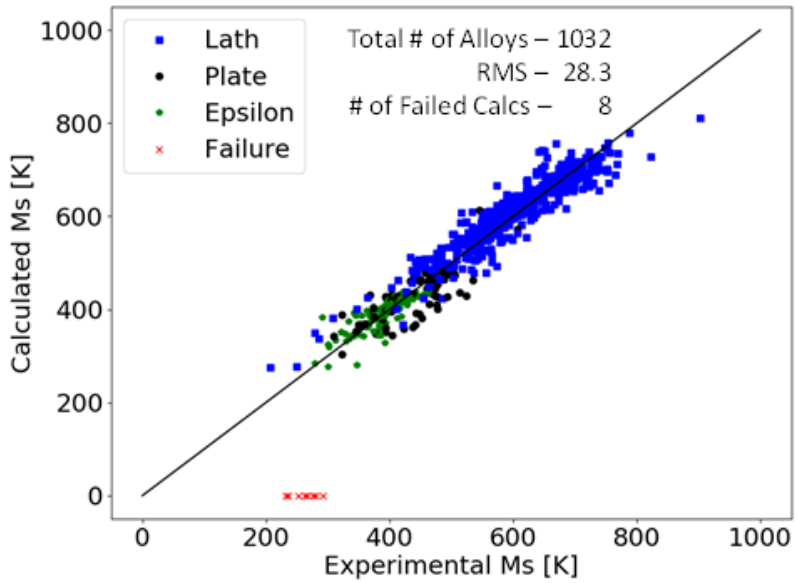
Additional barrier for transformation to Martensite
→ how to model?



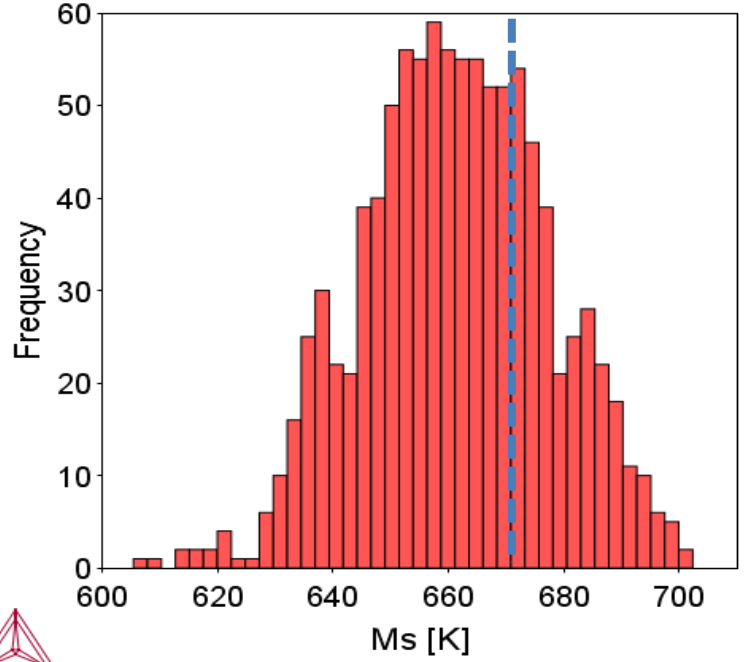
Semi-empirical model for describing the additional barrier (Stormvinter et al. Met. Mater Trans. 43A (2012)):

- takes into account the driving force to form martensite calculated by the CALPHAD method, with additional parameters added for various Fe-X binary systems

Modeling Martensite start temperatures (I)



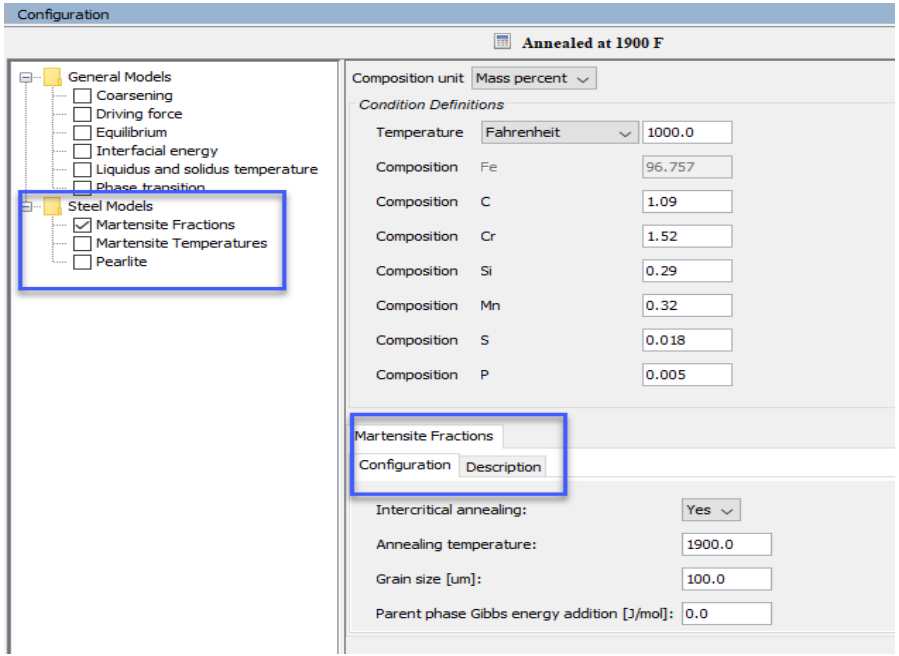
Comparison of calculated Ms against experimental Ms temperatures. Alloy compositions and Ms temperatures compiled from literature by Hanumantharaju.

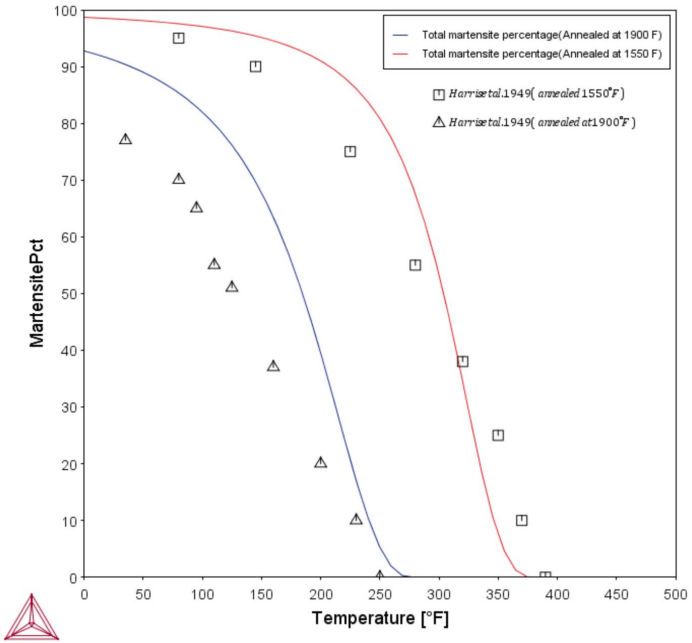


Calculated Ms temperature variation in 410 Stainless Steel composition specification

Measured value of 672K by Stone (OSU), 2017

Modeling Martensite fractions





- Based on model of Huyan et al. Met. Mat. Trans. A 2016
- Assumes first forming martensite morphology is only forming one.
- Austenite composition from eqm calc. at annealing temperature
- Grain size of austenite
- Austenite with smaller grain size is more stable

Dynamic and Kinematic Viscosity for TCFE10 and TCHEA4

Dynamic viscosity

- End-members $RT \ln \eta = RT \ln \eta_0 + E$

- The SI unit of viscosity is pascal.second (Pa.s). The viscosity parameters are expanded via Redlich-Kister polynomials

$$RT \ln \eta_{\text{alloy}} = x_A\left(E_A + RT \ln \eta_0^A\right) + x_B\left(E_B + RT \ln \eta_0^B\right) + x_A x_B [L_0 + (x_A - x_B).L_1]$$

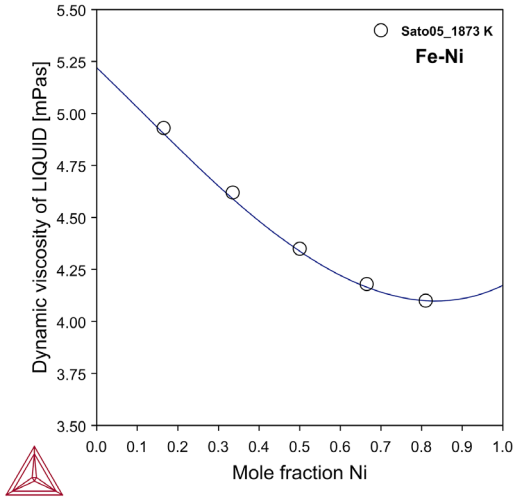
Kinematic viscosity

Kinematic viscosity, ν, is the ratio of the dynamic viscosity to the density, ρ, of the alloy:

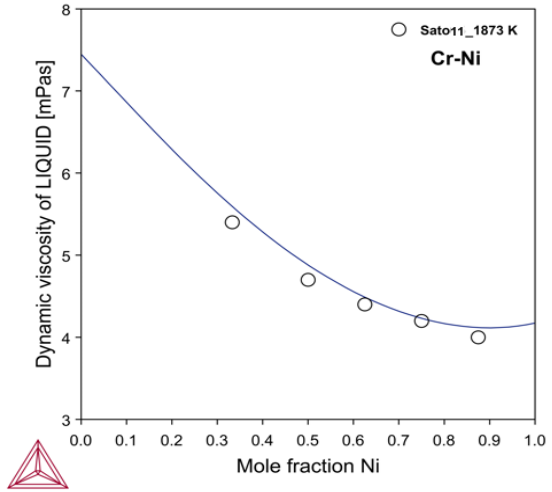
$$\nu = \eta/\rho \quad (\text{m}^2/\text{s})$$

Viscosity of Liquid Metals: Viscosity Curve Examples

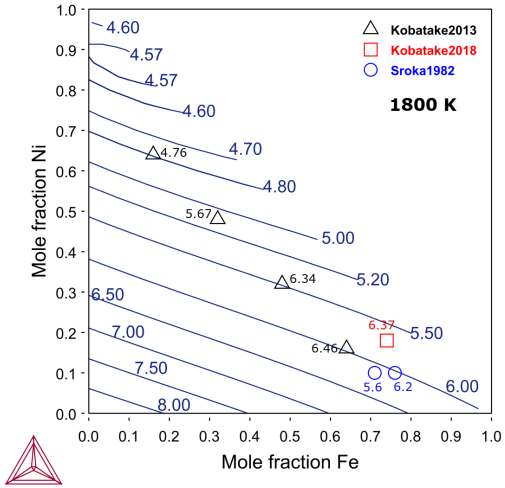
Fe-Ni, 1873 K



Cr-Ni, 1873 K



Cr-Fe-Ni, 1800 K



[1] Sato, Yuzuru; Sugisawa, Koji; Aoki, Daisuke; Yamamura, Tsutomu (2005) Measurement Science and Technology, 363-371

[2] Sato, Yuzuru (2011), Jpn J Appl Phys 50, 11RD01

[3] Kobatake, Hidekazu; Brillo, Jurgen (2013) J Mater Sci 48, 6818-6824

[4] Kobatake, Hidekazu; Brillo, Jurgen (2018) High Temp High Press 47, 465-477

[5] Sroka, M; Skala, J.; Freiberg Forschungsh (1982) 229, 17

Property Model Calculator: General Model for Yield Strength

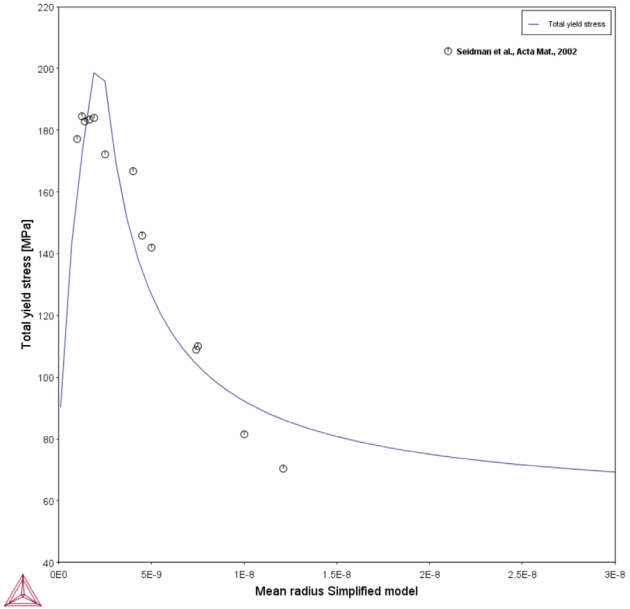
A new general model called the *Yield strength* model is added to the Property Model Calculator.

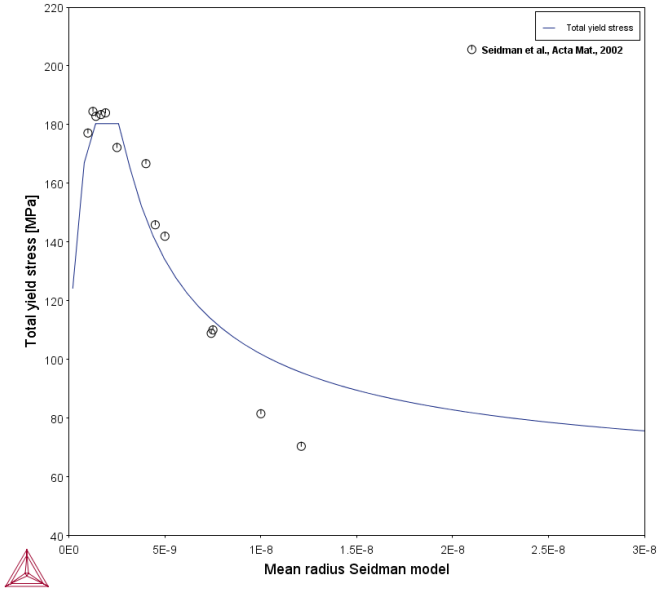
This model considers four contributions to the overall yield stress of the material:

- intrinsic strength for the pure elements
- grain boundary strengthening
- solid solution strengthening
- precipitation strengthening

A user-set temperature is used to evaluate the equilibrium of the system, and the resulting compositions and phase fractions are subsequently used in the evaluation of mechanical properties.

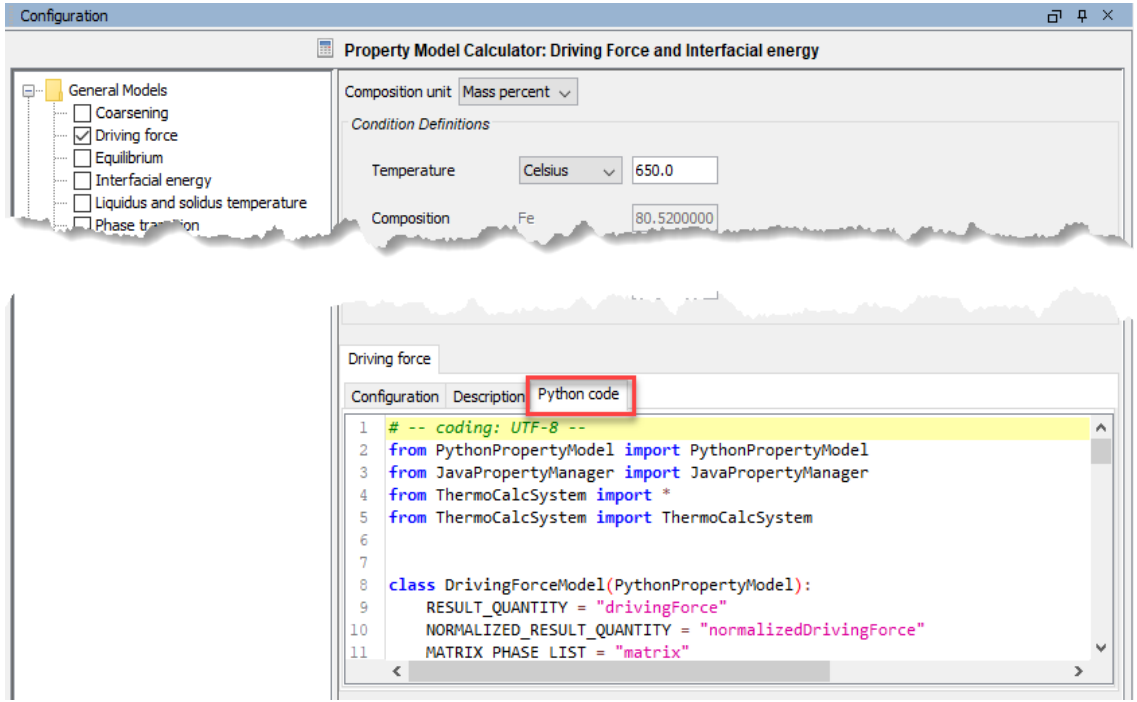
Property Model Calculator: General Model for Yield Strength

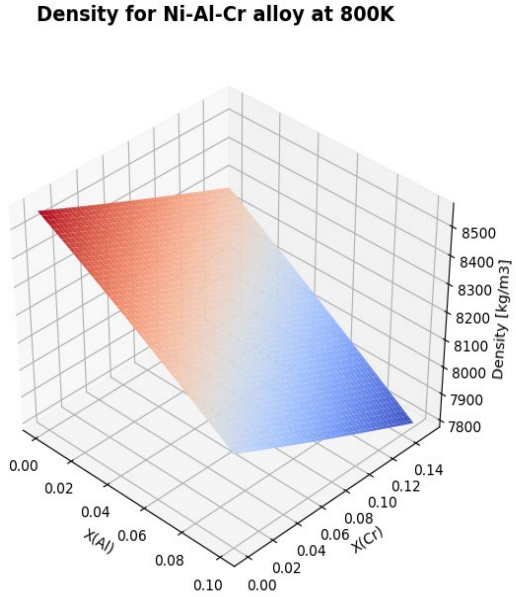




These plots are from the G_04 Yield Strength example which compares the **Simplified** and **Seidman** models yield strength versus precipitate radius to experimental data for an Al-0.3wt%Sc alloy homogenized at 648 °C for 24 hours and subsequently aged at 350 °C. Although the experimental set up is designed to eliminate grain boundary and solid solution strengthening, these are also included in the examples but give a negligible contribution to the total strength.

TC-Python: SDK for Thermo-Calc, DICTRA, TC-PRISMA





The batch equilibrium calculation type is similar to single equilibrium calculations, but it offers significant performance improvements when calculating a lot of fast single equilibria, which are systems with few or non-complicated phases.

Ab Initio and CALPHAD

Thermo-Calc Software

- **CALPHAD needs theoretical data**
  - wherever experimental data are sparse
  - wherever experiments are difficult, extreme conditions…
  - wherever experiments are impossible, metastable phases and endmembers…
- **First principle calculations help to predict**
  - Pure elements or end-member compounds
    - H, S, Cp
    - volume, thermal expansivity
    - elastic constants, shear, Young's, bulk modulus
    - Debye temperatures, Grueneisen parameters,…
  - Mixing or interaction properties
- **First principle calculations should be combined with CALPHAD**
  - It is not sufficient to predict phase equilibria with first principle values alone.

Machine Learning and CALPHAD

Thermo-Calc Software

Ocean of Data: Integrating First-Principles Calculations and CALPHAD Modeling with Machine Learning

Zi-Kui Liu

ELSEVIER

Acta Materialia
Volume 164, 1 February 2019, Pages 636-647

Full length article

Bayesian uncertainty quantification and information fusion in CALPHAD-based thermodynamic modeling

P. Honarmandi [a], T.C. Duong [a, b], S.F. Ghoreishi [b], D. Allaire [b], R. Arroyave [a, b]

ELSEVIER

Acta Materialia
Volume 186, March 2020, Pages 425-433

Full length article

Accelerated design of novel W-free high-strength Co-base superalloys with extremely wide γ/γ′ region by machine learning and CALPHAD methods

Jingjing Ruan [a, e], Weiwei Xu [b], Tao Yang [c], Jinxin Yu [a], Shuiyuan Yang [a], Junhua Luan [d], Toshihiro Omori [e], Cuiping Wang [a], Ryosuke Kainuma [e], Kiyohito Ishida [e], Chain Tsuan Liu [c, d], Xingjun Liu [a, f, g]

Show more

Machine learning needs data and often these data are lacking. Using CALPHAD predictions can help fill the data gaps and provide better correlated models.

Machine learning can also help build better CALPHAD databases and models for property predictions.

Summary

Thermo-Calc Software

Simulation is an essential component of Industry 4.0. Simulation software relies on good data which includes materials data. However, these data vary with how the material is processed and its chemical composition. Handbook data and repositories typically do not capture such variations. When the data are not available there are three choices:

Do an experiment which can be costly or time consuming
Live with the uncertainty
Or simulate / predict the data

CALPHAD is a phase based approach to modeling material properties for multicomponent systems and is an important foundation to ICME and the MGI. For more than 30 years CALPHAD based tools have been used to accelerate alloy design and improve processes with applications throughout the materials life cycle.

Four years ago we stated that there would be a shift to predicting more properties and examples of this has been presented here. Future developments are likely to be focused on more properties, better integration, improved visualization and optimization which allow materials scientists and engineers to “trade off” properties based on design parameters. We should also expect to see more combined use of Ab initio, CALPHAD and Machine Learning as three legs on a stool that drive better and more efficient predictability of material properties.