Thermo-Calc Software

Database NEWS

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Computational Thermodynamics and Kinetics Seminar
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Introduction

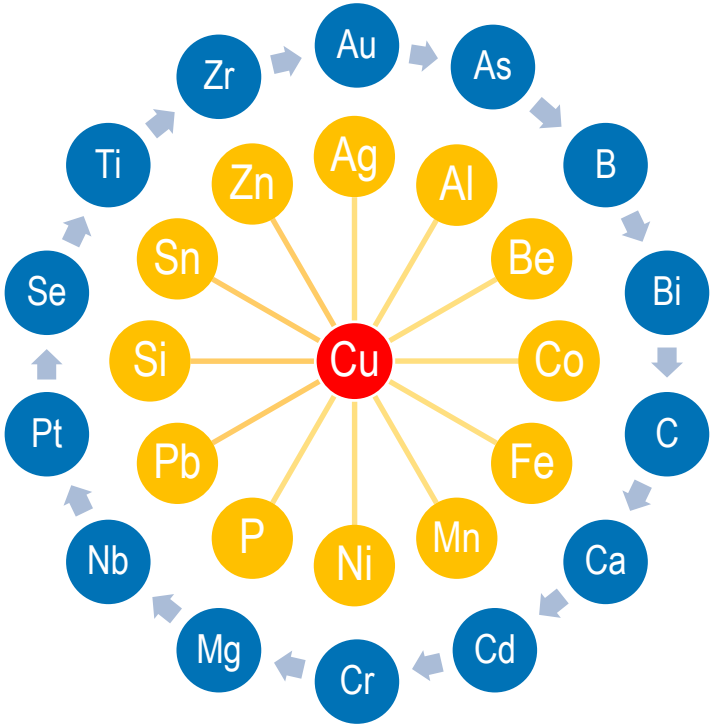
- **New and updated databases**
  - TCCU1
  - MOBCU1
  - SLAG4
  - SSOL6
  - TCNI6, 7, 8
  - Demo-databases

- **On-going database development**
  - TCFE9
  - TCNI9
  - TCOX7
  - TCTI1

TCCU1

Thermodynamic database for Cu-based alloys

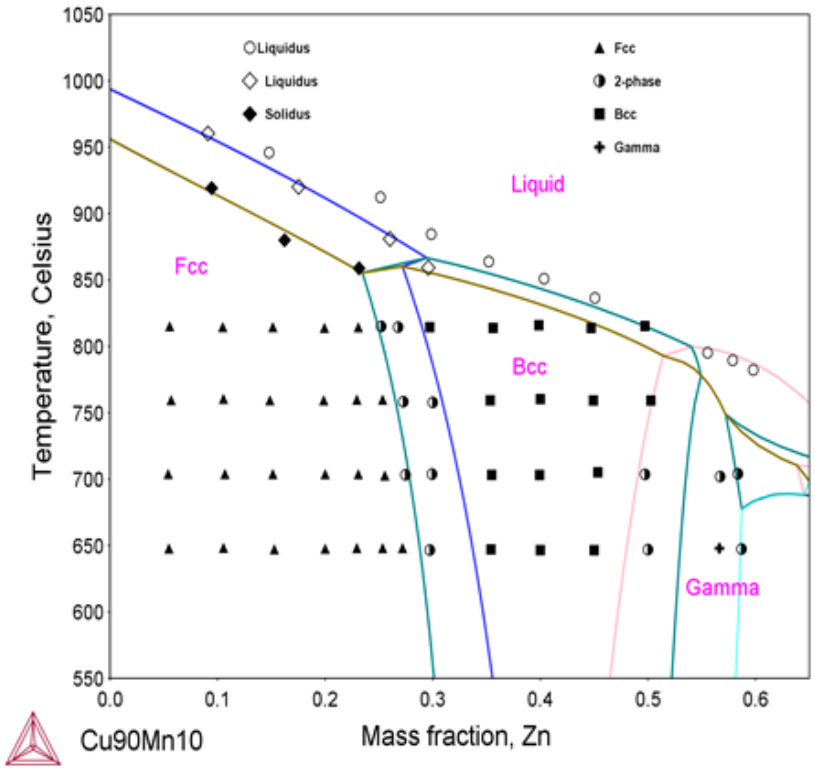
- 27 elements
- 113 assessed binary systems
- 40 assessed ternary systems
- 219 phases



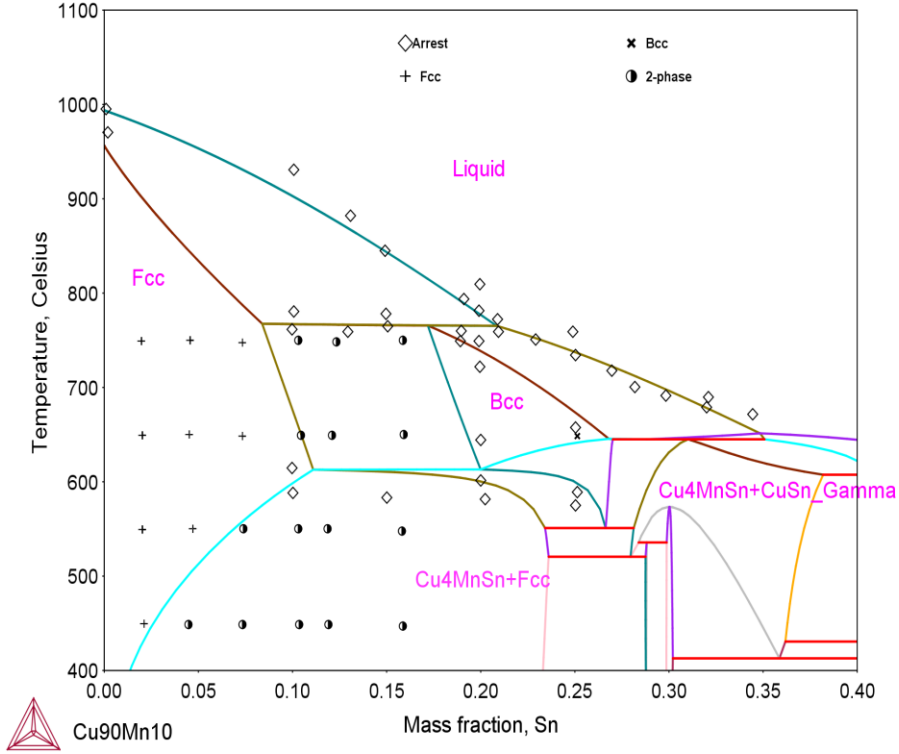
TCCU1

Thermo-Calc Software

Cu-Mn-Zn system

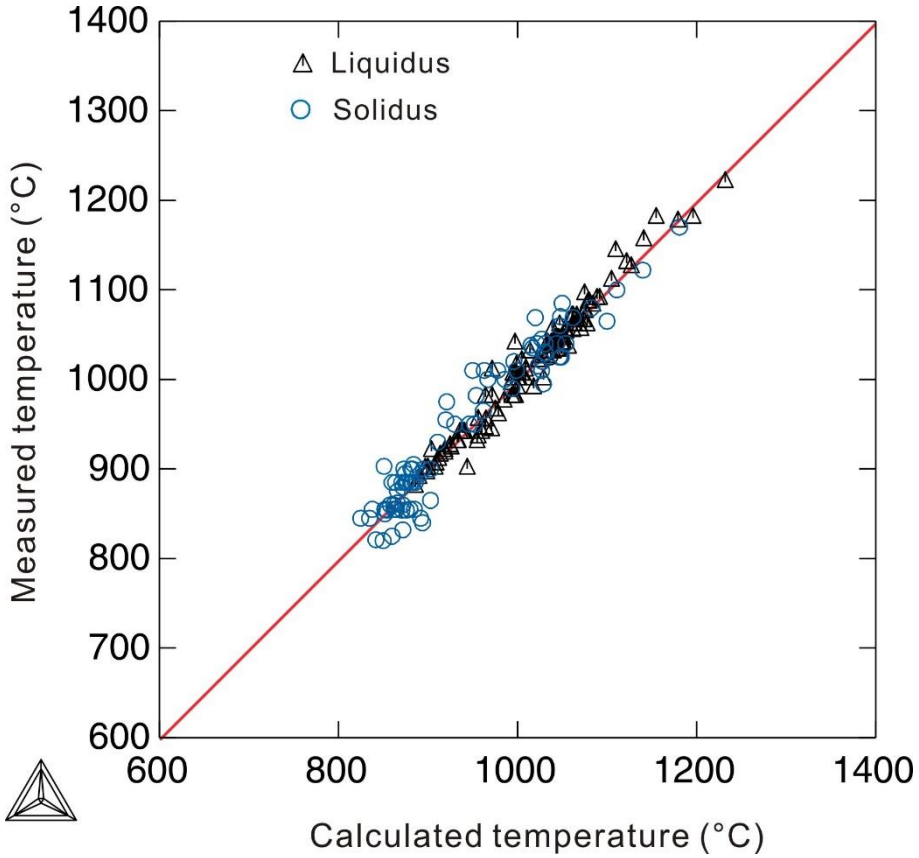


Cu-Mn-Sn system



Calculated vertical sections of 10wt.% Mn in (a) Cu-Mn-Zn and (b) Cu-Mn-Sn systems along with experimental data.

TCCU1



105 multi-component industry alloys

- Cu-Al-Fe-Ni based alloys
- Cu-Fe-Ni-Mn based alloys
- Cu-Pb-Sn-Zn based alloys
- Cu-Al-Si based alloys
- Cu-Fe-P based alloys
- Cu-Be-Co based alloys
- .....

MOBCU1

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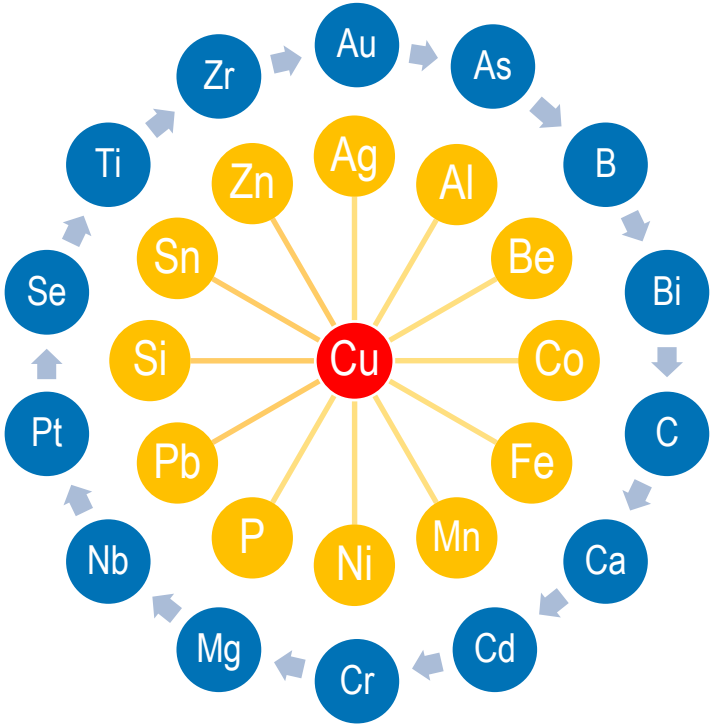
Atomic mobility database for Cu-based alloys

- 27 elements
- Liquid and fcc phases
- 37 binary systems
- 26 ternary systems
- 1 quaternary systems

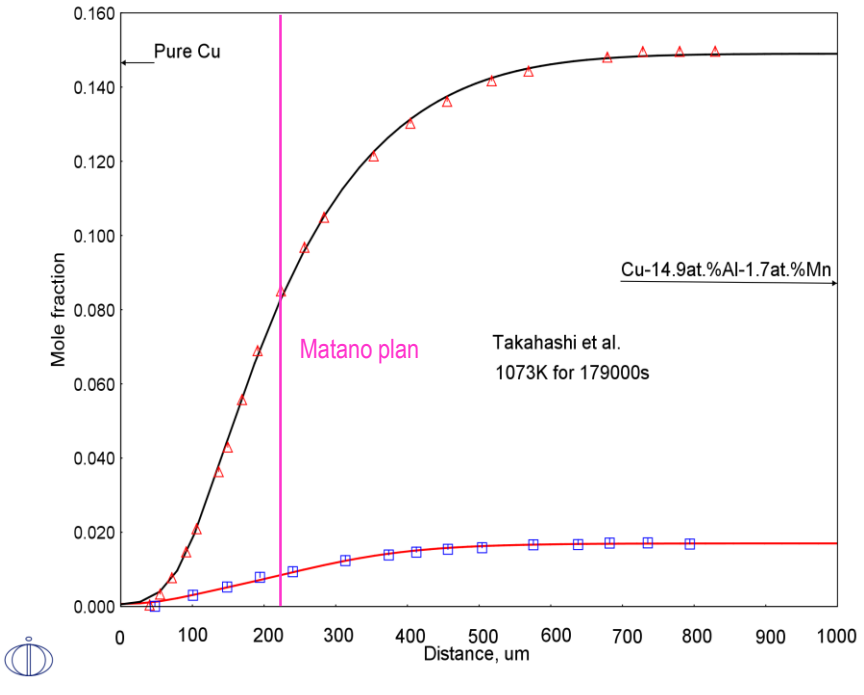


MOBCU1

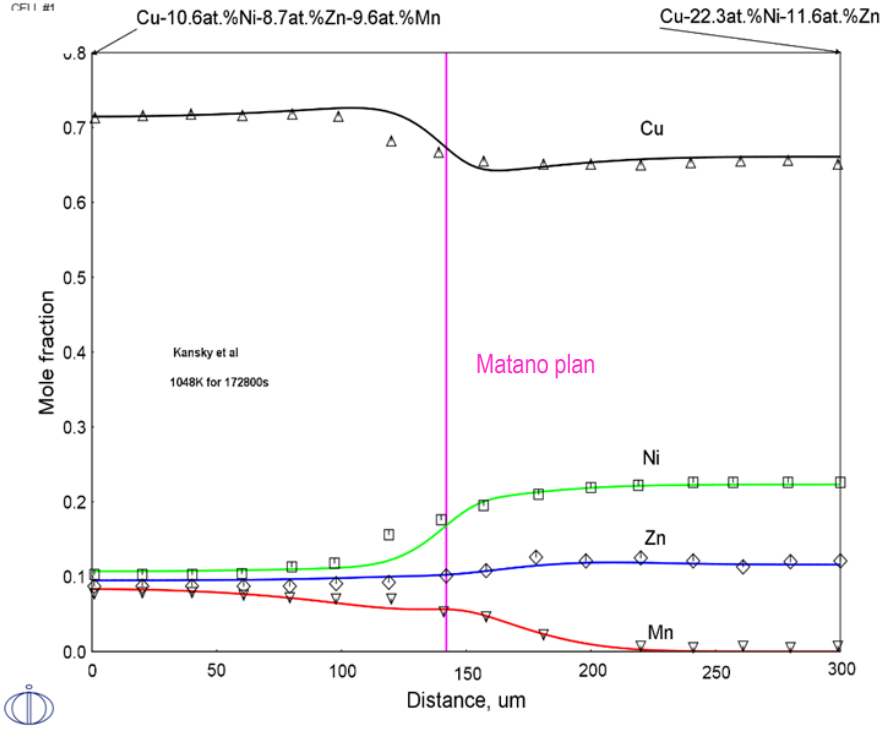
Thermo-Calc Software

❑ Diffusivity in solid (fcc) phase

Cu-Al-Mn system



Cu-Ni-Mn-Zn system



Calculated concentration profile compared with experimental data **(a)** Cu//Cu-14.9Al-1.7Mn diffusion couple, **(b)** Cu-10.6Ni-8.7Zn-9.6Mn//Cu-22.3Ni-11.6Zn diffusion couple

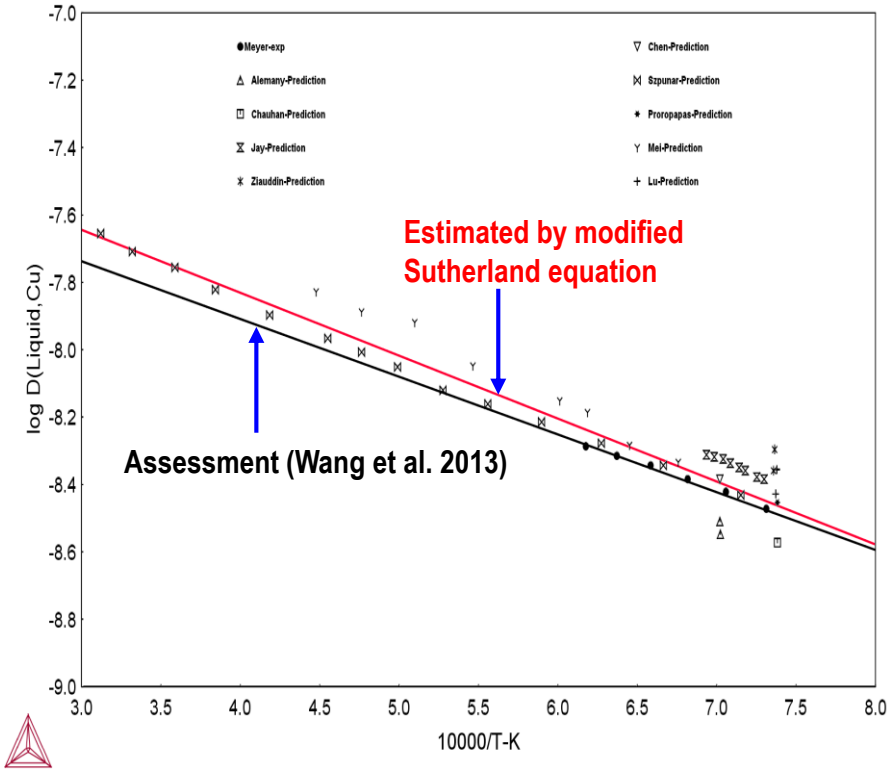
Experiments from Takahashi et al. , Defect. Diffus. Forum. 95 (1993) 641

Kansky et al. Metall. Mater. Trans. A 16 (1985) 1123

MOBCU1

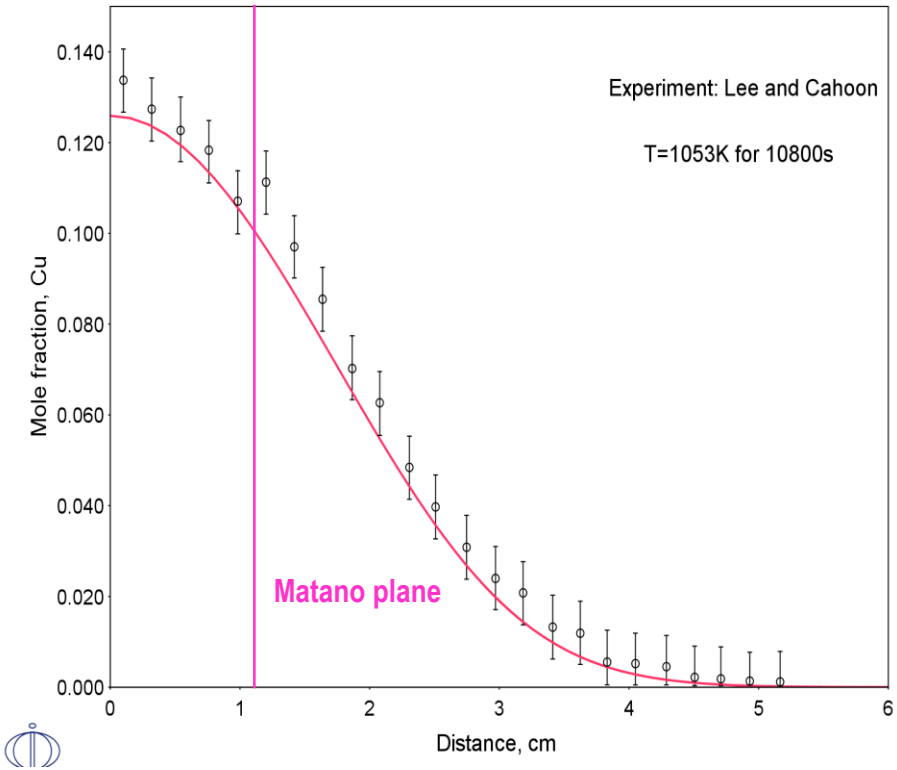
❑ Diffusivity in liquid phase

Self-diffusivity of liquid Cu



Calculated self-diffusivity of Cu in liquid phase compared with experimental data.

Cu-Al system



Calculated concentration profile compared with experimental data Al-0.231Cu // Al diffusion couple annealed at 1053 K for 10800 s.

SLAG4

- Phosphorus was added.
- The gas phase was simplified to accelerate the equilibrium calculation.
- Better description of some solid fluorides such as AlF3, FeF2, FeF3, MgF2, and MnF2.
- Oxygen solubility in liquid iron and FeO stability corrected.

SLAG4

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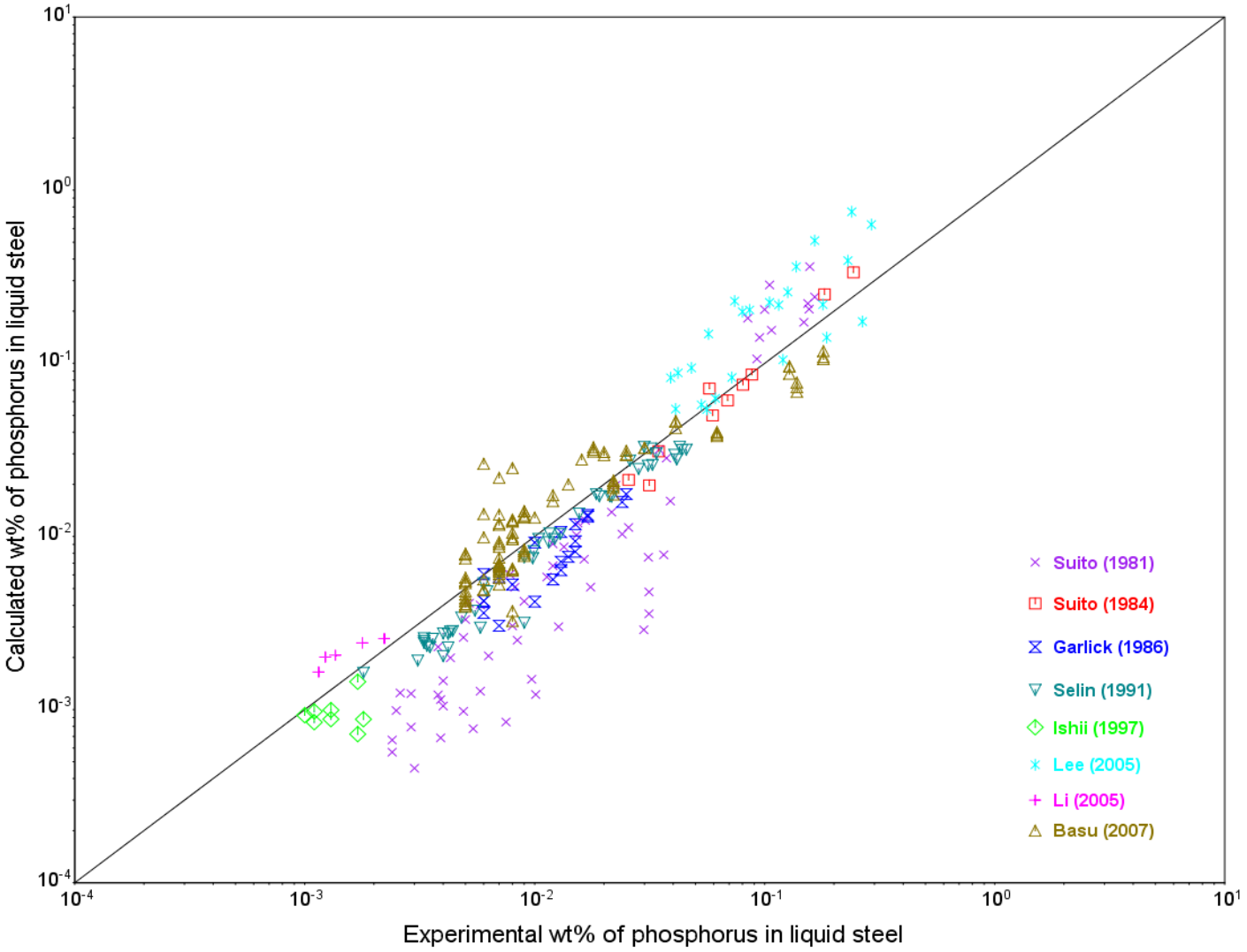
Phorsphorus solubility in liquid iron in equilibrium with steelmaking slag



SSOL6

SSOL6 contains assessed thermodynamic data from the literature and provided by SGTE members. SSOL6 includes 729 alloy systems consisting of:

- 575 binary systems
- 133 ternary systems
- 20 higher-order systems
- 1331 phases.

The key changes from SSOL5 to SSOL6 are listed below:

- Hydrogen (H) is added to the database – now 79 elements.
- Many binary and ternary systems are added or updated in SSOL6.

TCNI6, TCNI7, TCNI8

- The TCNI6, TCNI7, TCNI8 databases have been slenderized.
  - Loading the databases is now 2 times faster.
  - Saving calculation time by as high as 50%.

DEMO-Databases

New DEMO-databases

- NIDEMO: Includes Ni, Al and Cr (full ternary description)
- MNIDEMO: Includes mobility data for Ni, Al and Cr in BCC_B2 and FCC_L12
- MALDEMO: Includes mobility data for Al, Cu, Sc and Si in FCC_A1.

Updated DEMO-databases

- ALDEMO: Includes Al, Cu, Sc and Si. Sc has been added to the database.

- **New and updated databases**
  - TCCU1
  - MOBCU1
  - SLAG4
  - SSOL6
  - TCNI6, 7, 8
  - Demo-databases

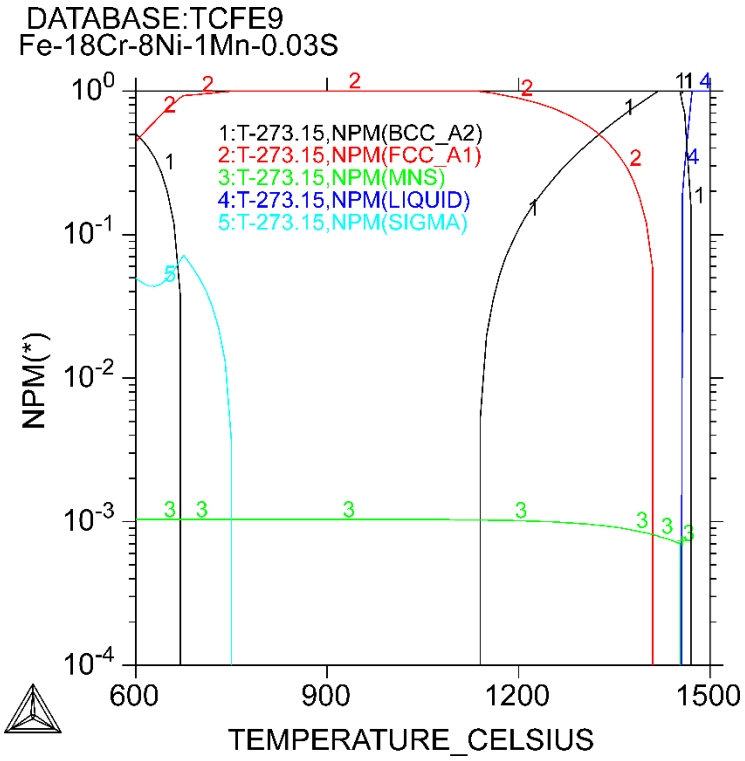
- **On-going database development**
  - TCFE9
  - TCNI9
  - TCOX7
  - TCTI1

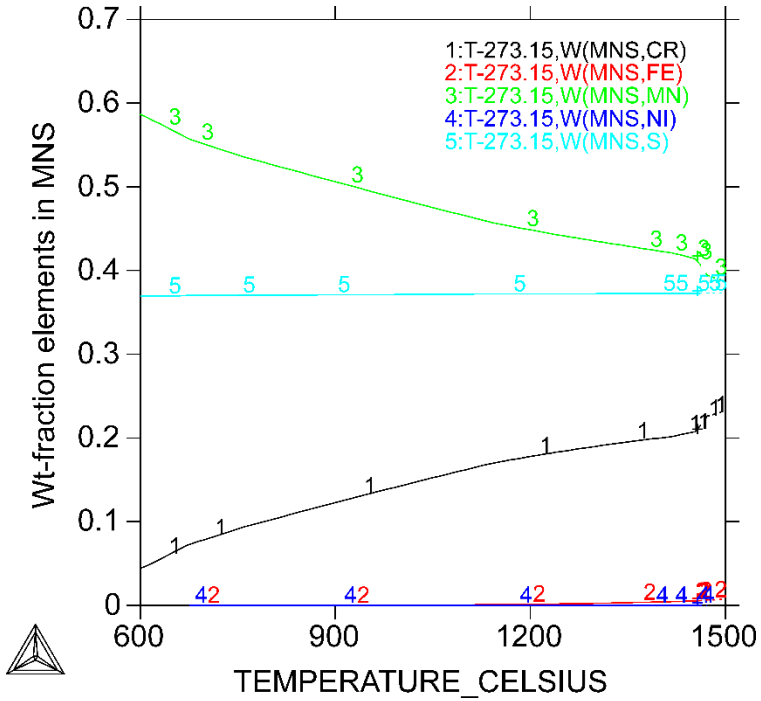
TCFE9 and FROST

- Ongoing work:
  - Improved sulfides description.
  - Improved Laves phase prediction.
  - Improved Sigma phase prediction.
  - Improved Fe-Cu-X systems.
  - Improved high Mn-high Al systems.
  - Extended Kappa phase description.
  - Improved ordered phases BCC_B2 and FCC_L12 descriptions.
  - Improved Borides description.
  - To include Ce and Gd

TCFE9 development

Improved sulfides description.

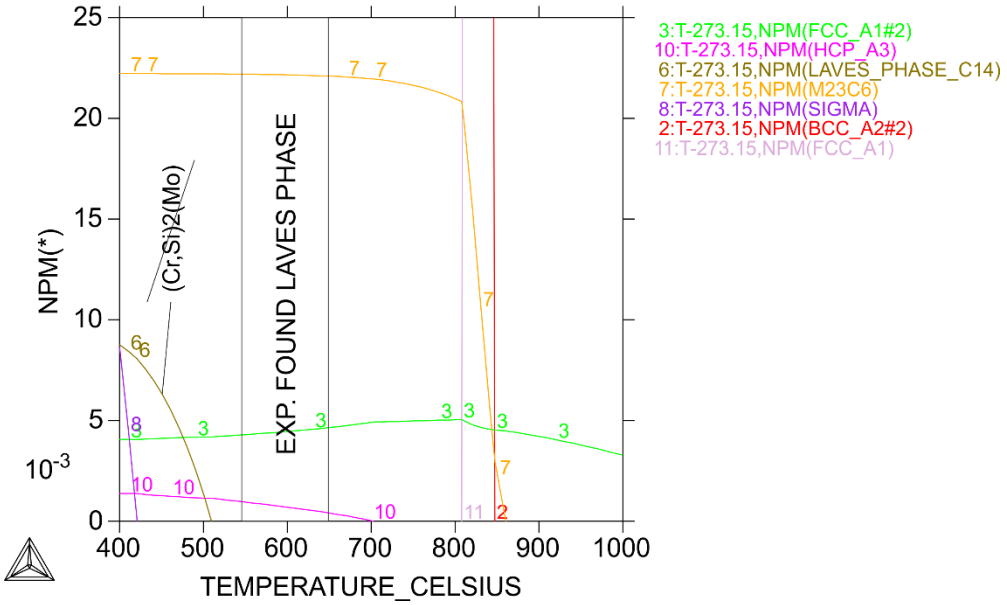




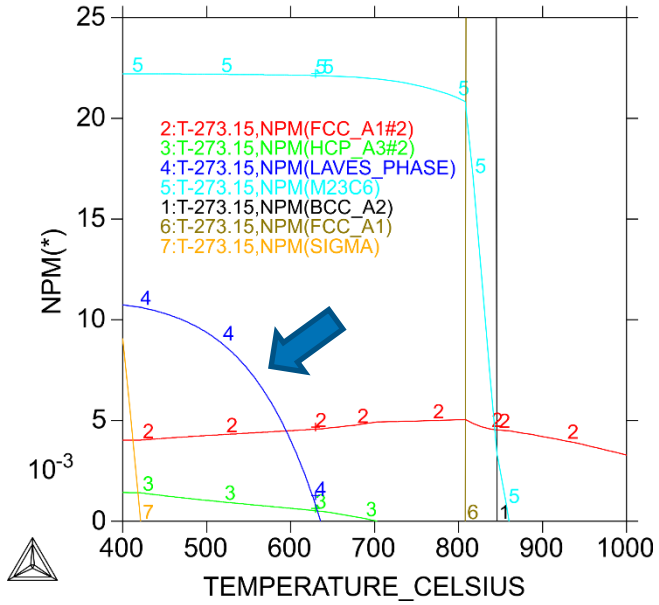
TCFE9 development

Improved Laves phase prediction.

DATABASE:TCFE7



DATABASE:TCFE9



	C	Cr	Mn	Mo	N	Nb	Ni	V	Si
ASME91	0.1	8	0.5	1	0.06	0.05	0.1	0.2	0.4

Thermo-Calc Software

- *Equilibria at liquidus - solidus*
- *Equilibria of matrix phases at high temperature*
- *Equilibria of secondary phases at intermediate temperature*

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Database modifications

Binary

Cu-N Fcc	Ni-N Bcc	Si-N Fcc, Bcc	Mn-Ni Fcc, bcc, liq		

Ternary

Cr-Fe-Mn Fcc	Cr-Fe-Mo Sigma, Laves	Cr-Fe-N Bcc, Fcc	Cr-Fe-Si Sigma	Cr-Mn-N Bcc	Cr-Ni-N Bcc, Fcc
Fe-Mn-Mo Bcc, Fcc, Laves	Fe-Mn-N Bcc	Fe-Mo-Si Sigma, Laves	Fe-Ni-N Bcc	Fe-W-N Bcc	Fe-Mo-V Laves
Fe-Mo-Nb Laves	Fe-Ni-Mo Laves	Cu-Fe-N	Fe-Si-N	Fe-Mn-Ni Fcc, bcc, liq	

Quaternary

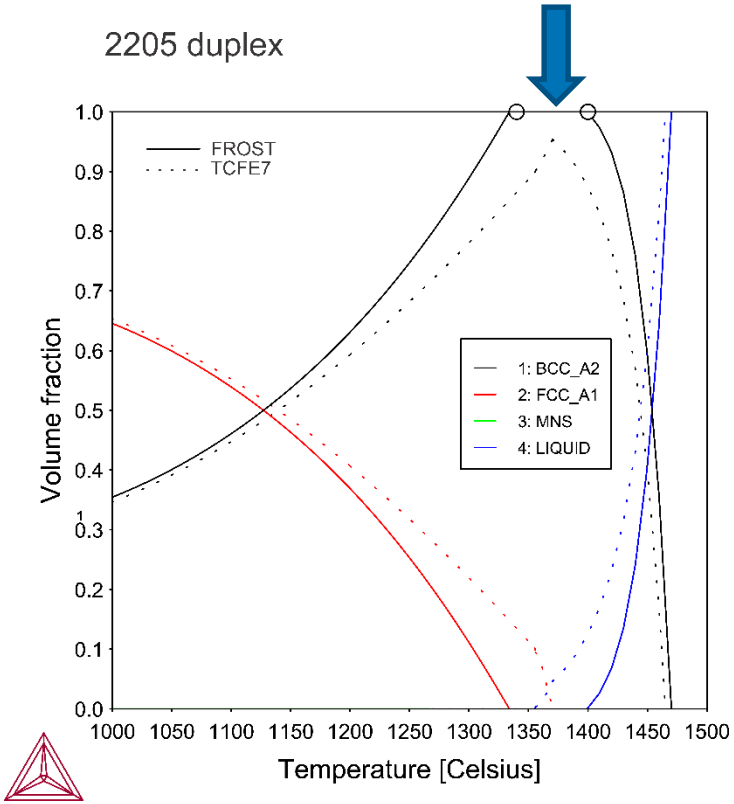
Cr-Fe-Mn-N Fcc, Hcp	Cr-Fe-Ni-N

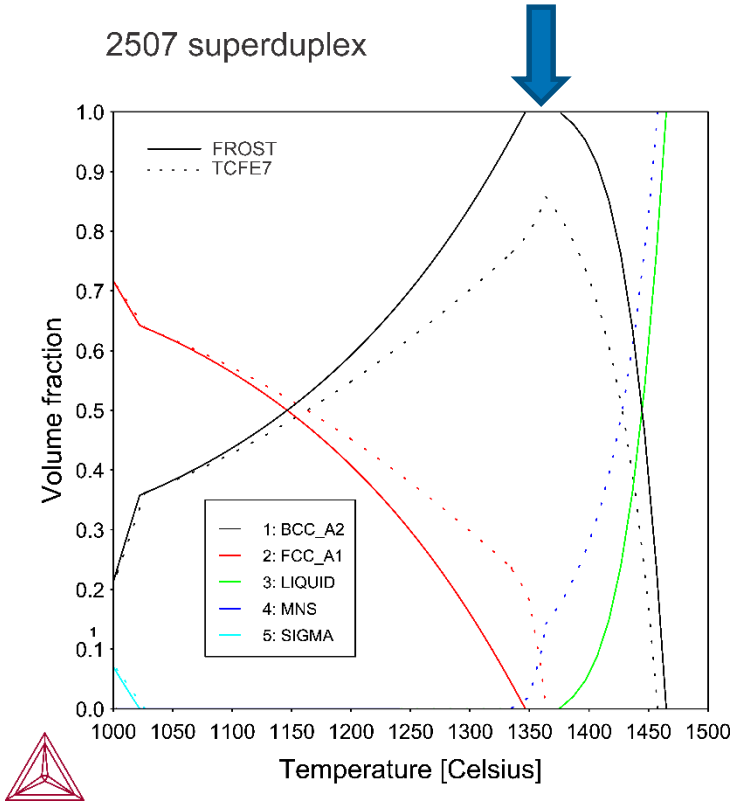
Quinary

Cr-Fe-Mo-Ni-N

A: Equilibria at liquidus - solidus

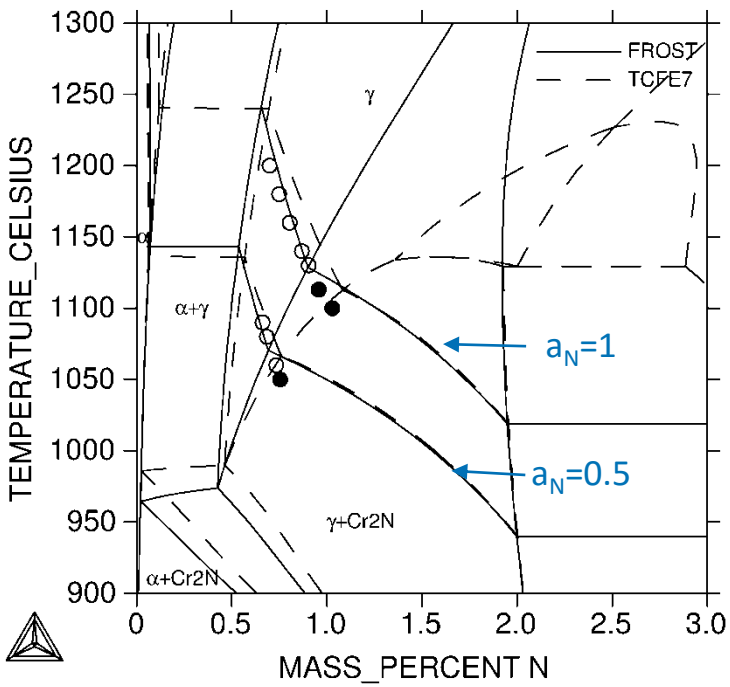
Phase fractions vs. temperature: 2205 duplex & 2507 superduplex



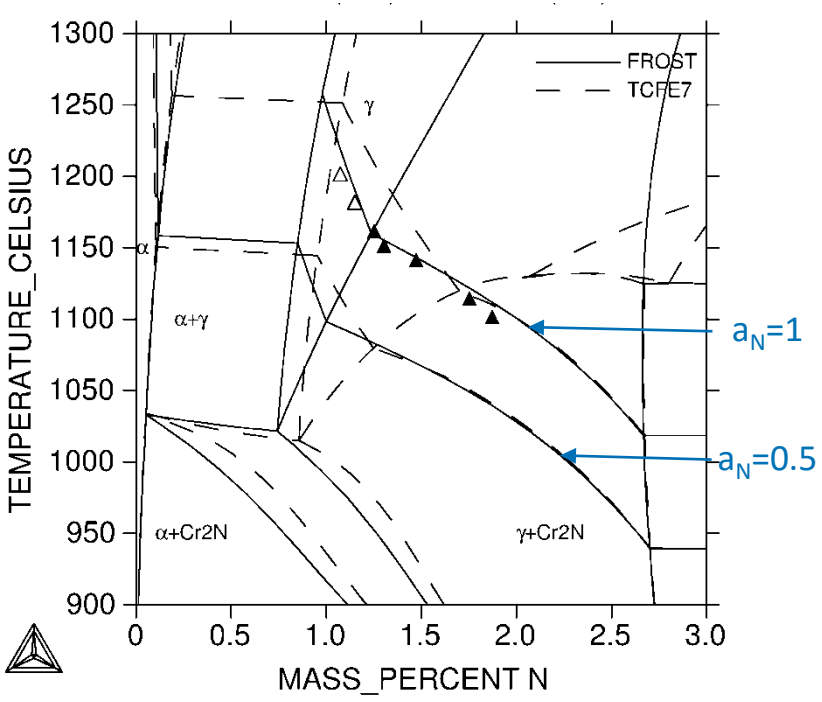


Thermo-Calc Software

C: Equilibria of secondary phases at intermediate temperature



Fe-19.8Cr-0.11Mn-N



Fe-24.3Cr-0.44Mn-N

Temperature [°C] vs. nitrogen content [wt-%] with isoactivity lines a_N=0.5 and 1 and experimental results.

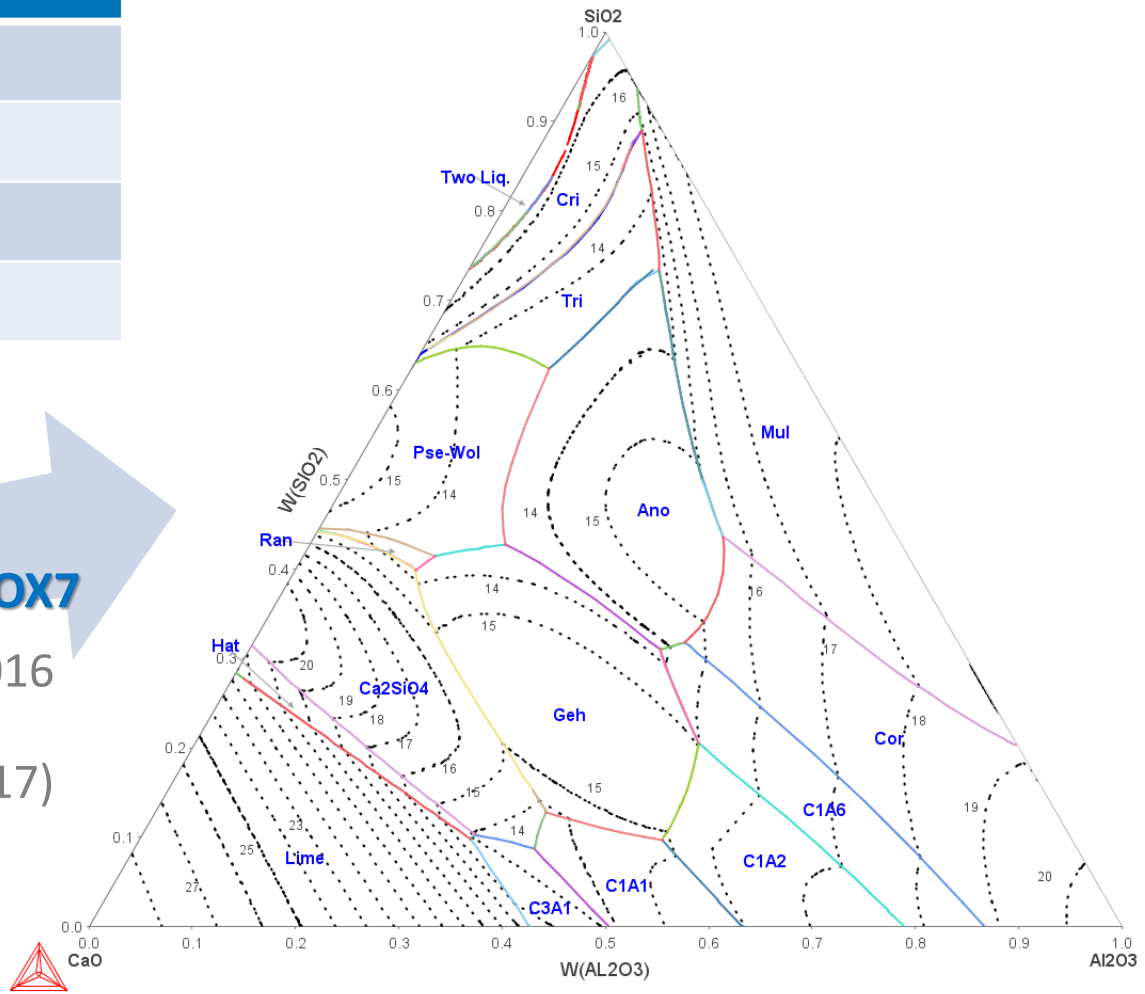
TCOX7

Al	C	Ca	Cr
Fe	Mg	Mn	Ni
O	Si	Y	Zr
F	Nb	S	Ti
Cu	La	Gd	

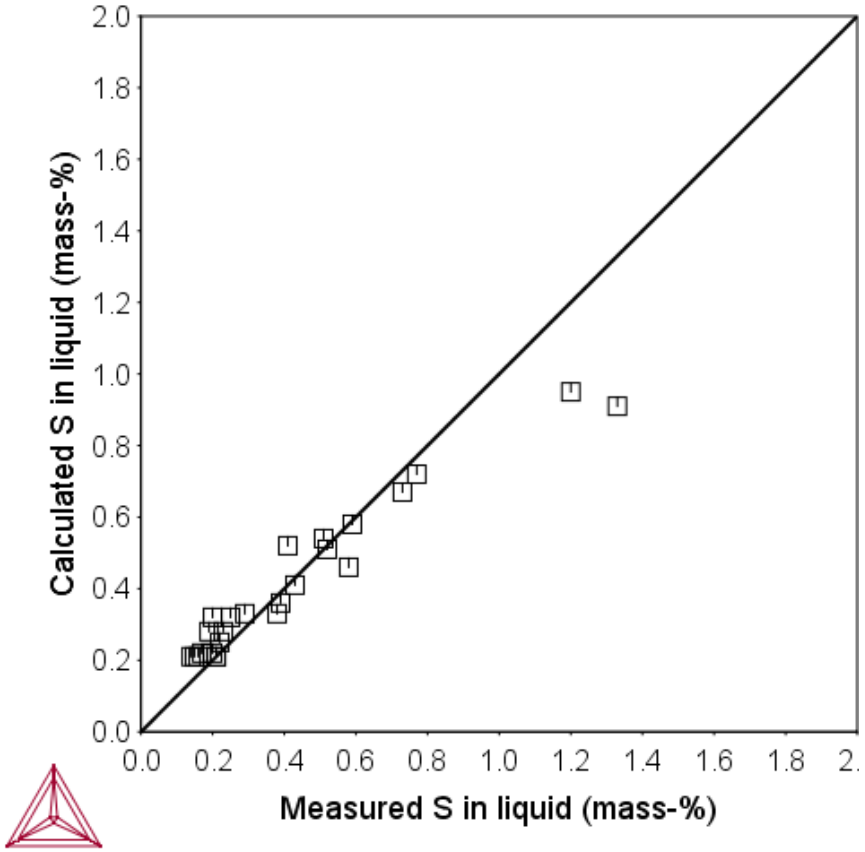
TCOX5 (2014)

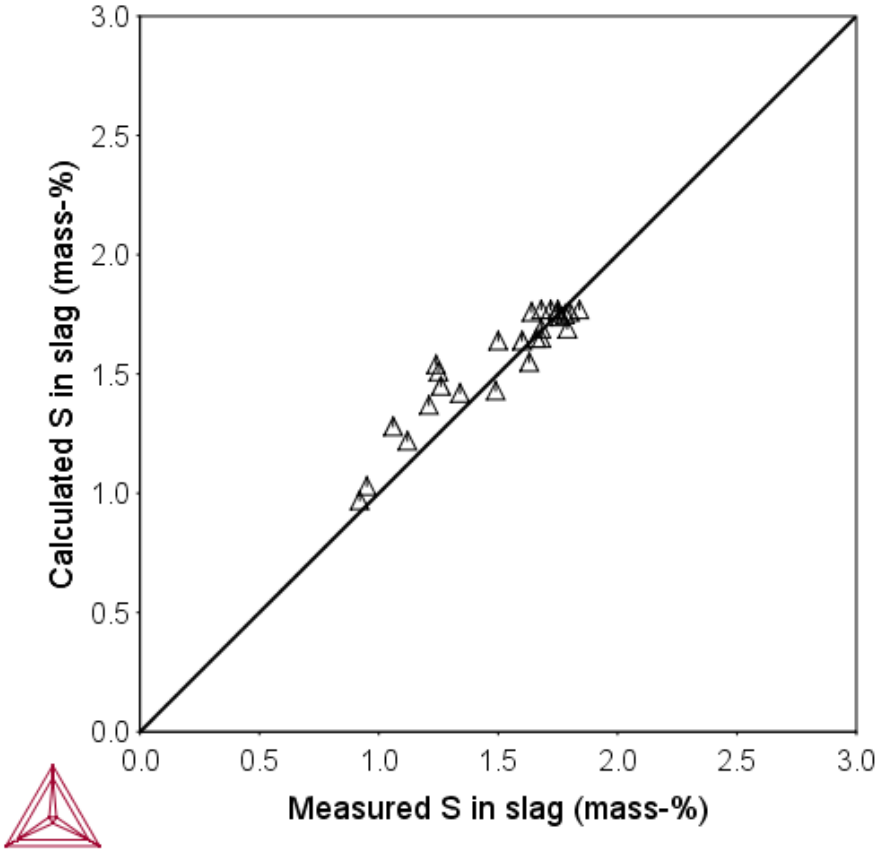
TCOX6 (2015)

TCOX7 (2016 or 2017)



TCOX7



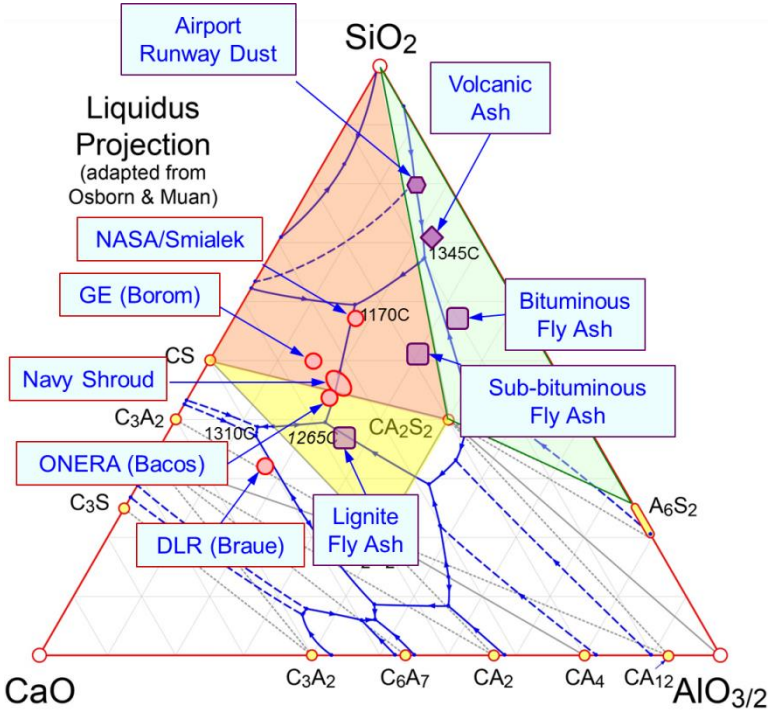


Computed Sulfur content in Cu liquid and slags in Cu-Al-Ca-Mg-Si-O-S system by mixing (liquid) Cu, Cu2S and a CMAS slag.
Experimental data are from C. Allertz's thesis (2016).

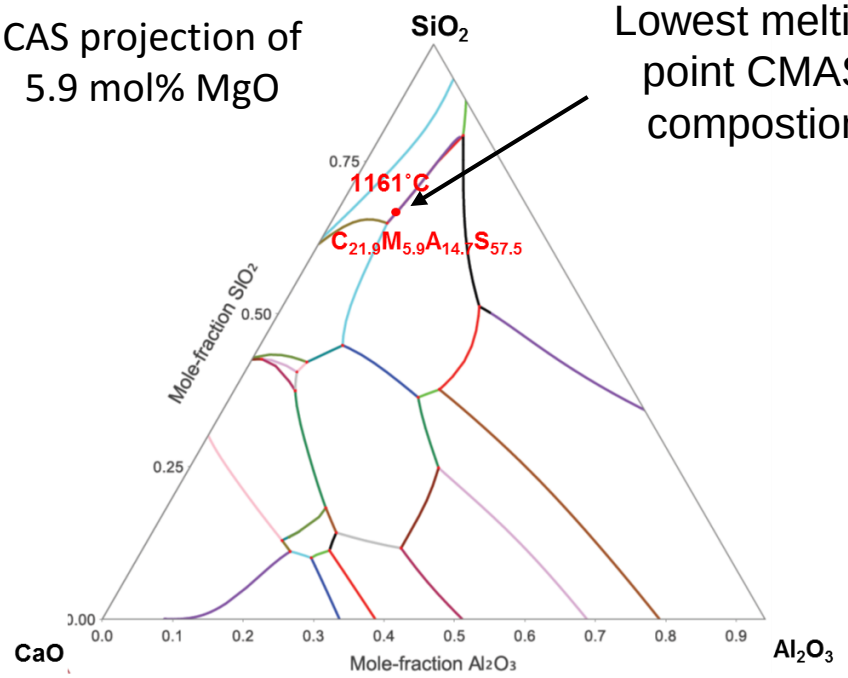
Thermo-Calc Software

Lowest melting point CMAS

- NASA/Smialek composition ($C_{23}M_9A_{13}S_{55}$) melts at 1170°C
- Database predicted lowest melting point at 1161°C CMAS composition: $C_{21.9}M_{5.9}A_{14.7}S_{57.5}$



CAS projection of 5.9 mol% MgO



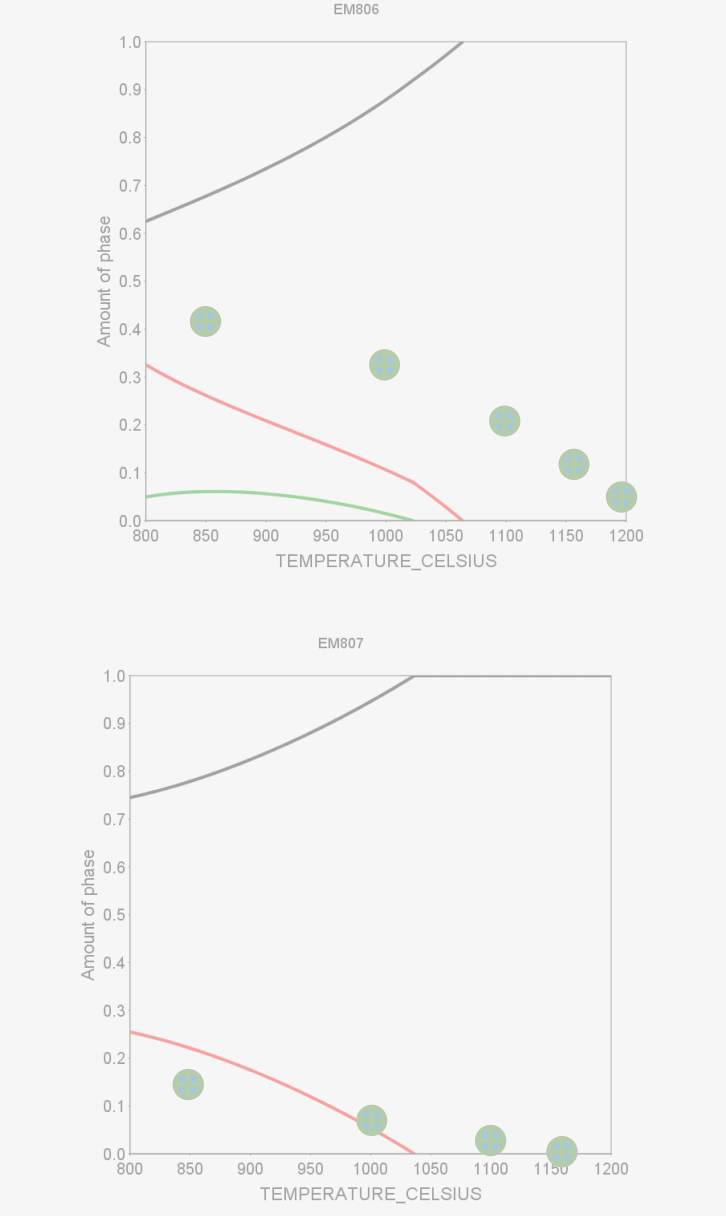
Lowest melting point CMAS compostion

TCNI9

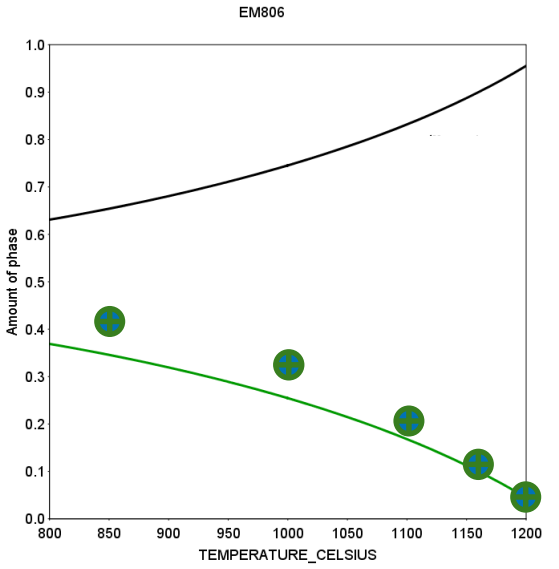
Experimental investigation in the Ni-Al-Co-Fe-Nb-Ti system was performed.

- All alloys showed high amount of eta-phase while TCNI8 predicts gamma-prime.
- Additional ternary and quartanary alloys were produced, heat-treated and analyzed for the TCNI9 development.
- After adjusting TCNI9 to this new experimental info, eta phase is predicted in the Ni-Al-Co-Fe-Nb-Ti alloys.

TCNI9



γ
γ'
η



γ
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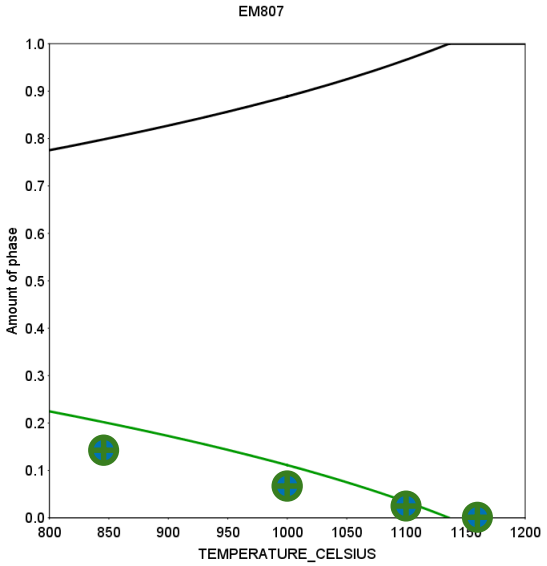
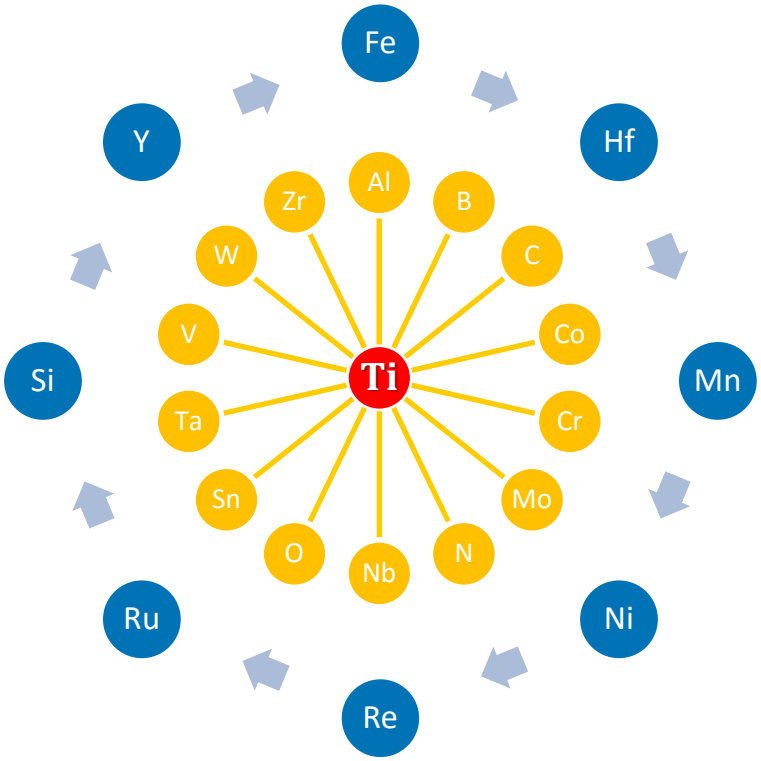


TCTI1

- **23 elements**
- **237 binary systems**
- **65 ternary systems**
  - 1 directly added
  - 29 to be reassessed
  - 35 to be assessed
  - 3 to be extrapolated



All important phases including ω phase and its variants

DFT calculations

ω, pure elements

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

ω , ordered structures, C32 and $B8_2$, Ti_2X + TiX_2

- X = Al, Co, Cr, Cu, Fe, Hf, Mn, Mo, Nb, Ni, Pd, Pt, Re, Ru, Si, Sn, Ta, V, W, Y, Zr

β Ti-X

- SQS @ 25, 50, 75 at.% X (20 * 3 = 60 structures)
- Supercell @ 25, 50 at.% X (20 * 2 = 40 structures)

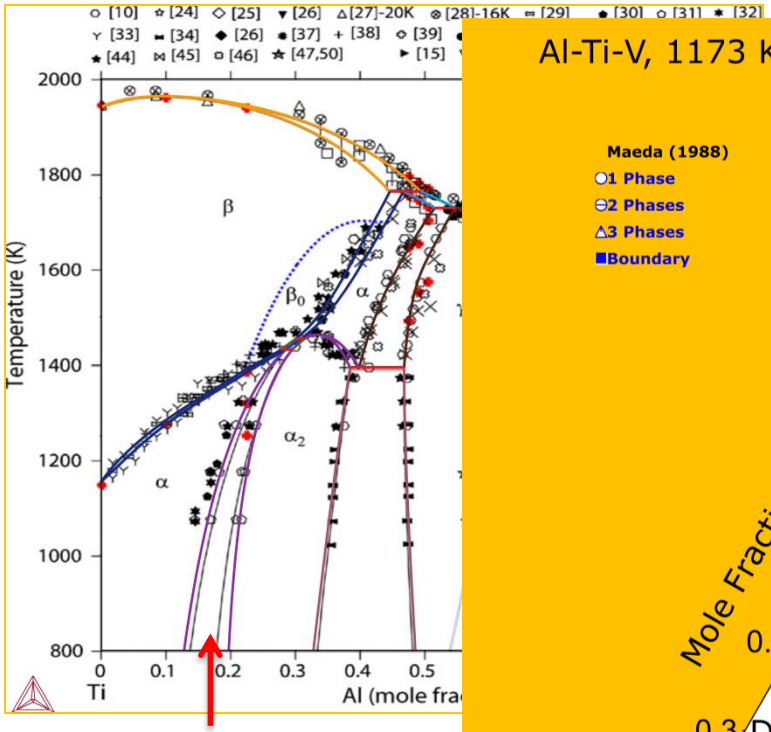
α Ti-X

- SQS @ 25 at.% X (19 structures)
- Supercell @ 25, 50, 75 at.% X (57 structures)

ω Ti-X (next step)

- SQS Ti36X12 (21 structures)
- Supercell $Ti_{96}X_{12}$, $Ti_{81}X_{27}$, $Ti_{54}X_{54}$ for X ≠ Z
- Supercell $Ti_{96}X_{12}$, $Ti_{81}X_{27}$, for Z=Cr, Mo, Nb, Ta, V, W

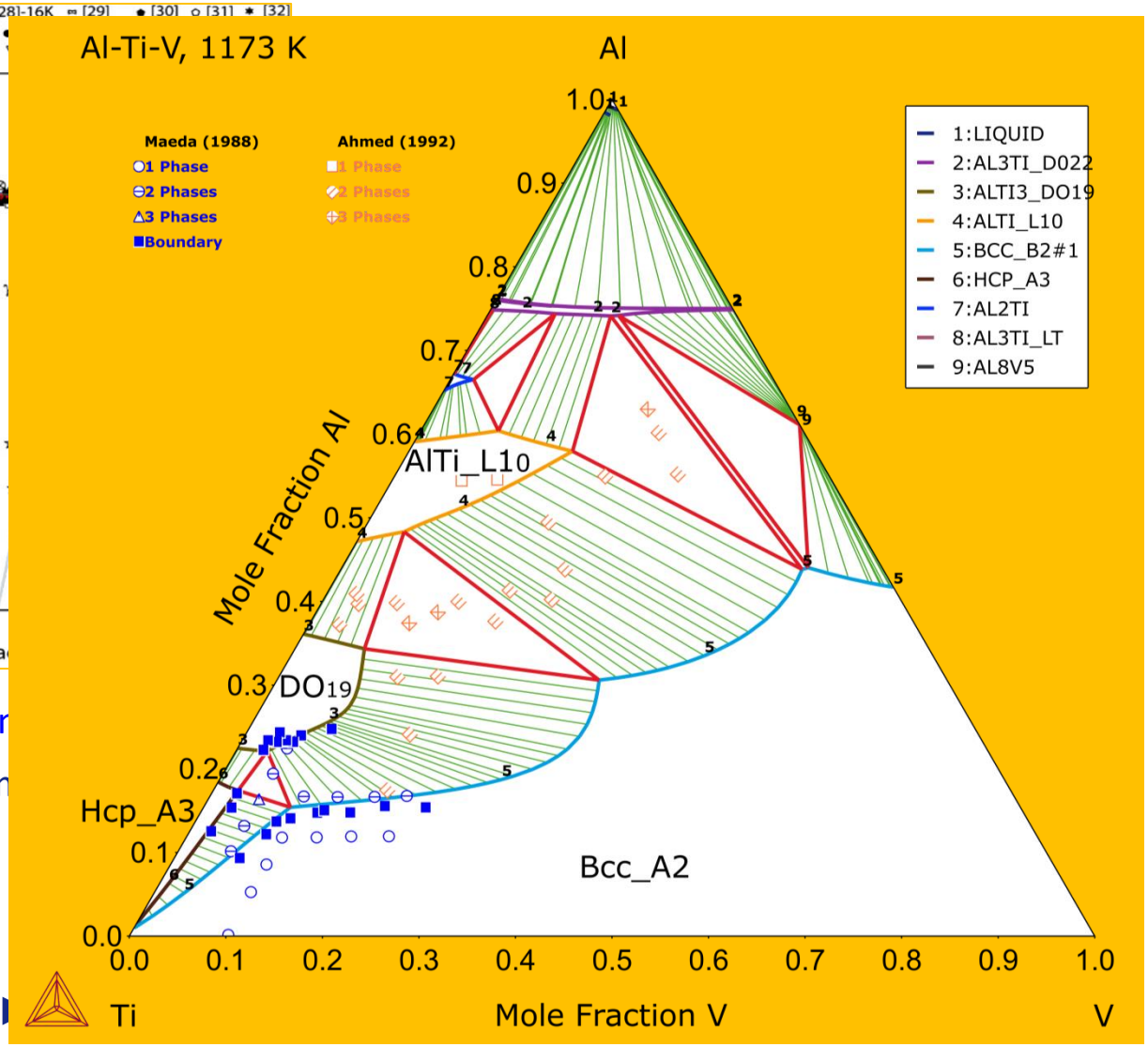
Example: Al-Ti-V



Al-Ti with modification or

Witusiewicz, J Alloys Com

Al-Ti -V, this work



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Thank You!

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