Thermodynamic modeling in HEAs

Calphad part of the project "High-throughput experimental and Calphad screening of CCAs (Hi-TeCC) – towards new alloys with exceptional mechanical properties".

With Christian Haase and Fabian Kies (IEHK, RWTH Aachen University)

Mehdi Noori, Bengt Hallstedt

Synthesis and Processing Subgroup Online Meeting, 8 October, 2021

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- Completed work
  - → Al-Co-Mn
  - → Al-Co-Fe
  - → Al-Ni-V (DFT)
- Database example calculations
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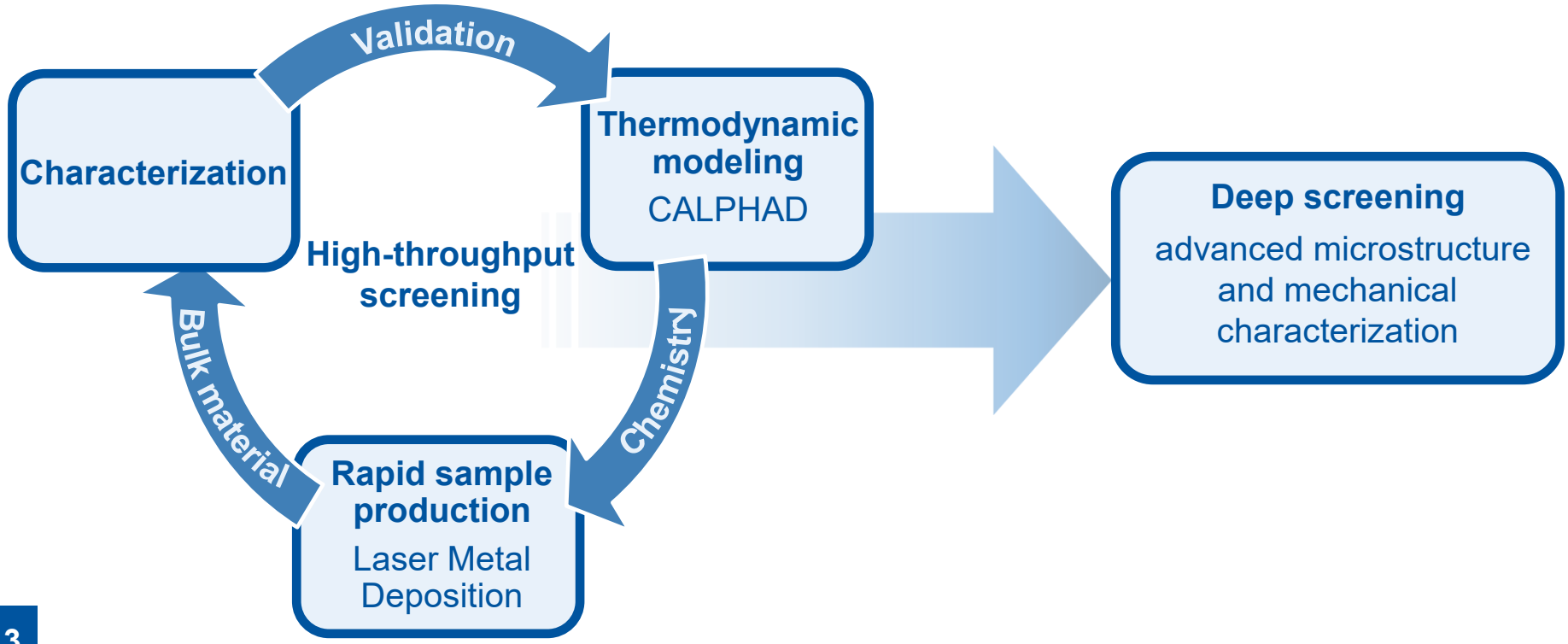
Goals

- Finding new alloys with exceptional mechanical properties
  - → Advancing from HEA to CCAs
- Alloy selection with 8 components
  - → Elements: Fe-Cr-Co-Mn-Ni-Al-C-V

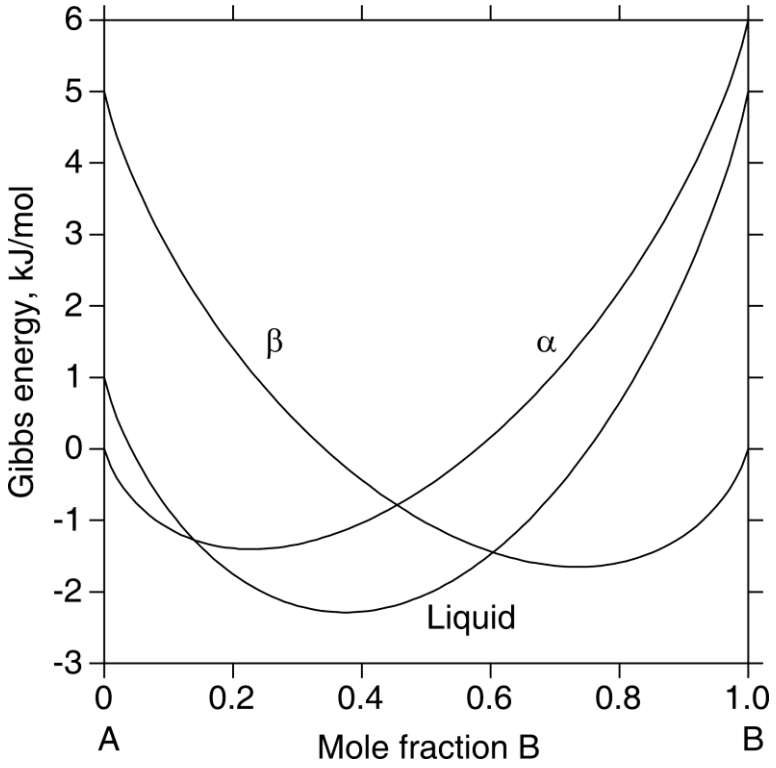
⚠ Not sufficient experimental data for HEA/CCA

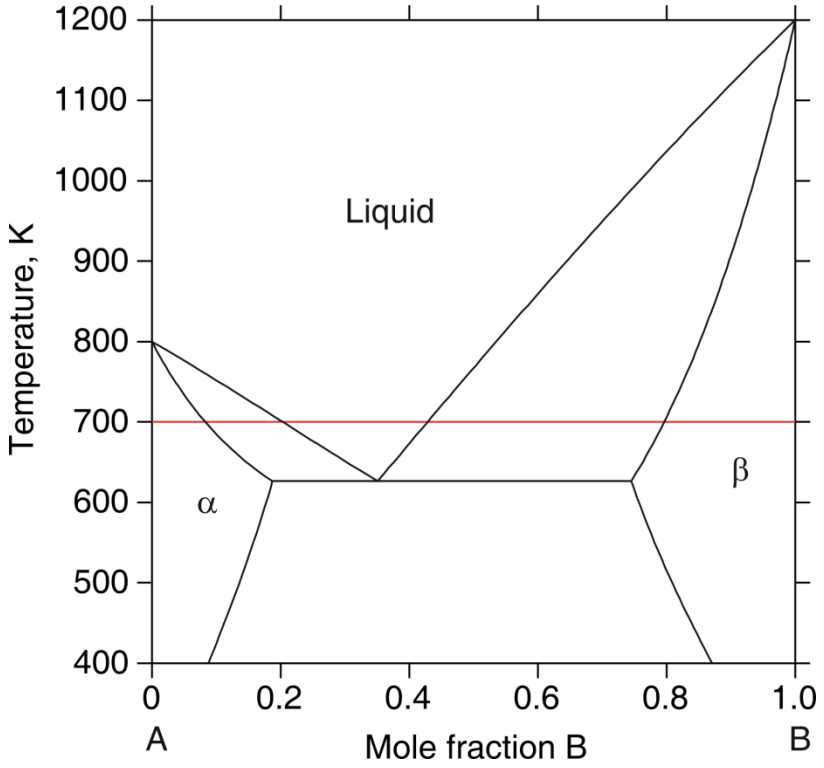


Goals

- Development of a thermodynamic database for CCAs
  - Al-C-Co-Cr-Fe-Mn-Ni database:
    → 21 binary systems included
    → 28 of 35 possible ternary systems included
  - Al-C-Co-Cr-Fe-Mn-Ni-V database:
    → 28 binary systems included
    → 39 of 56 possible ternary systems included
  - The addition of V related systems (preliminary database is constructed)
  - Thermodynamic modelling of Al-Co-Fe, Al-Co-Mn, Al-Mn-Ni, Ni-V-C, Al-Ni-V
- Calphad prediction of precipitates (e.g. B2, κ, VC) and phase stabilities

Thermochemistry and phase diagrams

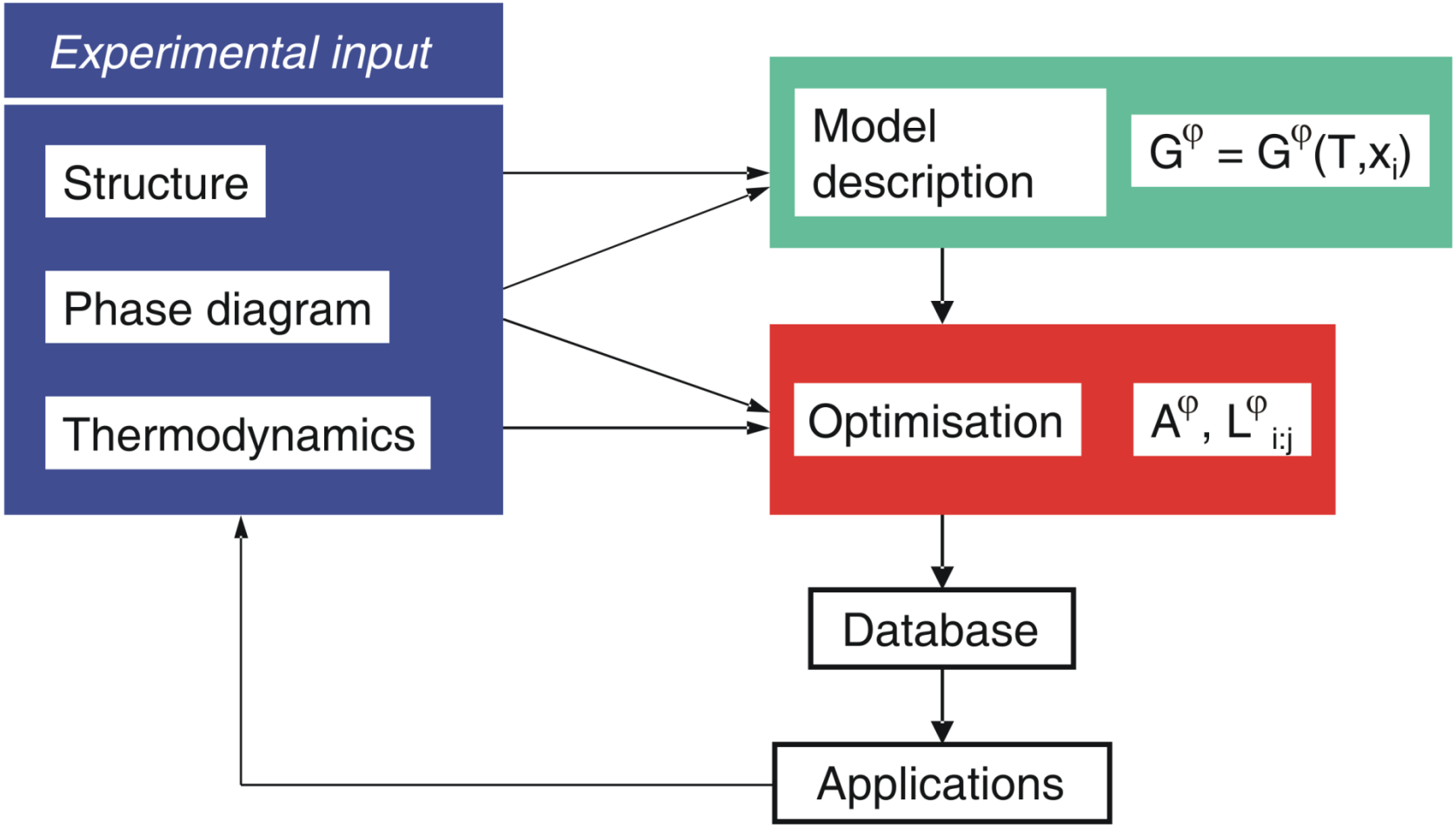




Thermochemistry ⟷ Phase diagrams

A Calphad database contains parameters for a mathematical description of the thermodynamic properties of a (multicomponent) system

The Calphad Method



General strategy, databases

Binary systems

+

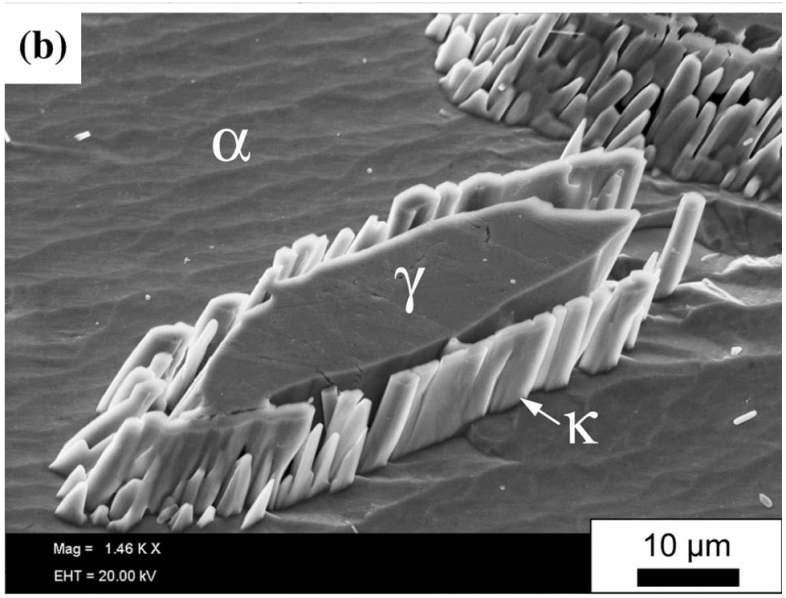
(Important)
Ternary systems

+

Extrapolations

=

Real alloys
(several elements)

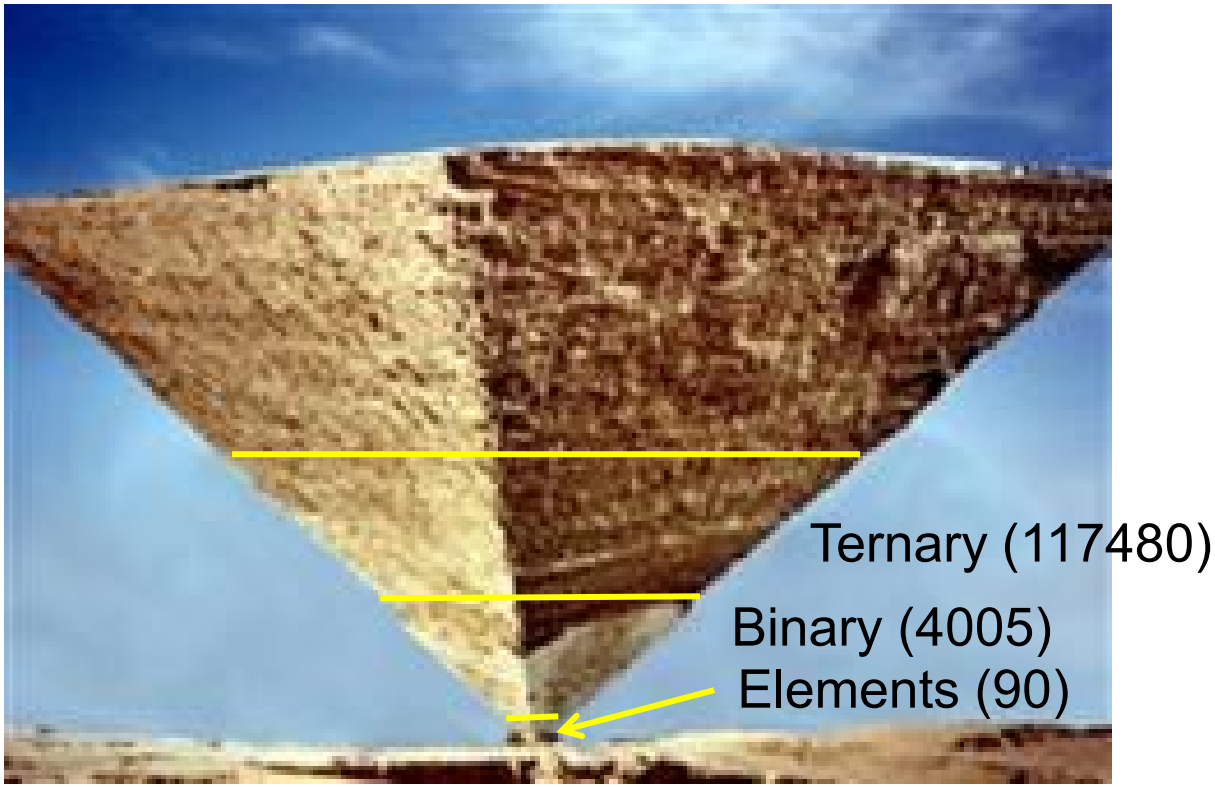


Fe-2%Mn-8%Al-0.2%C, cooling 10K/s from 1400 C, quenched from 870 C.

I. Zuazo et al, JOM 66 (2014) 1747–58.

MPEA particular challenge: All included elements are equally important; i.e. all (!!) ternary systems should be included in the database

The inverted pyramid



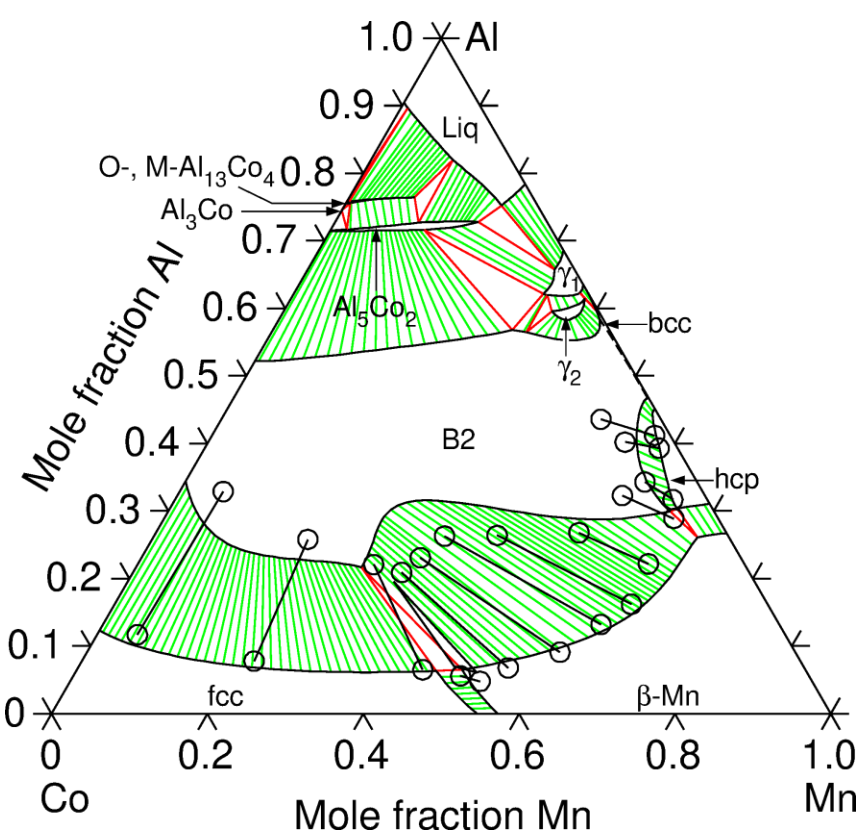
- A fair proportion of the binary systems have been modelled
- A large proportion of the ternary systems are not even known experimentally
- However, there are good databases for steels and many alloys

Completed work

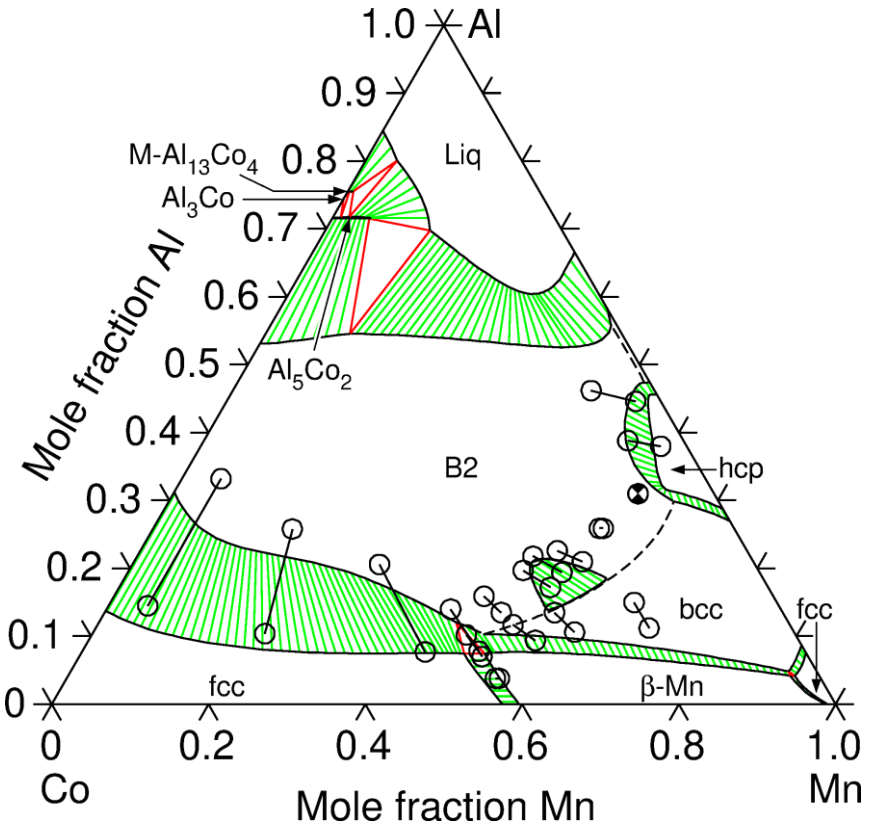
Al-Co-Mn Ternary system

Al-Co-Mn Isothermal Sections

- Isothermal section at 1000 C



- Isothermal section at 1100 C

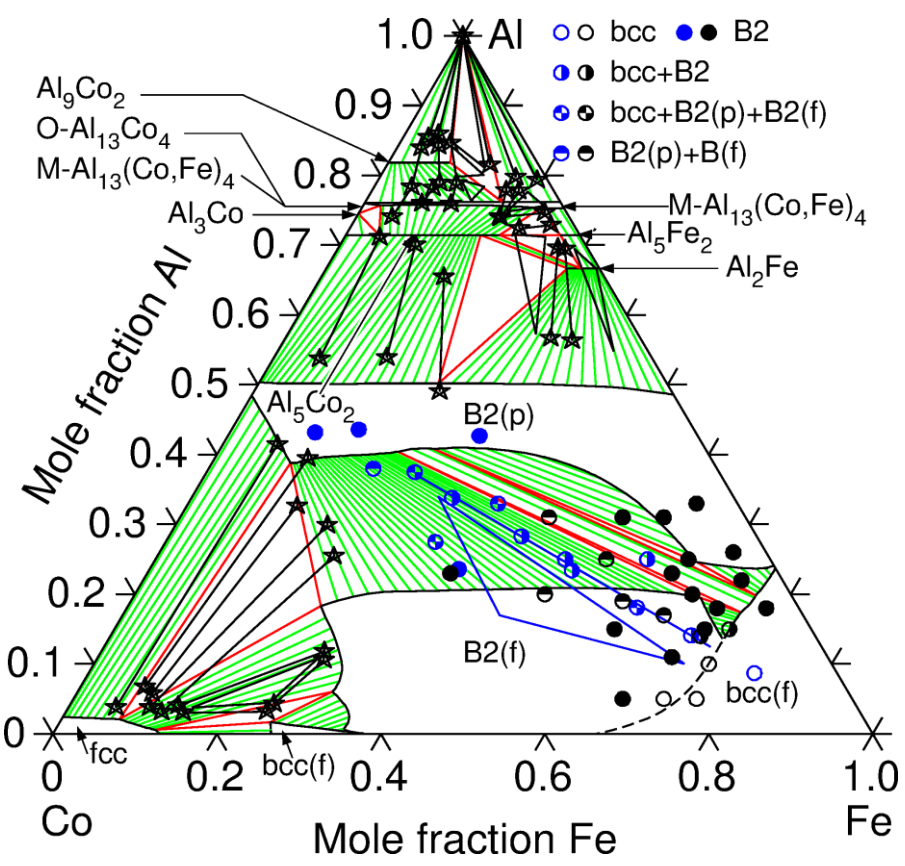


Thermodynamic modeling: M Noori and B. Hallstedt, *Calphad* 2020.
Experimental work: R. Kainuma et al., *J. Alloys Compd.* 1998.

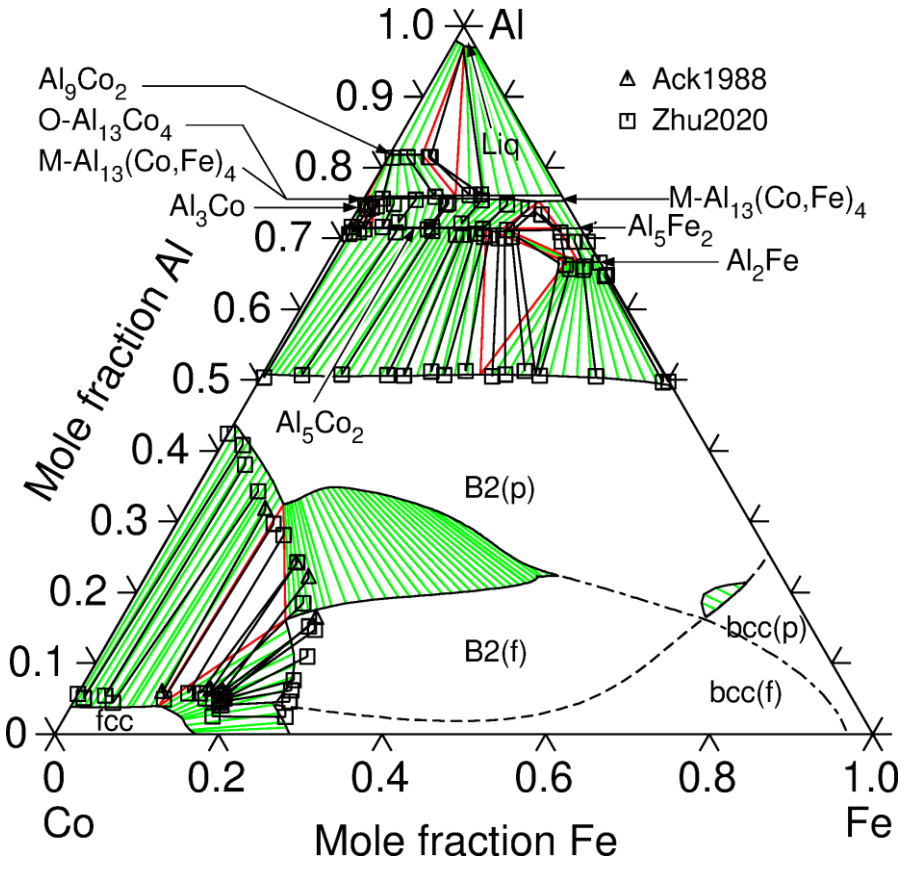
Al-Co-Fe Ternary system

Al-Co-Fe Isothermal Sections

- Isothermal section at 650 C



- Isothermal section at 800 C

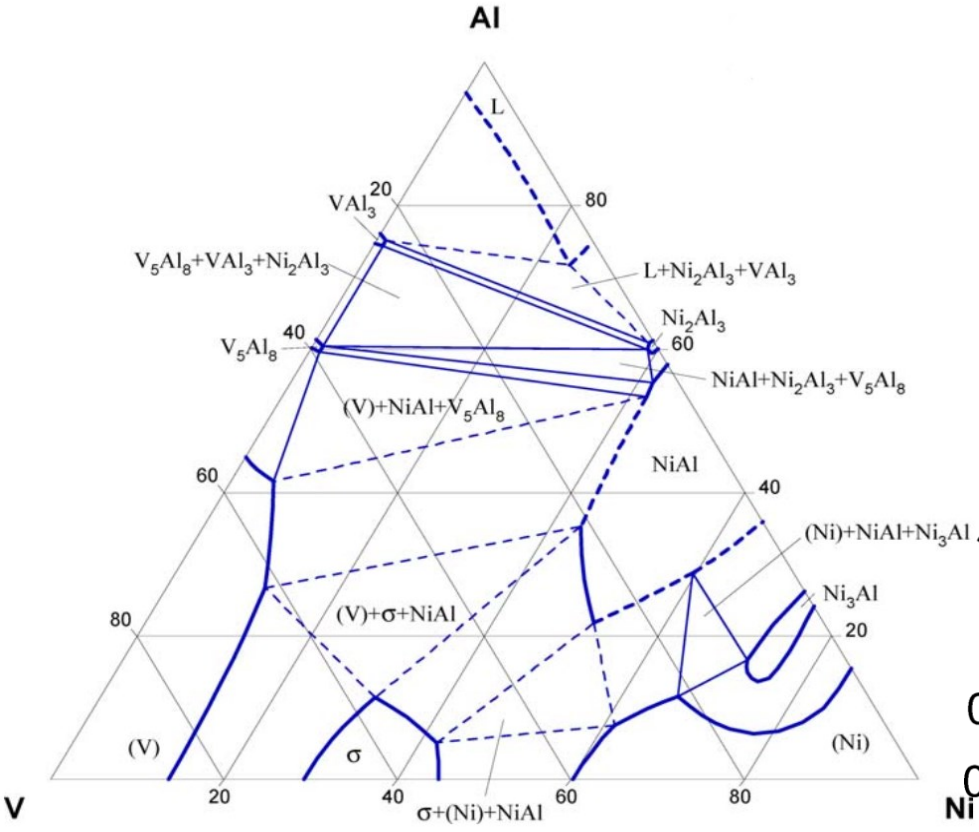


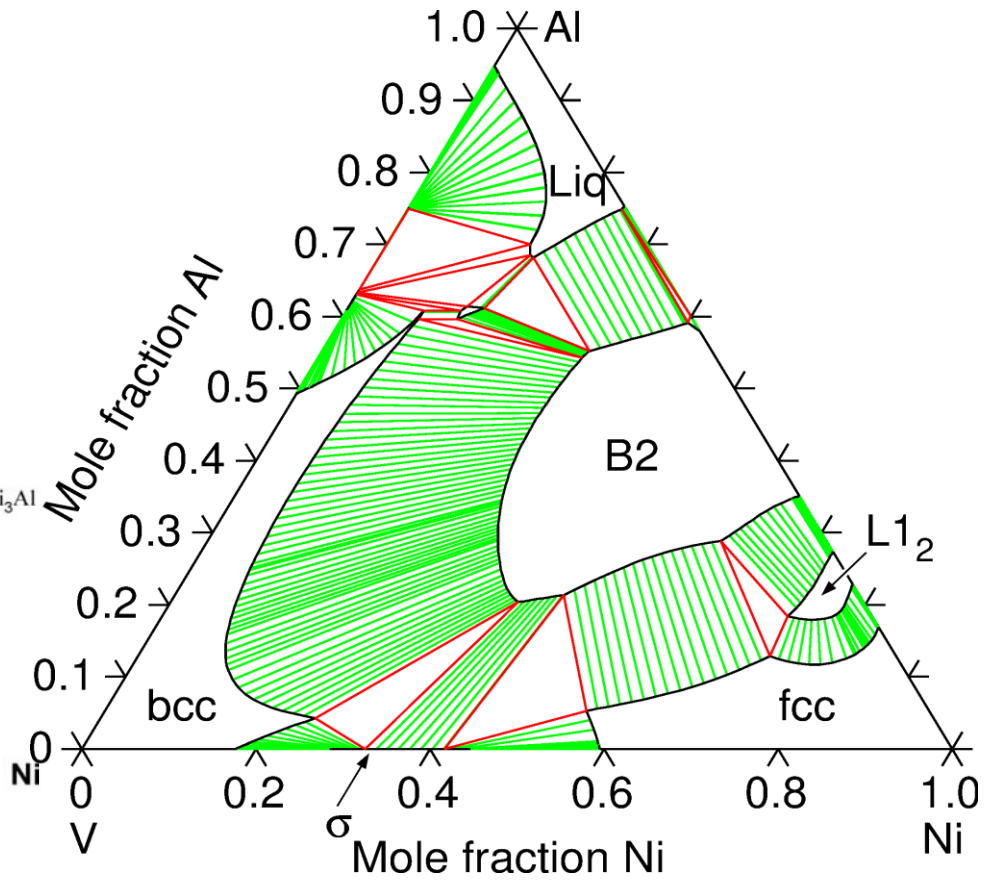
Thermodynamic modeling: M Noori and B. Hallstedt, *Calphad* 2021

Al-Ni-V (DFT)

Al-Ni-V 1100 C Isothermal section

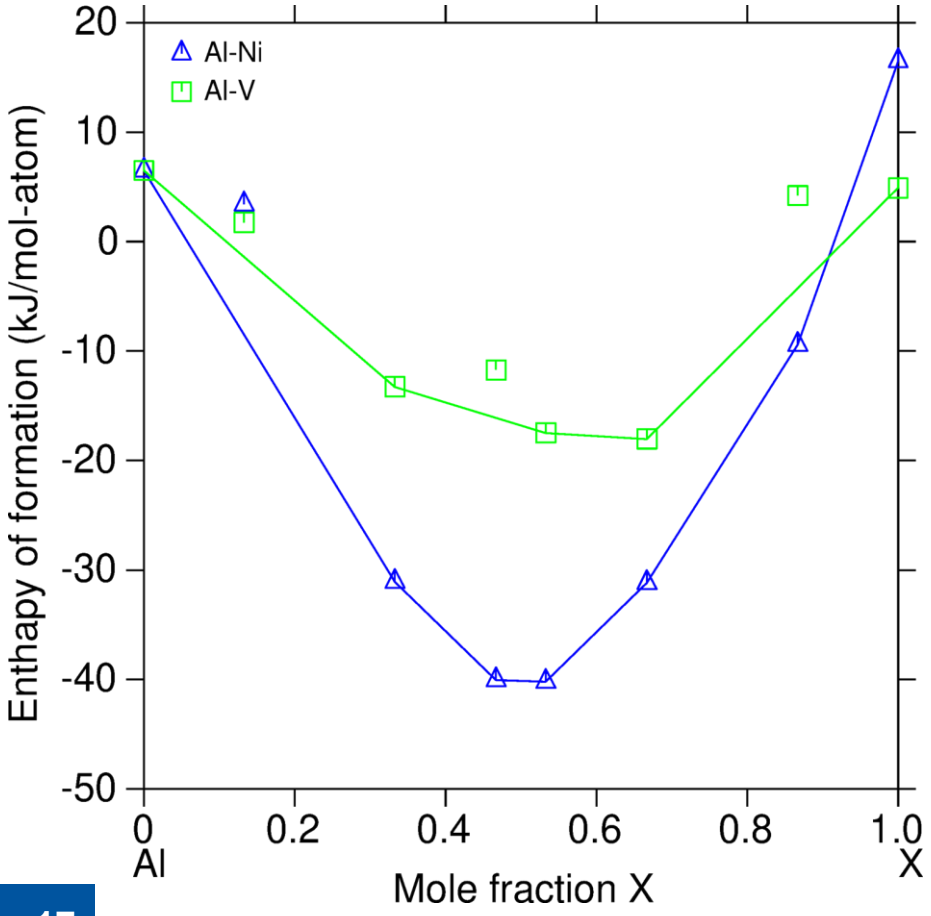
- Experimental work from K.P. Myasnikova et al., Russ. *Metall.* 1977.
- Thermodynamic extrapolation from the binaries



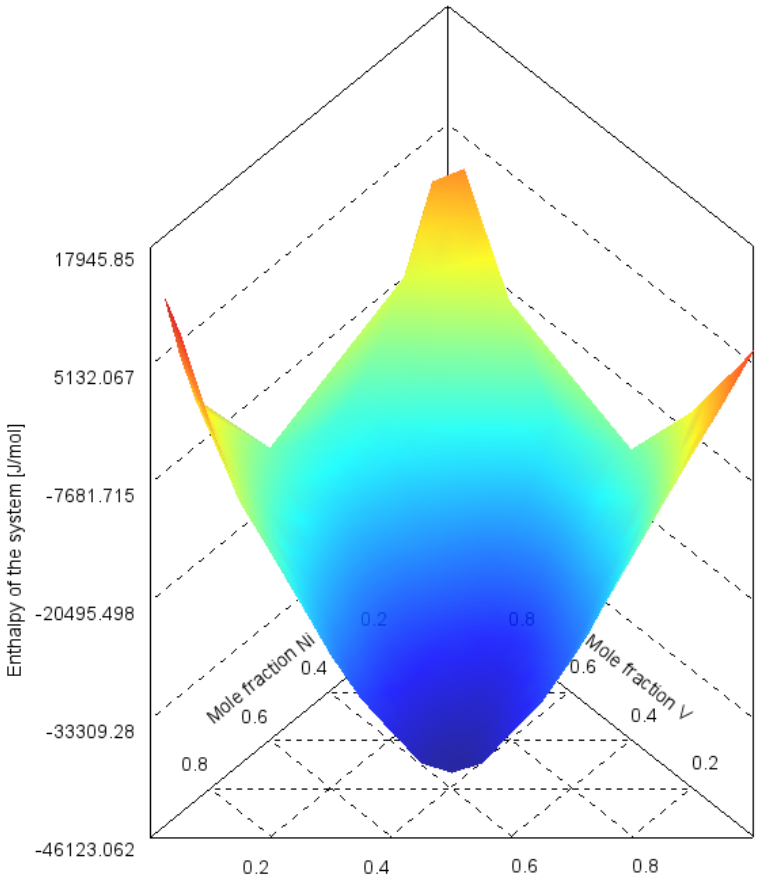


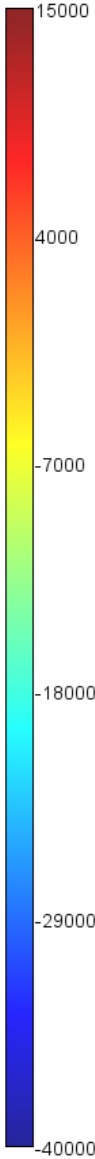
Al-Ni-V Ternary system

- Formation enthalpies for σ phase in Al-Ni and Al-V binary systems:



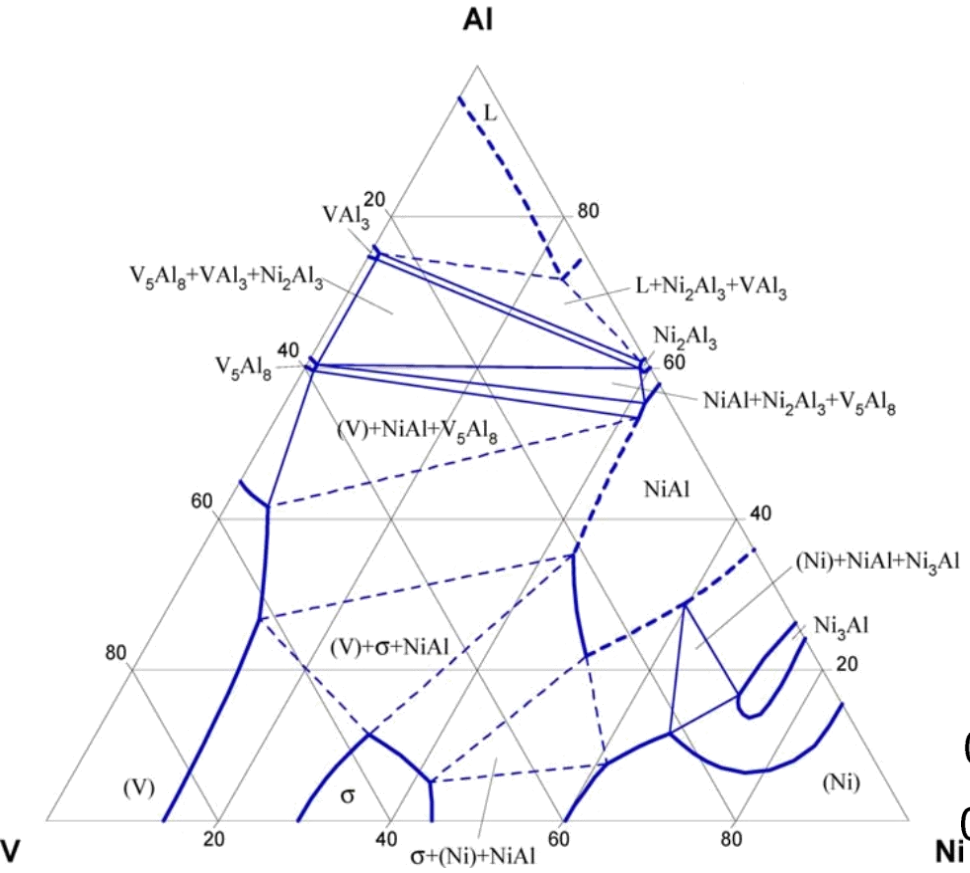
- Formation enthalpies for σ phase in the ternary system:



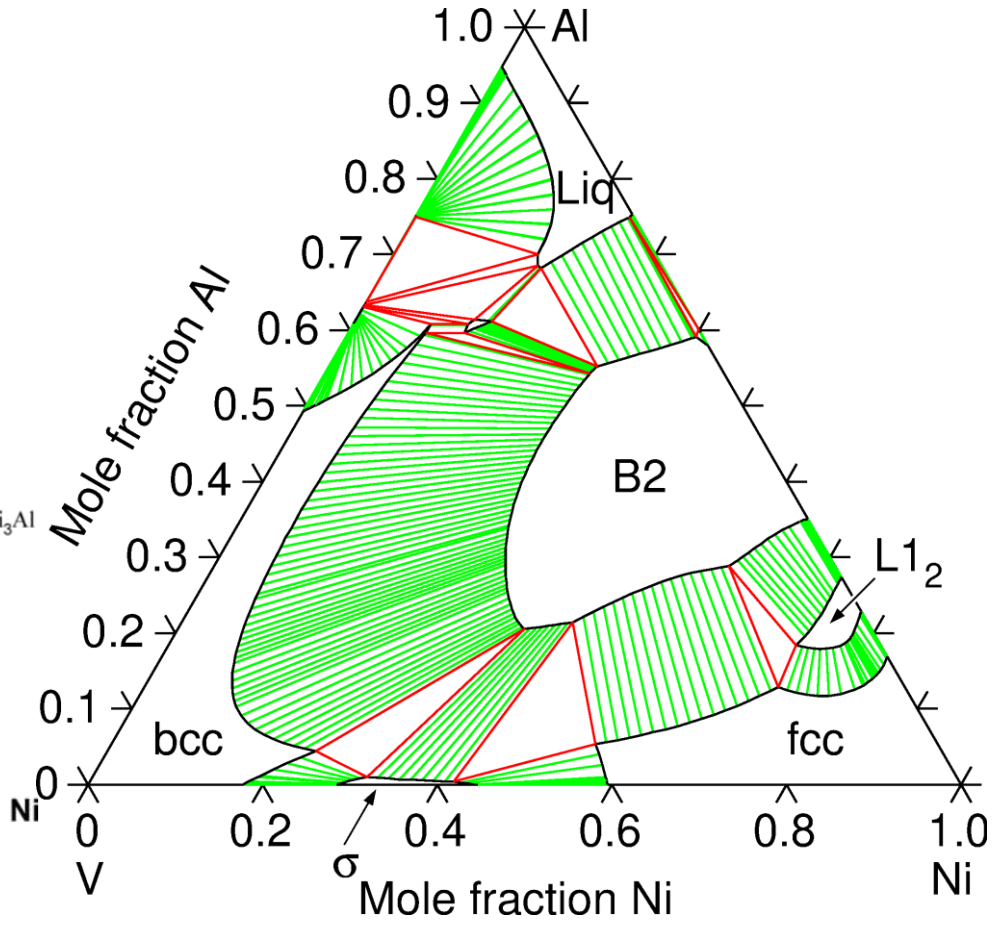


Al-Ni-V 1100 C Isothermal section

- Experimental work from K.P. Myasnikova et al., Russ. *Metall.* 1977.



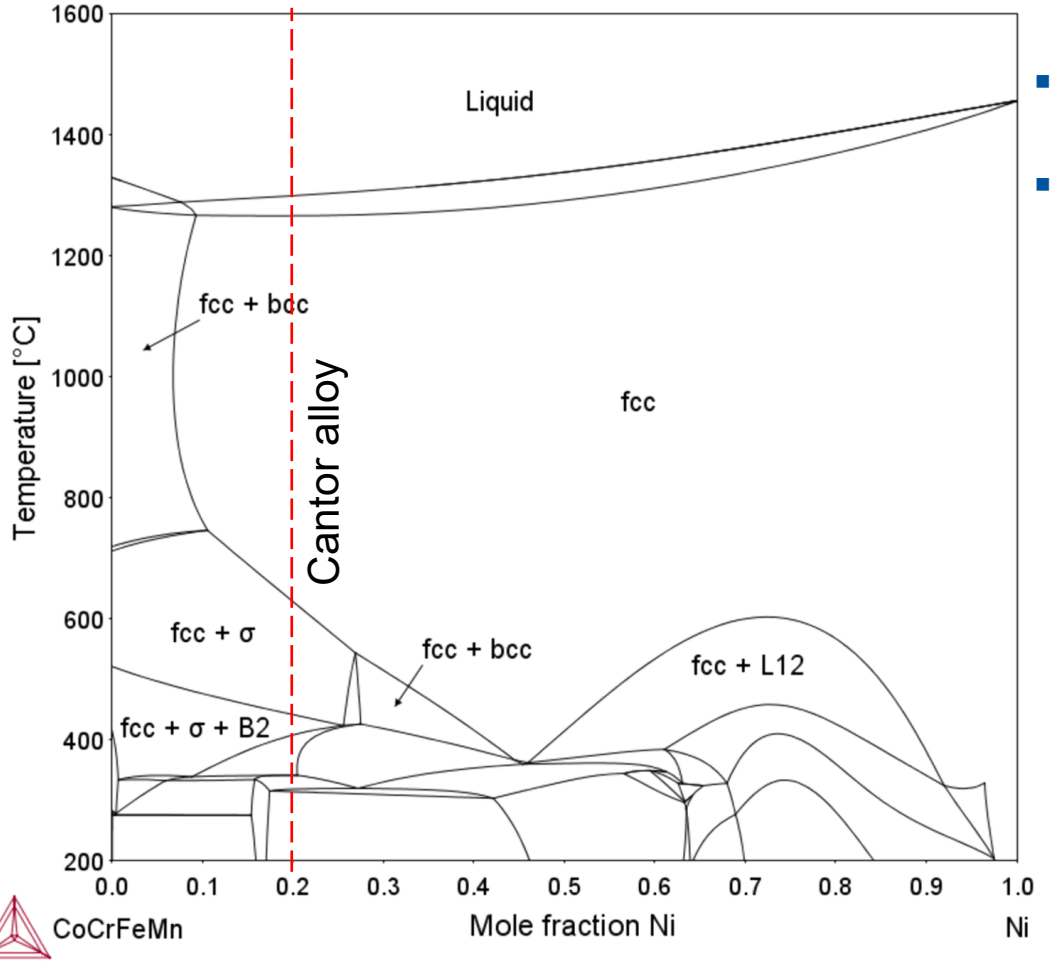
- Thermodynamic extrapolation from the binaries with ab initio calculations for the σ phase.



Constructed Databases

Co-Cr-Fe-Mn-Ni database

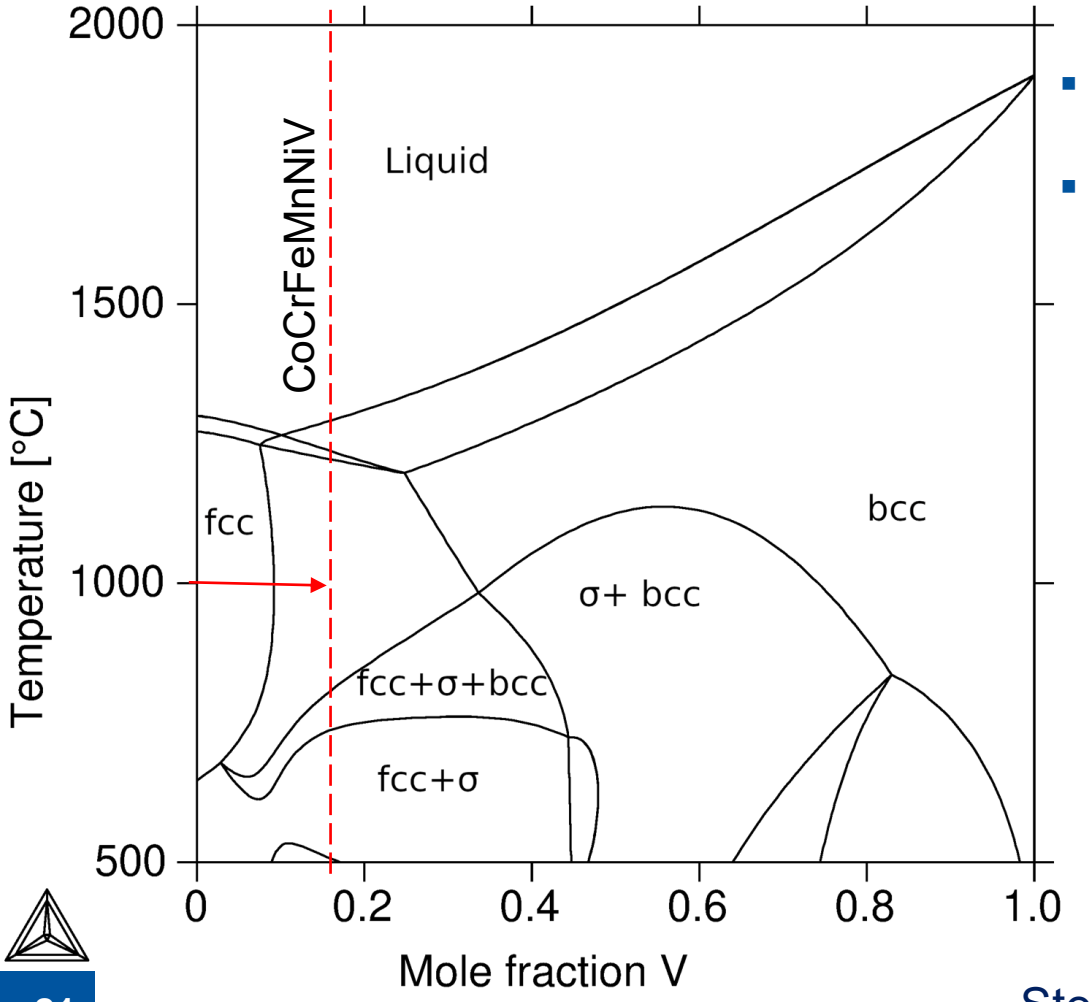
Constructed thermodynamic database for Cantor Alloy



- Fcc stable from pure Ni to Cantor alloy
- Max. stability of fcc is at x(Ni)=0.45
  NOT at equiatomic composition!

Co-Cr-Fe-Mn-Ni-V database

Constructed thermodynamic database for Cantor Alloy + V

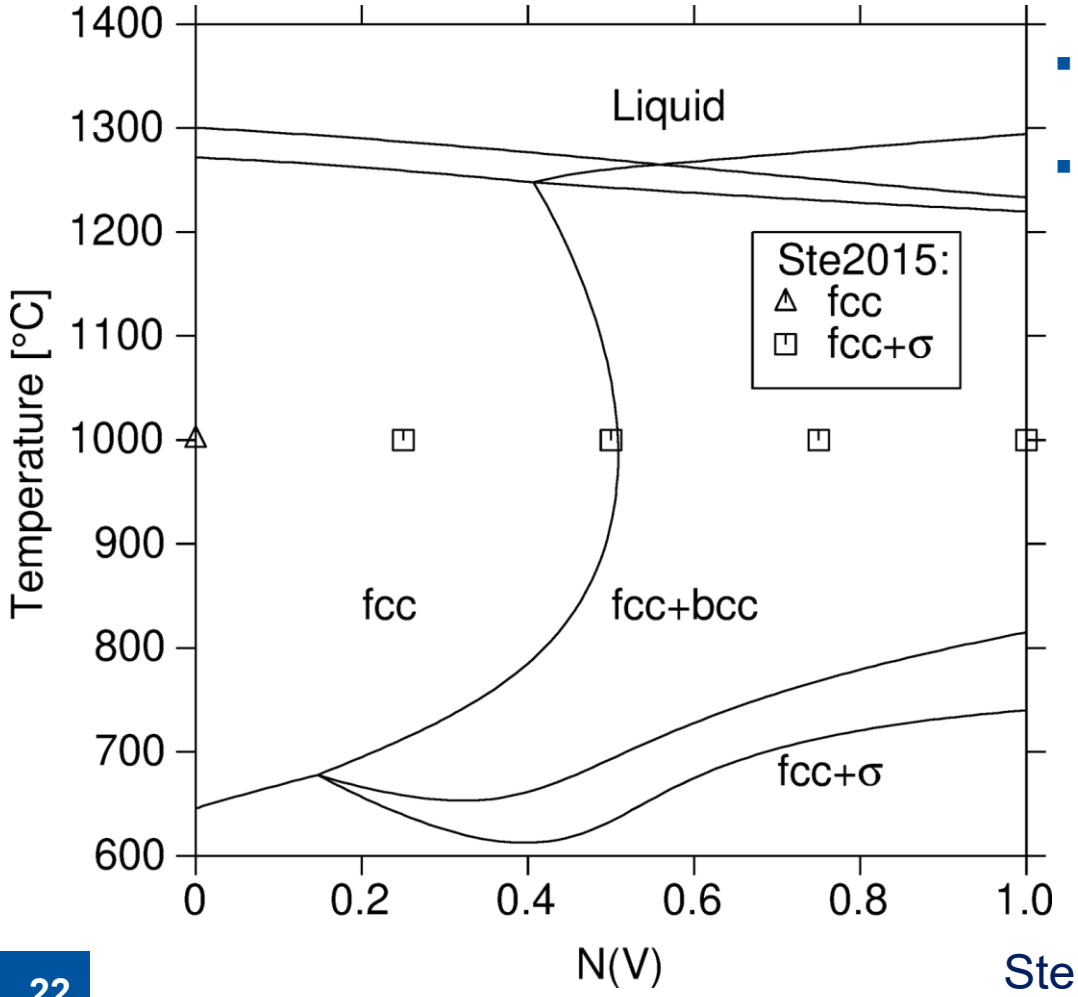


- Addition of V stabilizes the bcc phase
- Addition of V transforms fcc into duplex phase fcc+σ. Compared to the findings of Stepanov, our database underestimates the stability of the σ phase. The reason could be Cr-Co-Mn that is not experimentally investigated.

Stepanov et al., *J. Alloys Compd.(2015)*

Co-Cr-Fe-Mn-Ni-V database

Constructed thermodynamic database for Cantor Alloy + V



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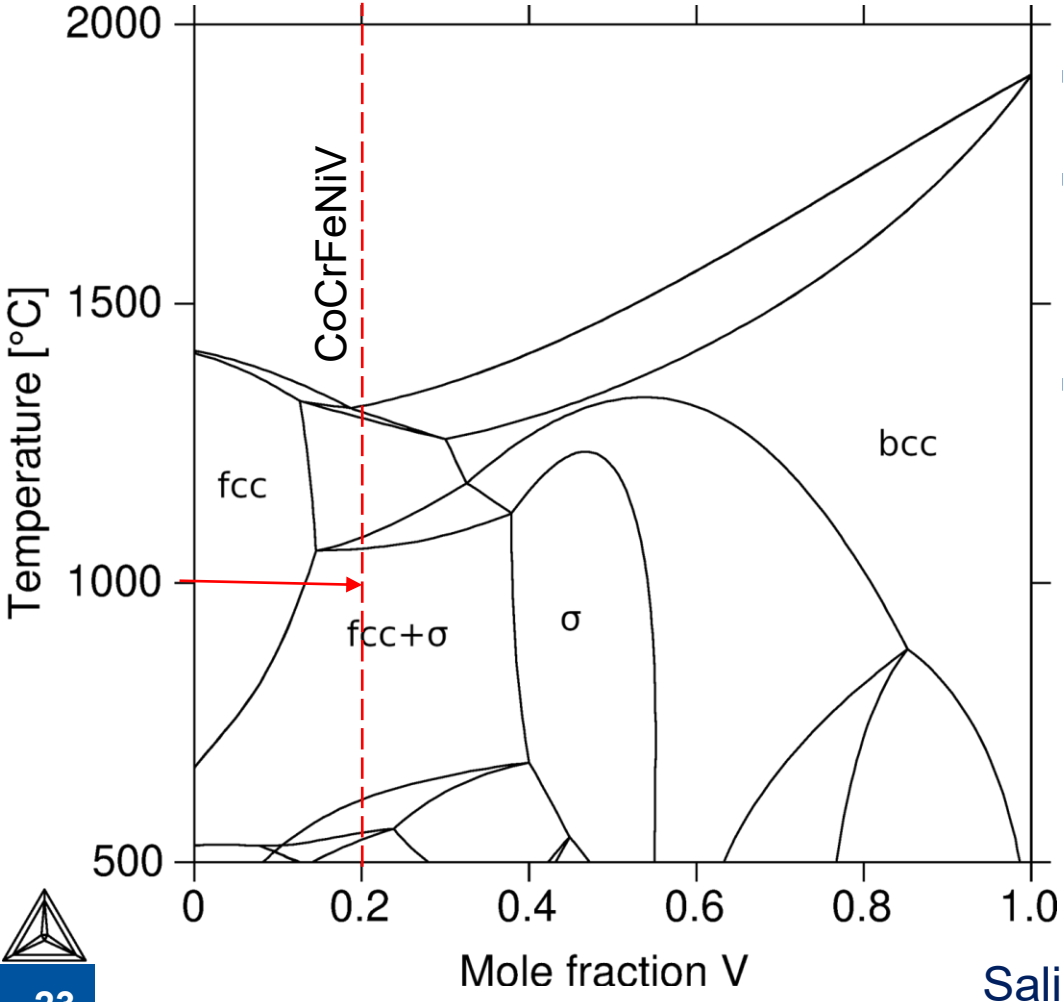
Stepanov et al., *J. Alloys Compd.(2015)*

Co-Cr-Fe-Ni-V database

Constructed thermodynamic database for Co-Cr-Fe-Ni-V:



- Addition of V stabilizes the bcc phase
- Addition of V transforms fcc into duplex phase fcc+Sigma. This is in agreement with the findings of Salishchev.
- It shows that the underestimation of the σ phase in Co-Cr-Fe-Mn-Ni-V database could arise from the Mn related systems that include σ phase.

Salishchev et al., *J. Alloys Compd.(2014)*

Conclusion

- Al-Co-Mn and Al-Co-Fe systems were thermodynamically modelled.
- A thermodynamic database for Co-Cr-Fe-Mn-Ni-Al-C was constructed.
- A preliminary database with V-content systems was constructed.
- A DFT calculation on σ phase of Al-Ni-V system was done.
- Al-Ni-V and Ni-V-C systems are planned to be modelled.

Thank you for your attention!

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