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".

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SPP CCA/HEA Online Meeting, 13-14 April, 2021

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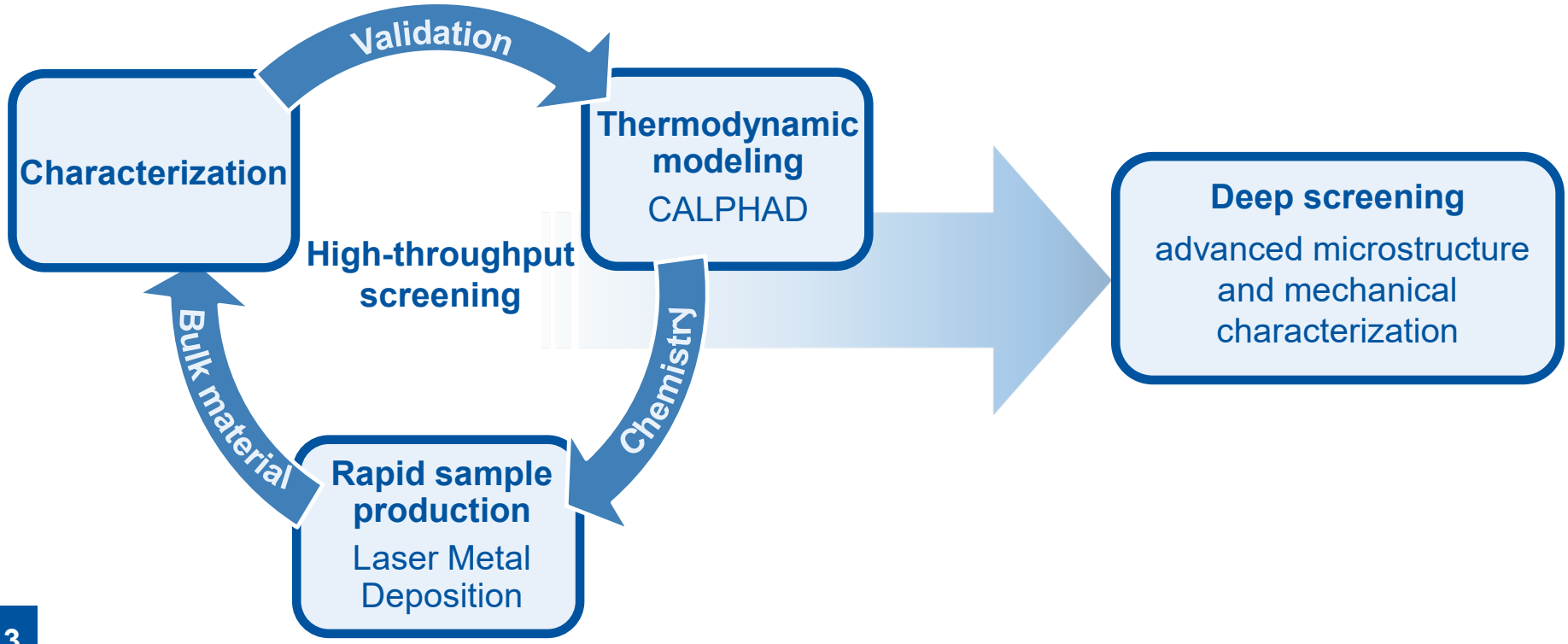
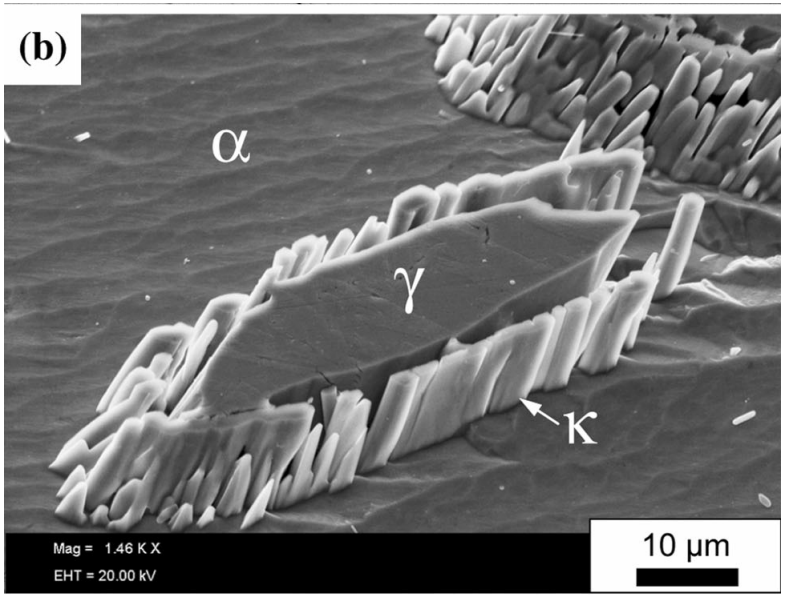
Goals

- 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

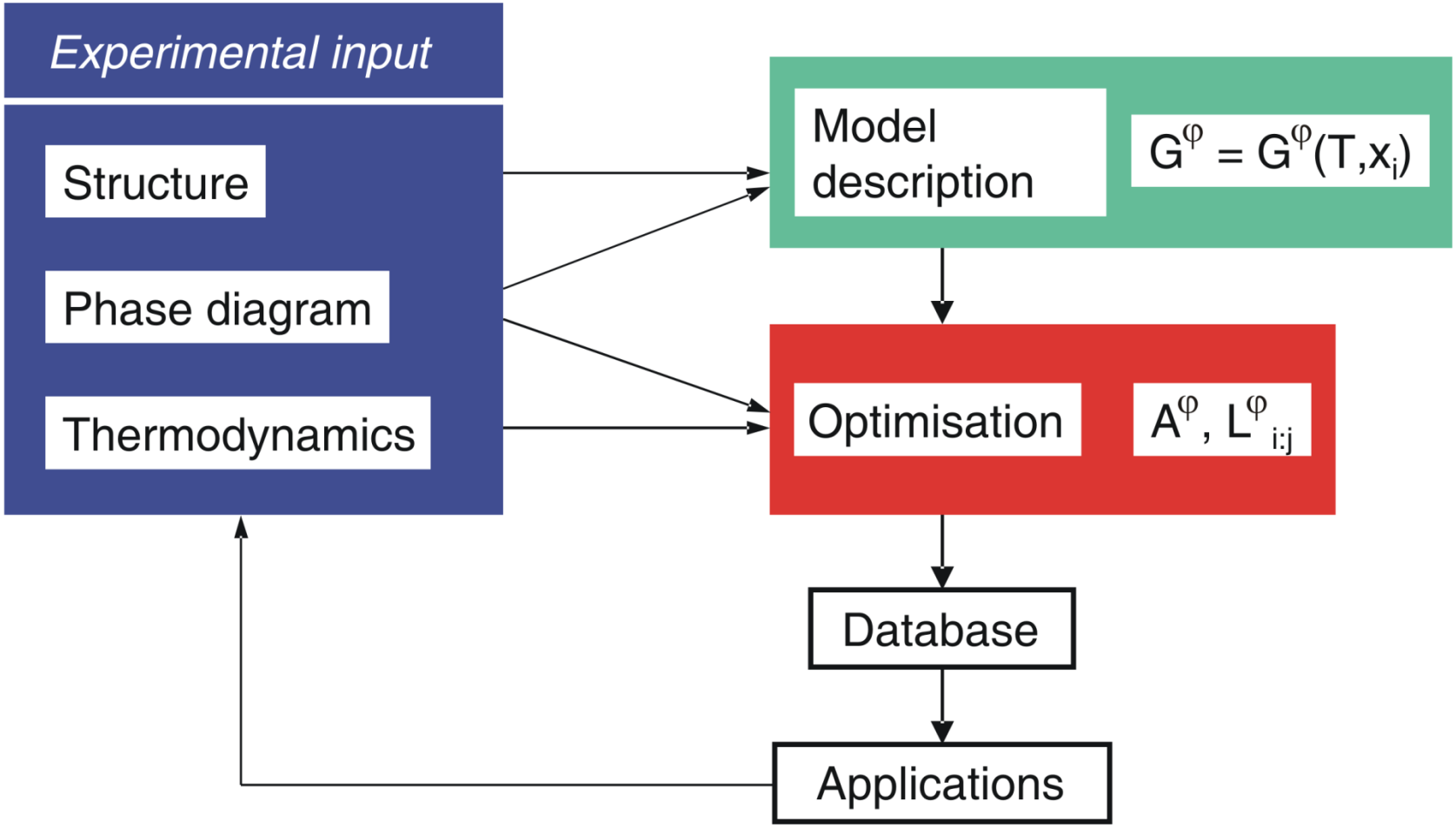
- Development of a thermodynamic database for CCAs
  - → 21 binary systems included
  - → 28 of 35 possible ternary systems included
  - → The addition of V related systems (preliminary database is constructed)
  - → Thermodynamic modelling of Al-Co-Fe, Al-Co-Mn, Al-Mn-Ni, Ni-V-C, Al-Ni-V
- Calphad prediction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



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.

The Calphad Method

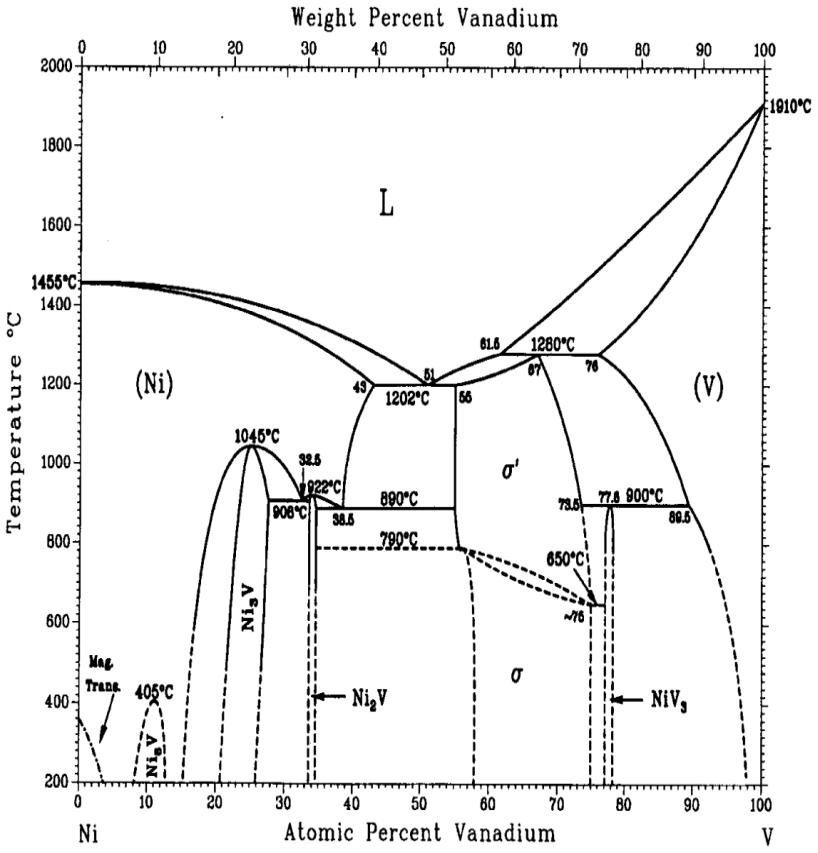


Completed work

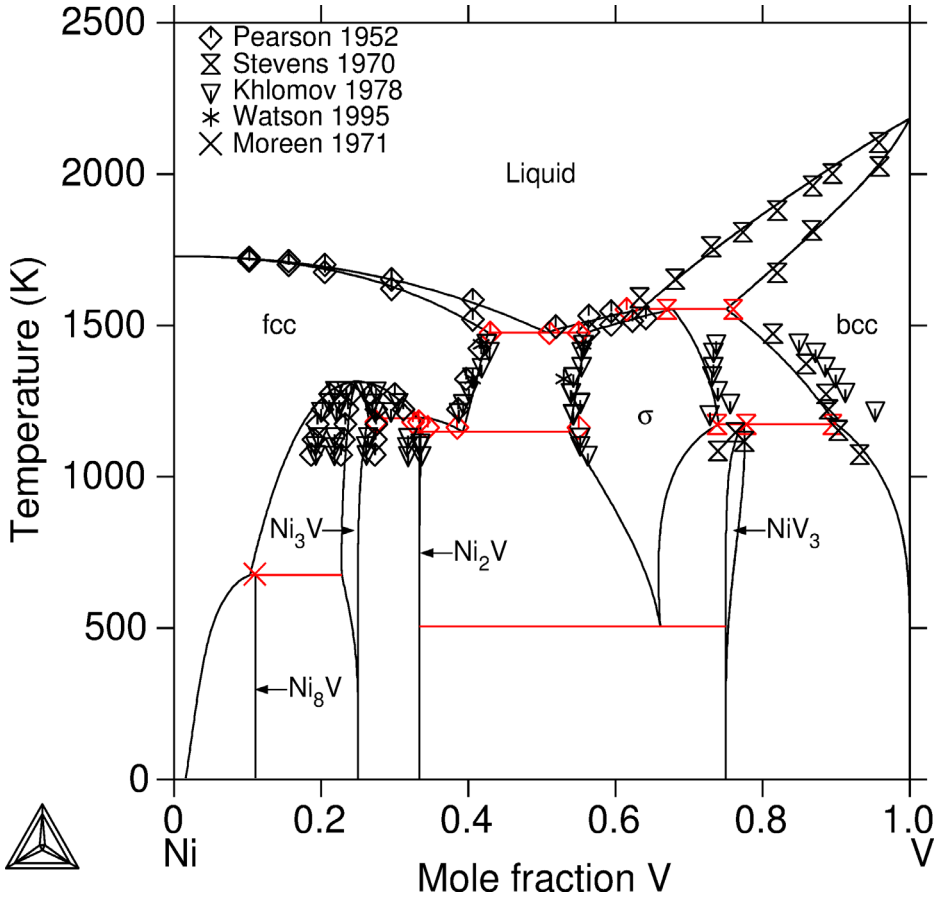
Ni-V binary system

Ni-V thermodynamic modelling

- The experimental work from J.F. Smith et al., *Bull. Alloy Phase Diagr.* 1982



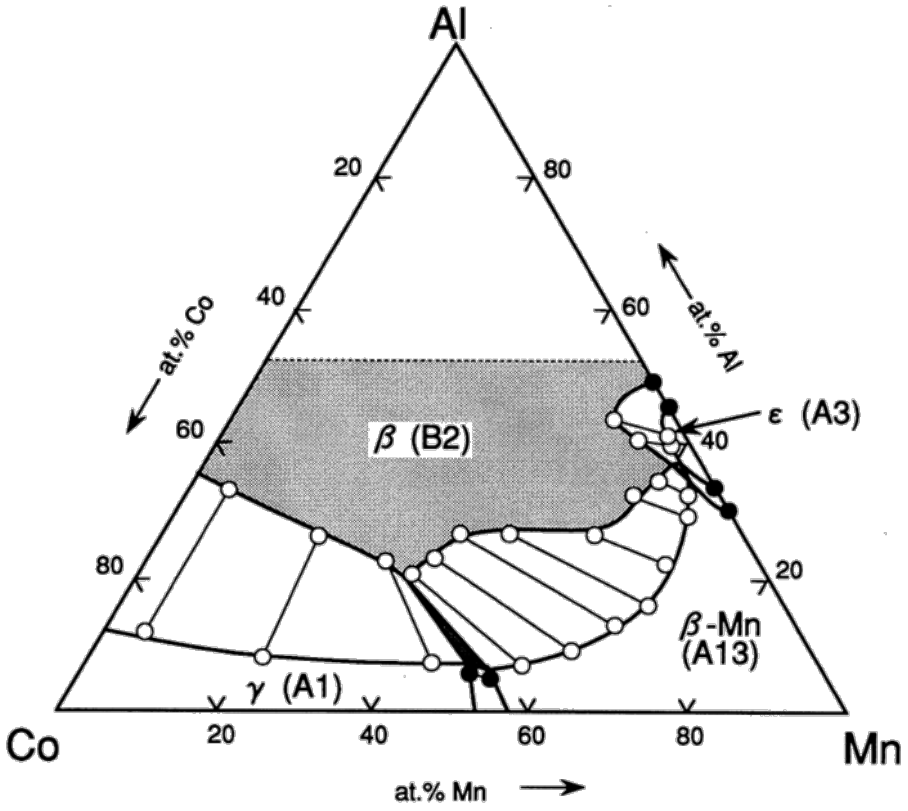
- The thermodynamic modelling



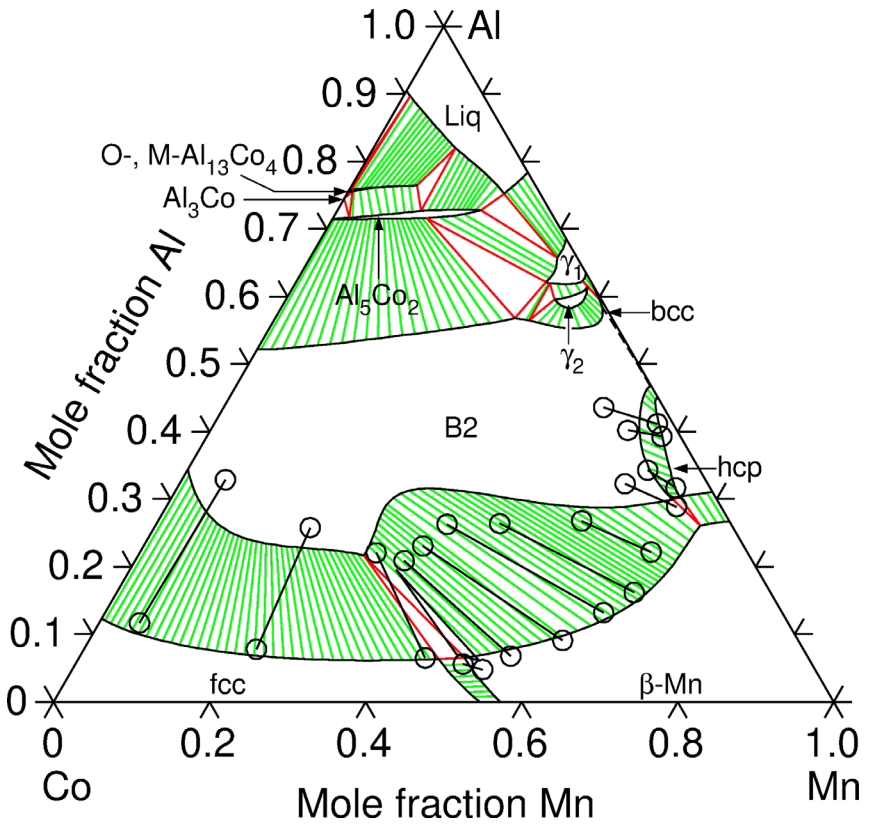
Al-Co-Mn Ternary system

Al-Co-Mn 1000 C Isothermal Section

- Experimental work from R. Kainuma et al., *J. Alloys Compd.* 1998.



- The thermodynamic modelling



Al-Co-Mn 1100 C Isothermal Section

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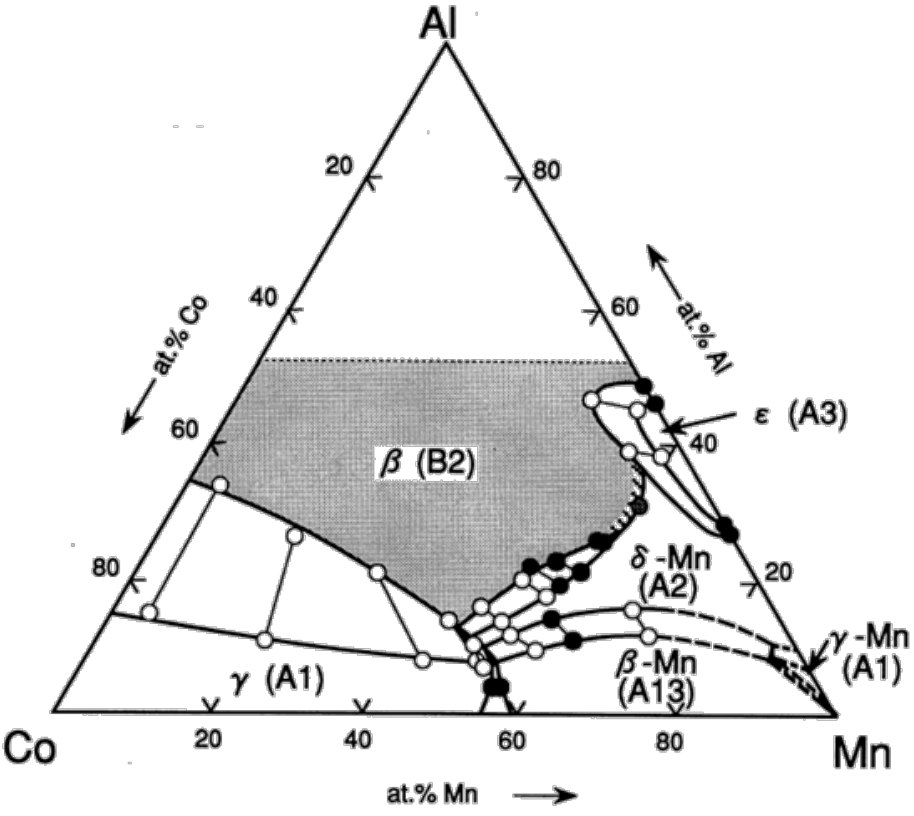
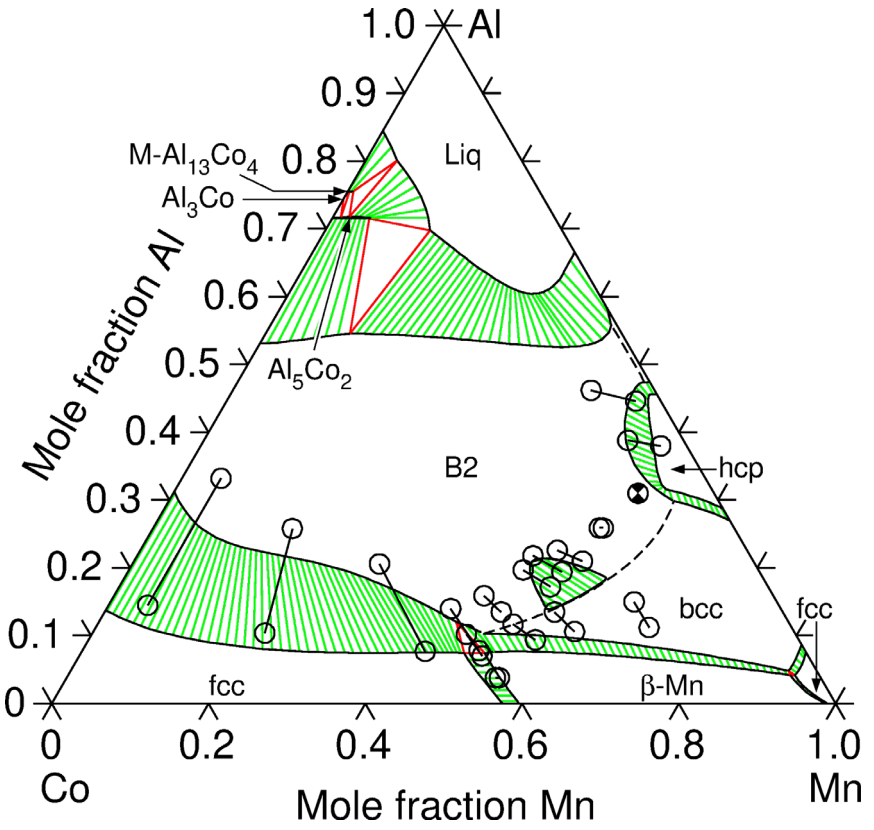


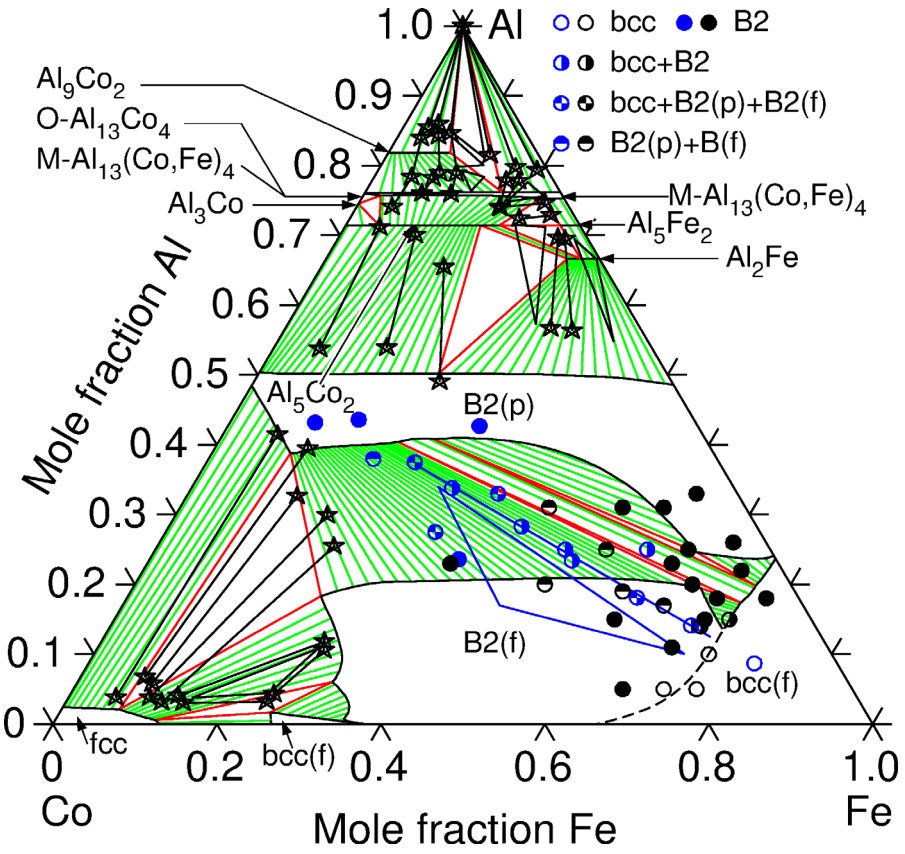
- The thermodynamic modelling



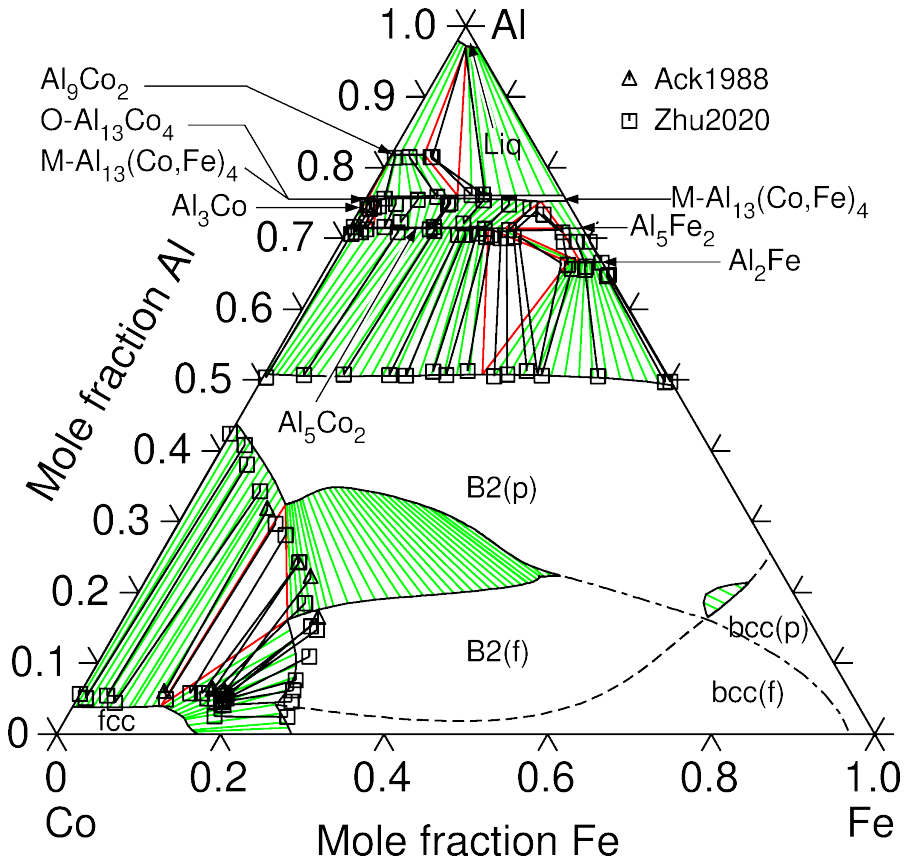
Al-Co-Fe Ternary system

Al-Co-Fe Isothermal Sections

- The thermodynamic modelling
- Isothermal section at 650 C



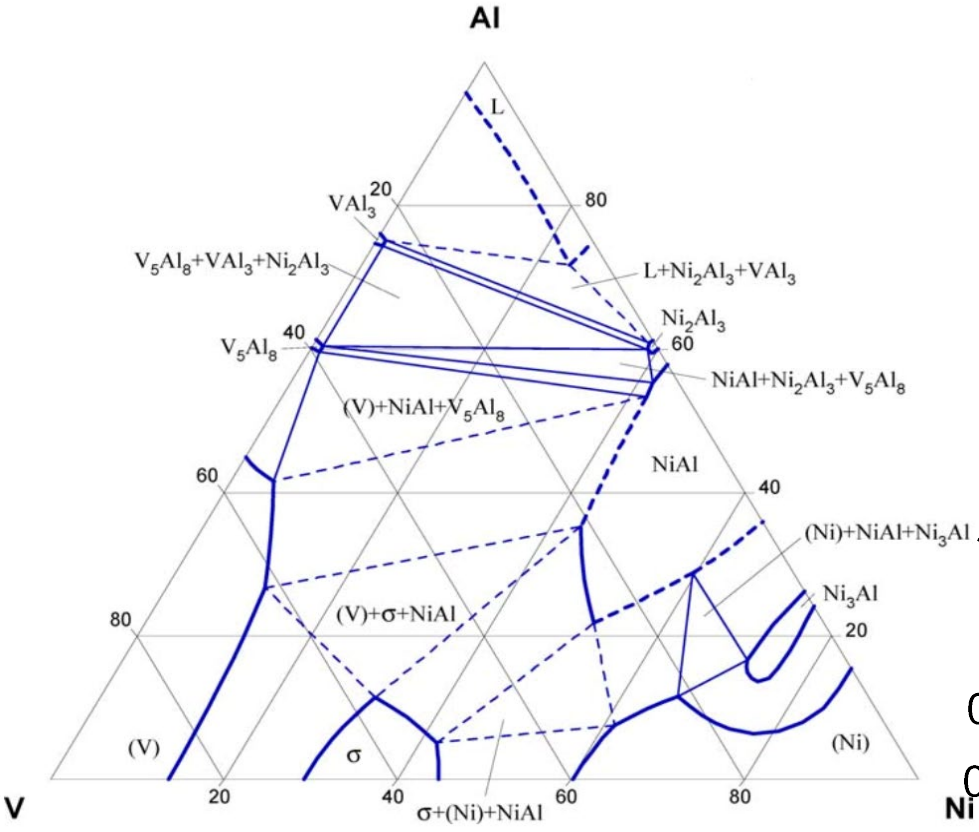
- The thermodynamic modelling
- Isothermal section at 800 C

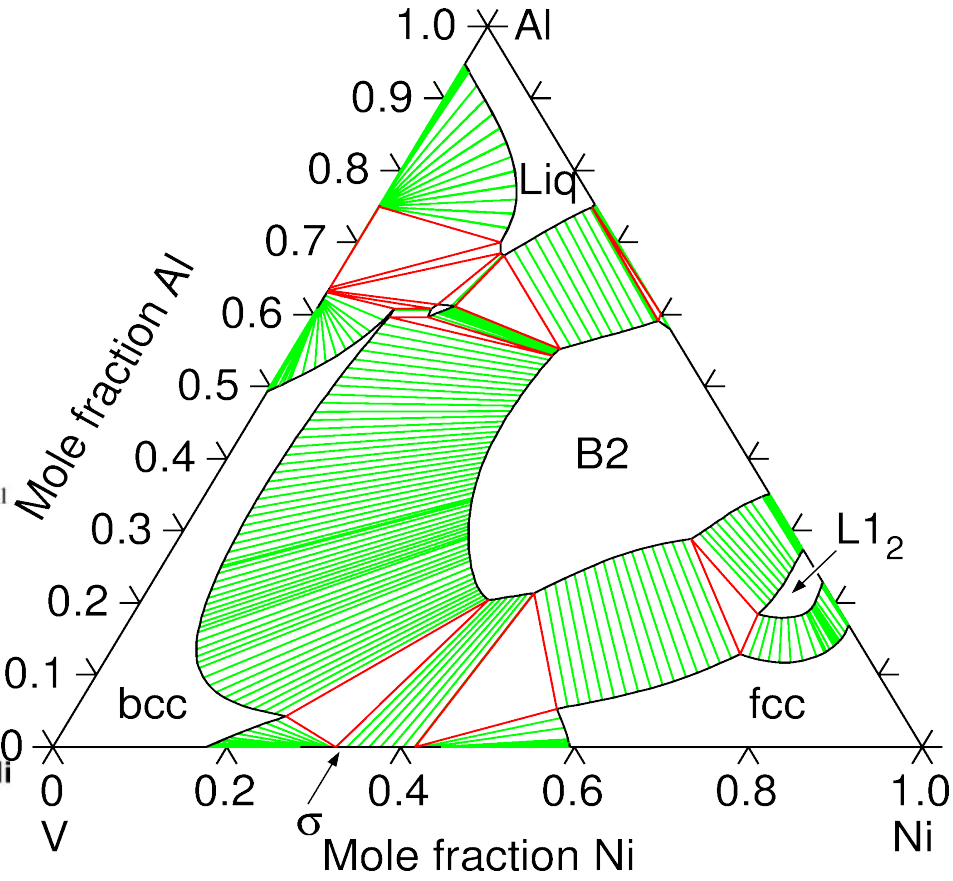


Al-Ni-V (DFT)

Al-Ni-V 1100 C Isothermal section

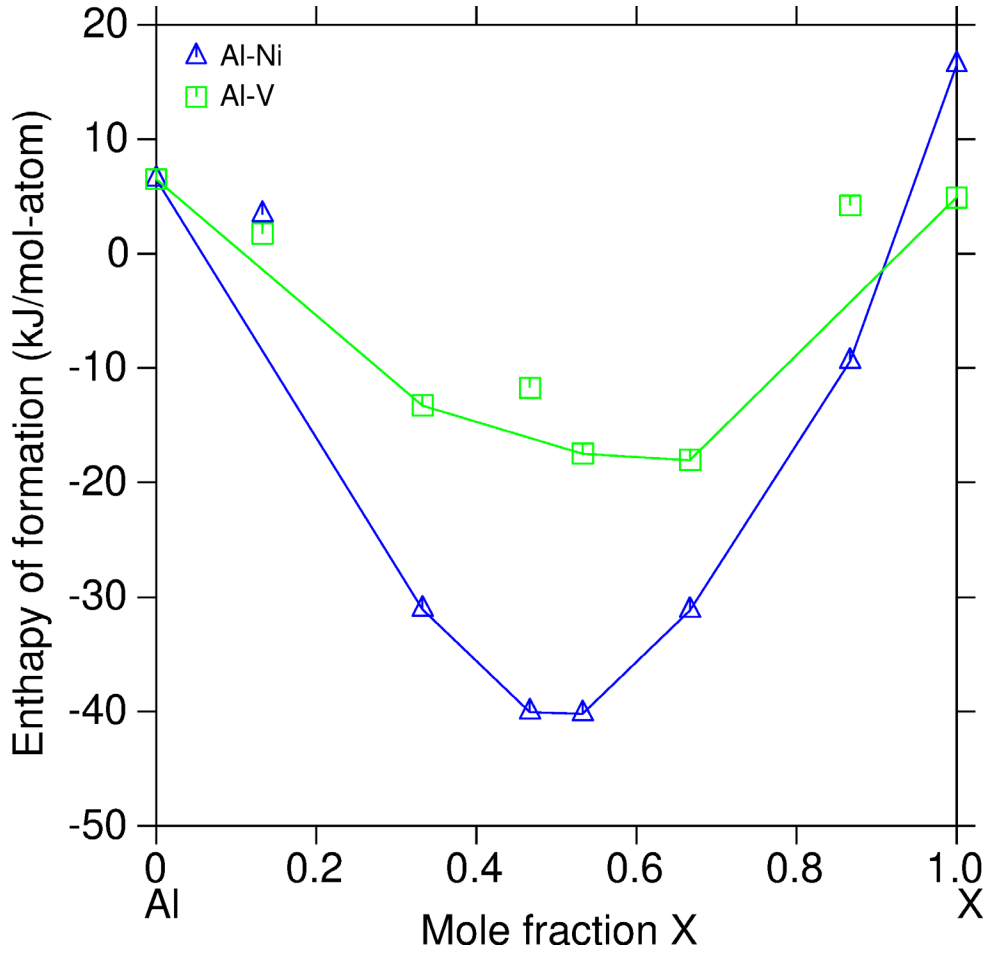
- Experimental work from K.P. Myasnikova et al., Russ. *Metall.* 1977.
- Thermodynamic extrapolation from the binaries





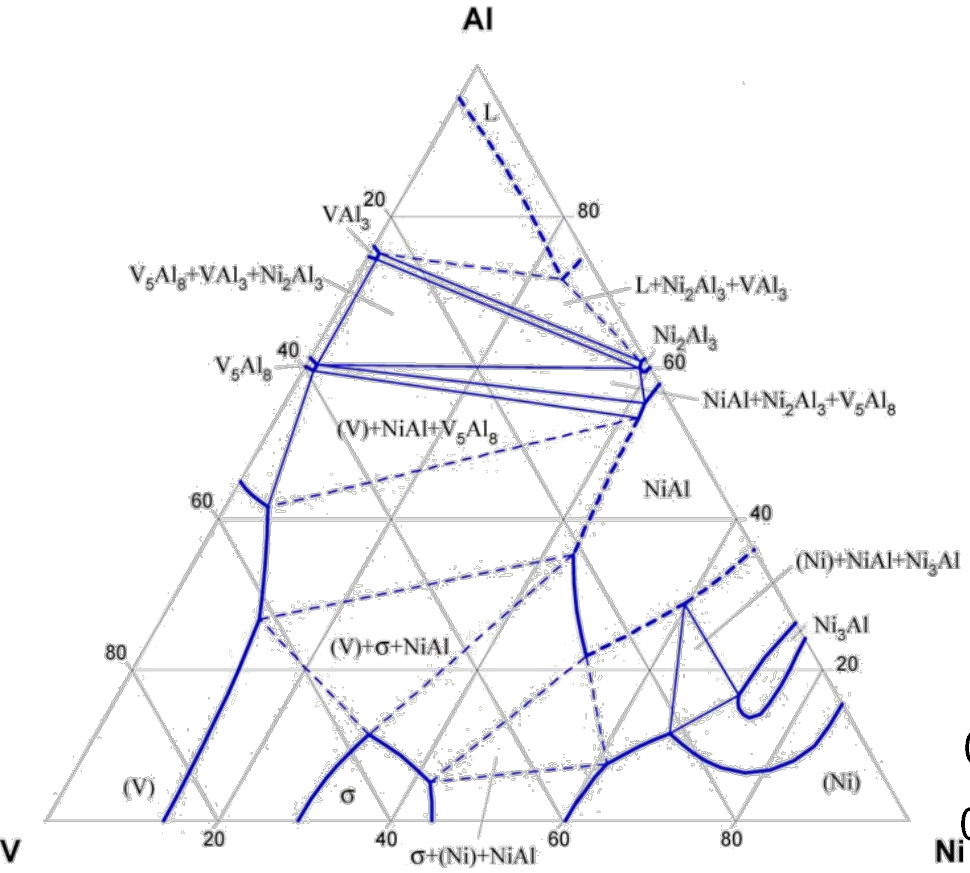
Al-Ni-V Ternary system

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

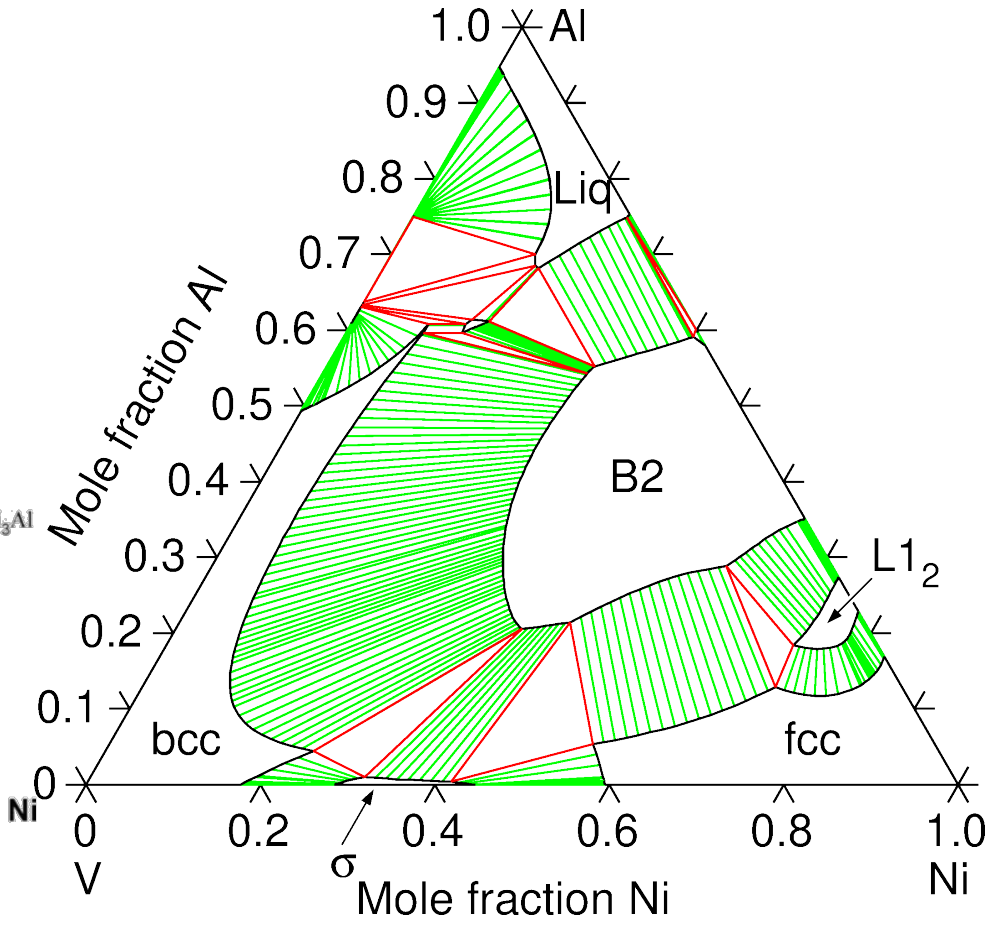


Al-Ni-V 1100 C Isothermal section

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



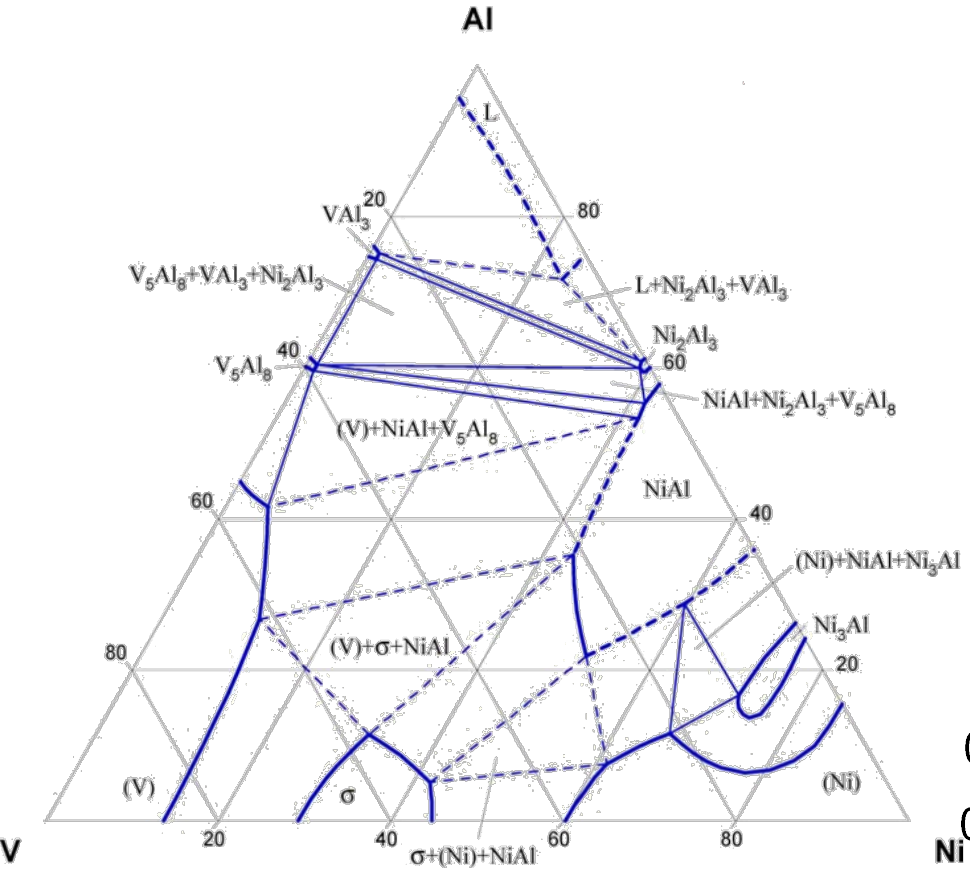
- Thermodynamic extrapolation from the binaries with ab initio calculations for the σ phase.



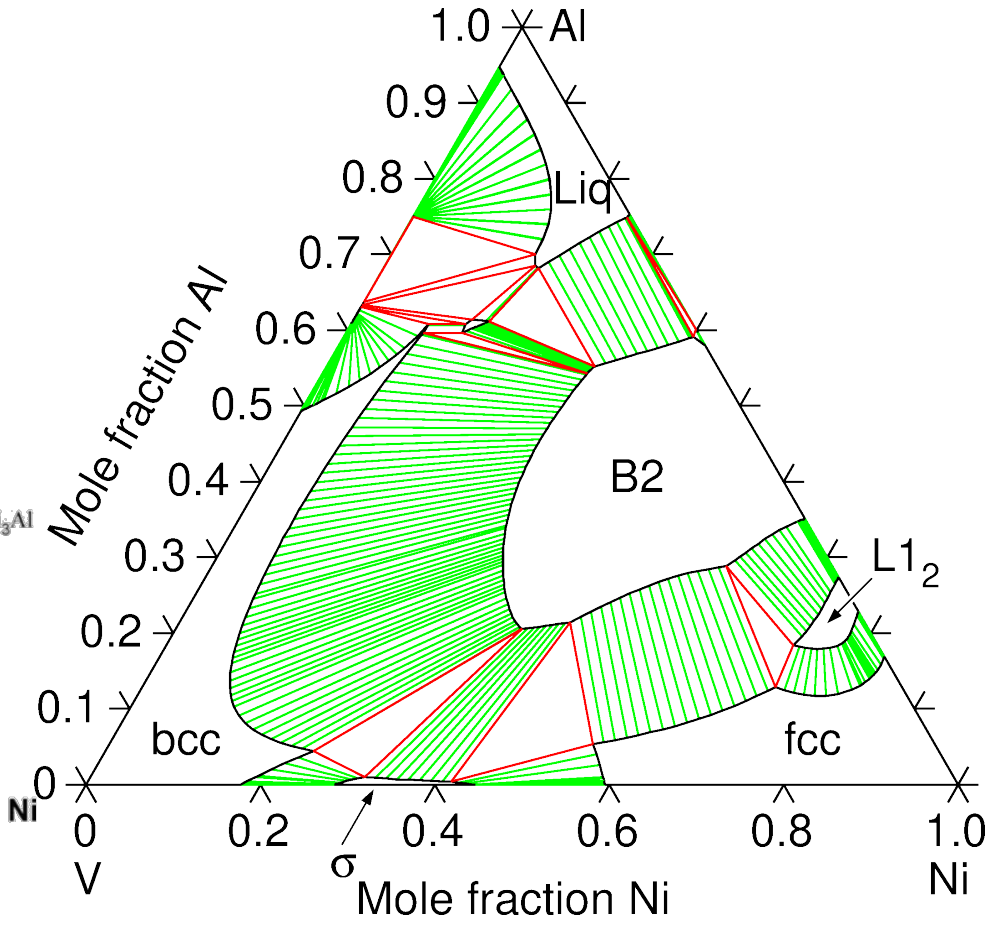
Planned work

Al-Ni-V 1100 C Isothermal section

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

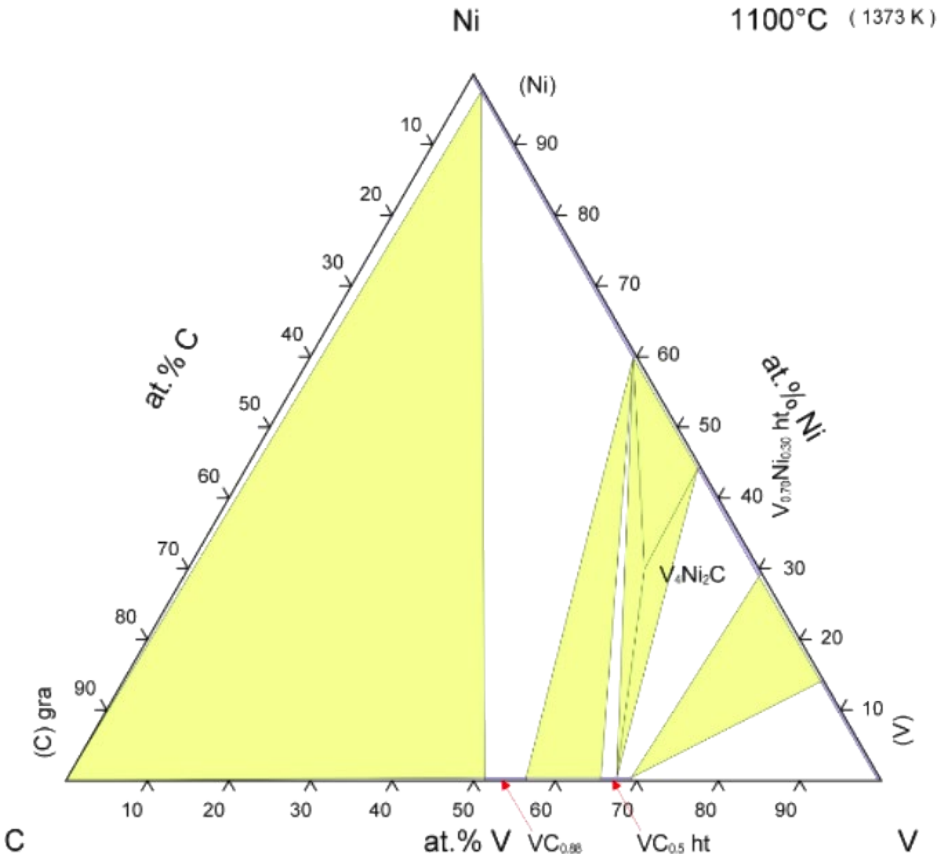


- Thermodynamic extrapolation from the binaries with ab initio calculations for the σ phase.

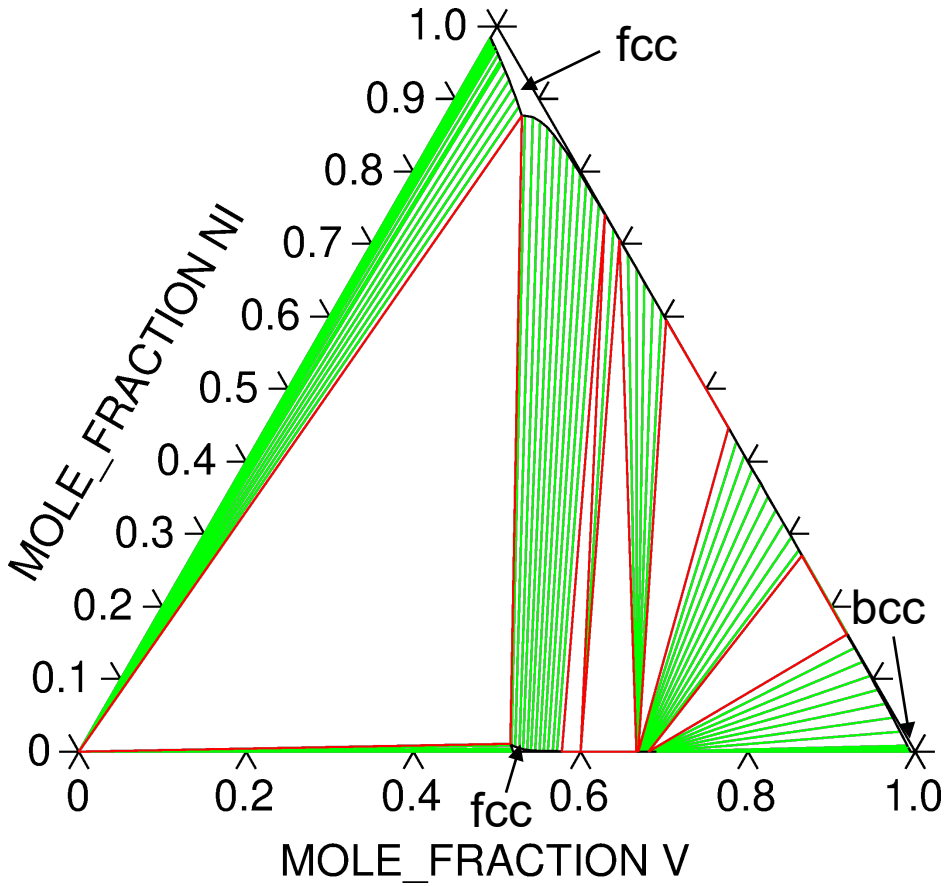


Ni-V-C 1100 C Isothermal section

- Experimental work from H. Holleck, pp. 170-196, 1981.

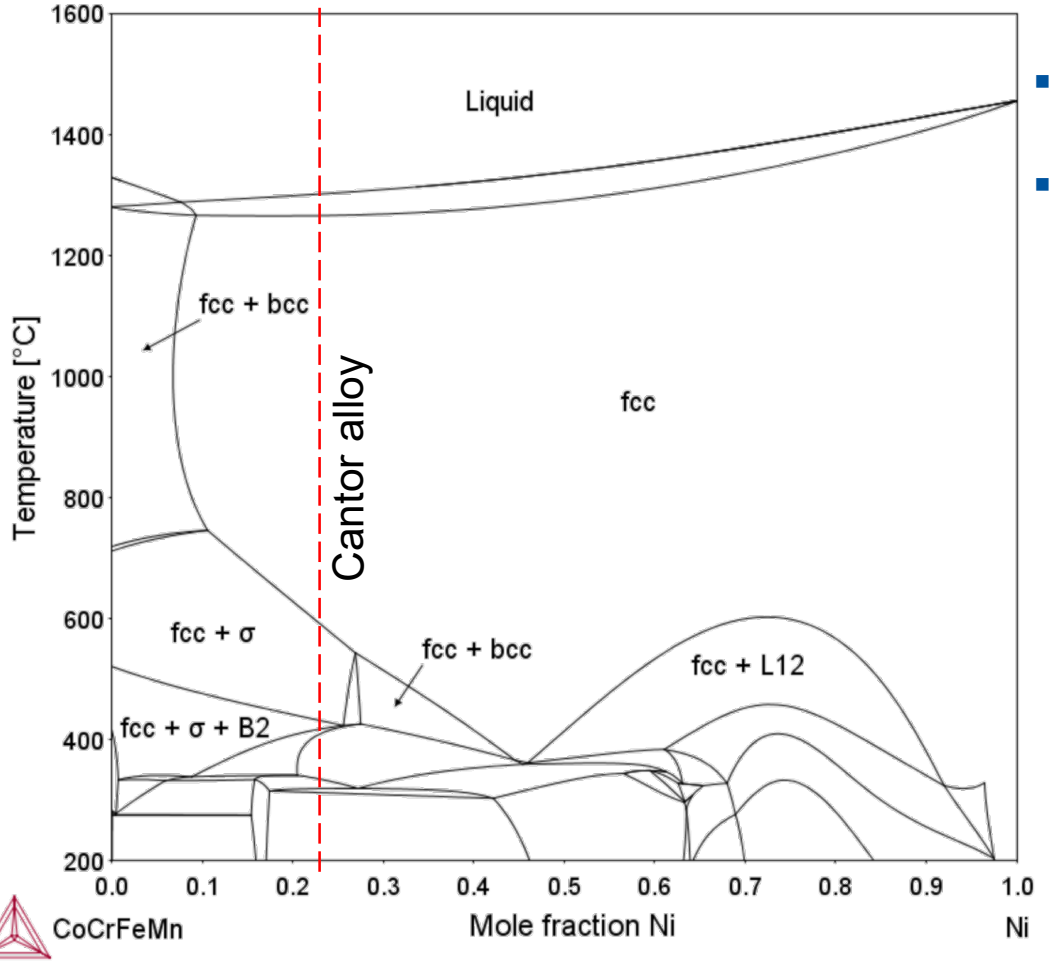


- Thermodynamic extrapolation from the binaries



Co-Cr-Fe-Mn-Ni-Al-C database

Constructed thermodynamic database for Cantor Alloy +Al+C



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

Conclusion

- Ni-V, 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 sigma 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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