# Calphad modeling in High Entropy Alloys (HEA)

**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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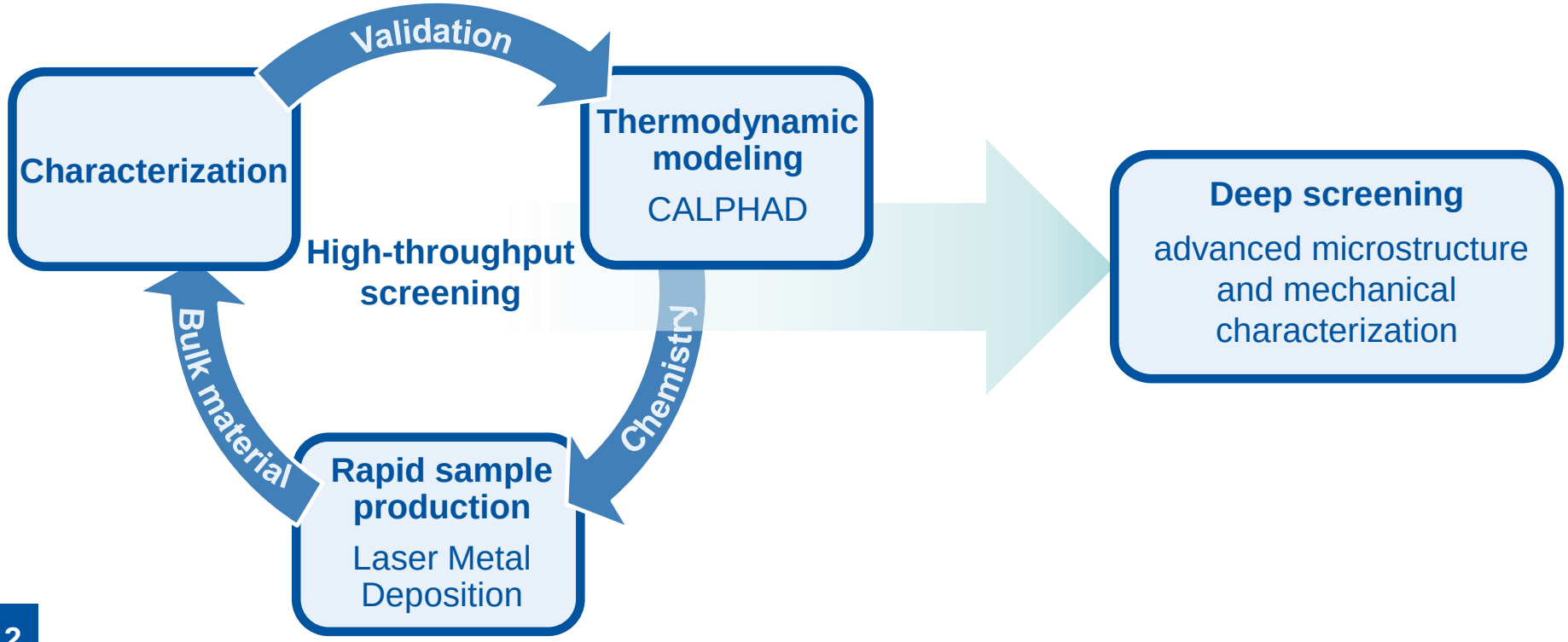
**SPP CCA/HEA Meeting Karlsruhe, 25-27 March, 2019**

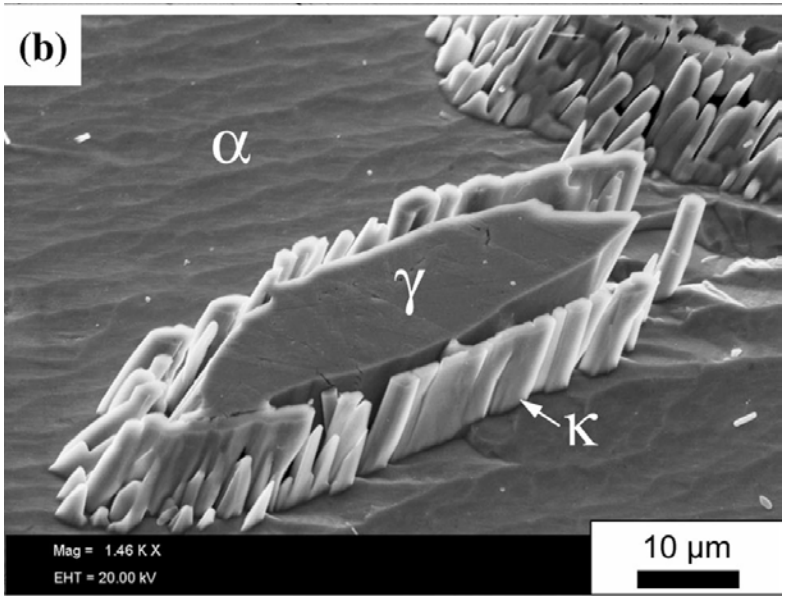
# Goals

- Finding new alloys with exceptional mechanical properties
  - → Advancing from HEA to CCAs
- Alloy selection with 7 components
  - → Elements: Fe-Cr-Co-Mn-Ni-Al-C
- Not sufficient experimental data for HEA/CCA



# Goals

- Development of database for CCAs
  - → 21 binary systems included
  - → 28 of 35 possible ternary systems included
  - → Thermodynamic modelling of Al-Co-Fe, Al-Co-Mn, Al-Mn-Ni
- Calphad prediction of precipitates (e.g. B2, κ) and phase stabilities

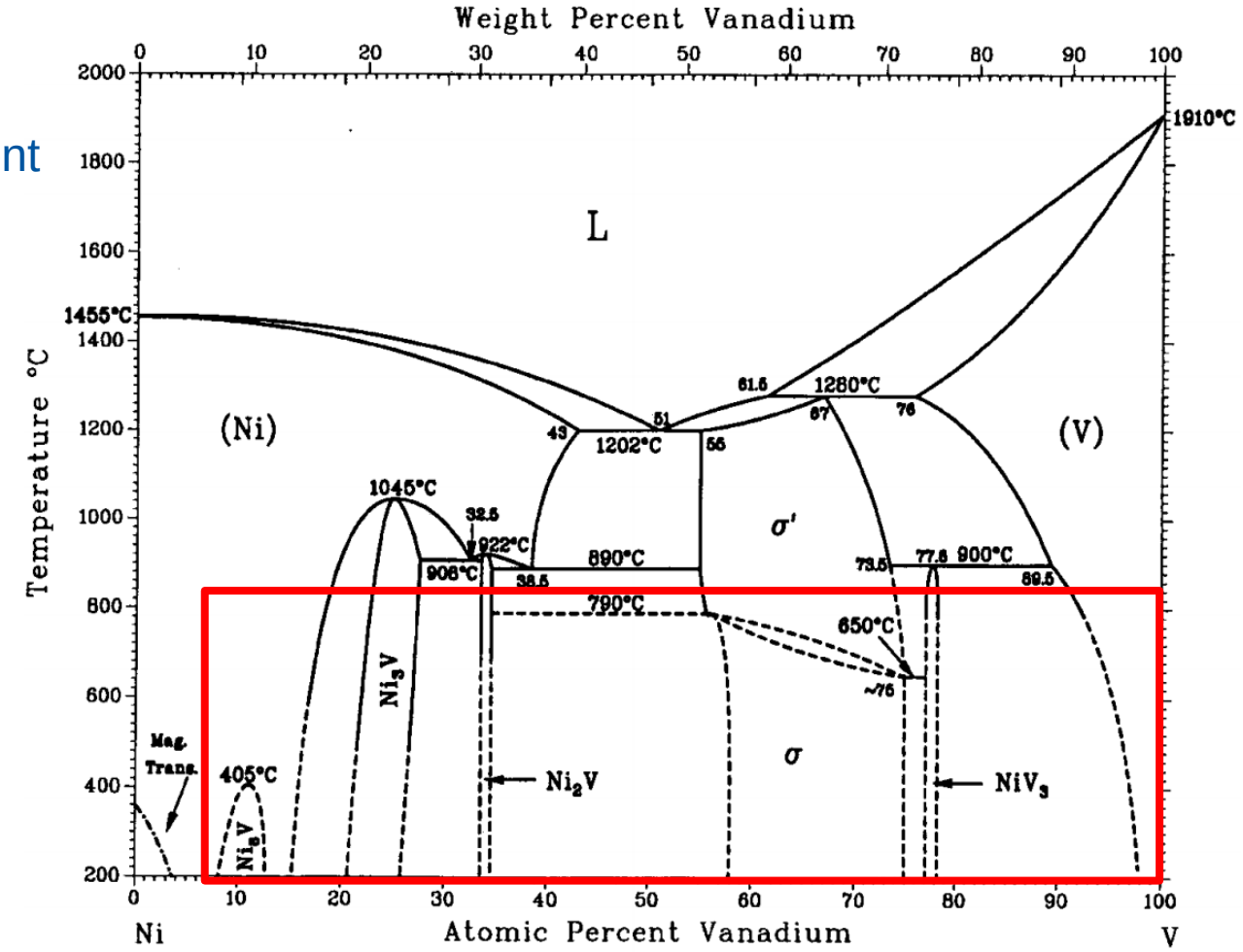



**Fe-2%Mn-8%Al-0.2%C**, cooling 10K/s from 1400 C, quenched from 870 C.

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

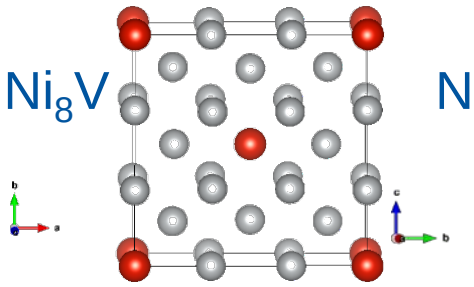
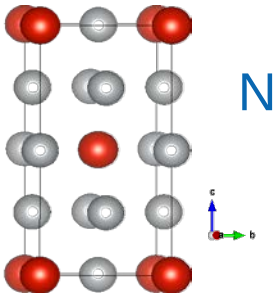
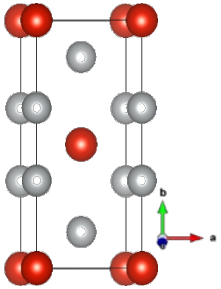
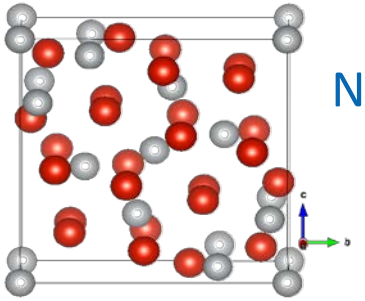
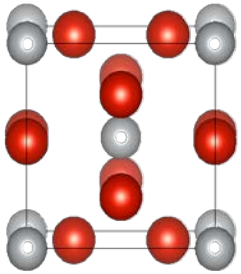
# Ni-V system

Experimental assessment from J. F. Smith et al., Bull. Alloy Phase Diagrams 1982.

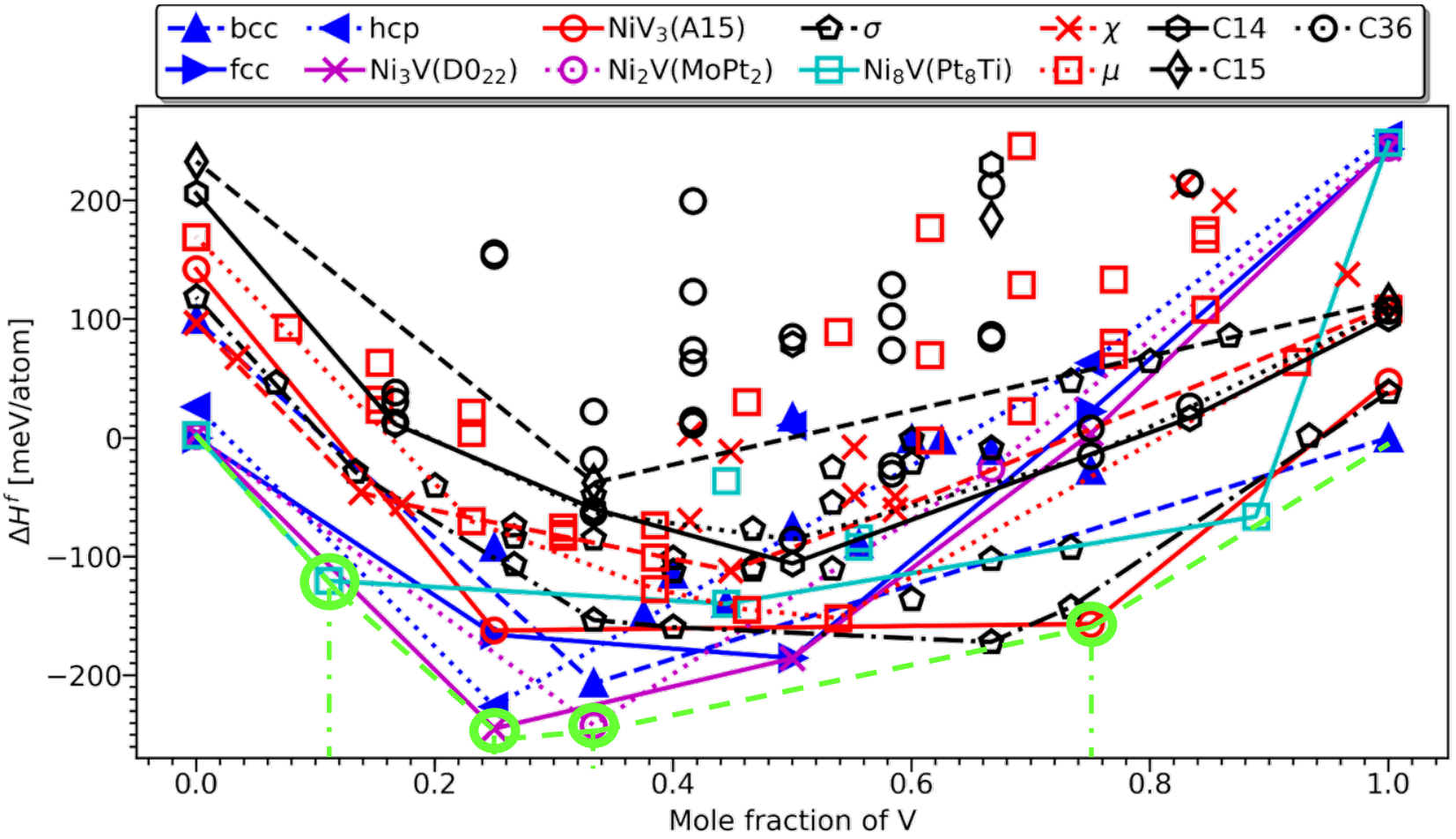


# Crystallographic info. of Ni-V system

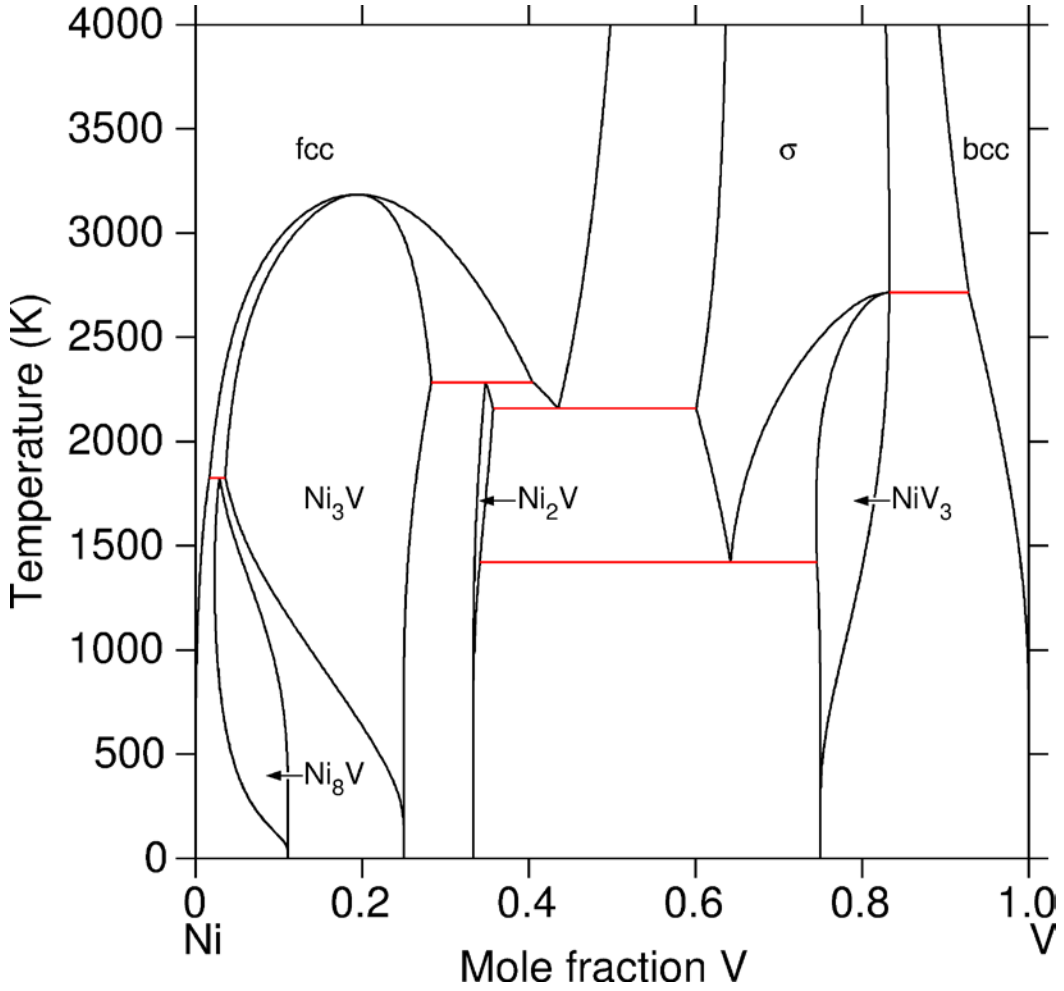
| Phase label | Prototype | Pearson symbol | Space group | Struktur-bericht | Wyckoff positions | Configu-rations |
|---|---|---|---|---|---|---|
| Ni-fcc | Cu | *cF4* | *Fm-3m* (225) | *A1* | | |
| $Ni_8V$ | $NbNi_8$ | *tI18* | *I4/mmm* (139) | - | 2a, 8h, 8i | 8 |
| $Ni_3V$ | $TiAl_3$ | *tI8* | *I4/mmm* (139) | $D0_{22}$ | 2a, 2b, 4d | 8 |
| $Ni_2V$ | $MoPt_2$ | *oI6* | *Immm* (71) | - | 2a, 4i | 4 |
| σ | $Cr_{0.49}Fe_{0.51}$ | *tP30* | $P4_2/mnm$ (136) | $D8_b$ | 2a, 4f, $8i_1$, $8i_2$, 8j | 32 |
| $NiV_3$ | $Cr_3Si$ | *cP8* | *Pm-3n* (223) | *A15* | 2a, 6c | 4 |
| V-bcc | W | *cI2* | *Im-3m* (229) | *A2* | | |

$Ni_8V$  $Ni_3V$  $Ni_2V$  σ  $NiV_3$ 

# *Ab initio* calculation

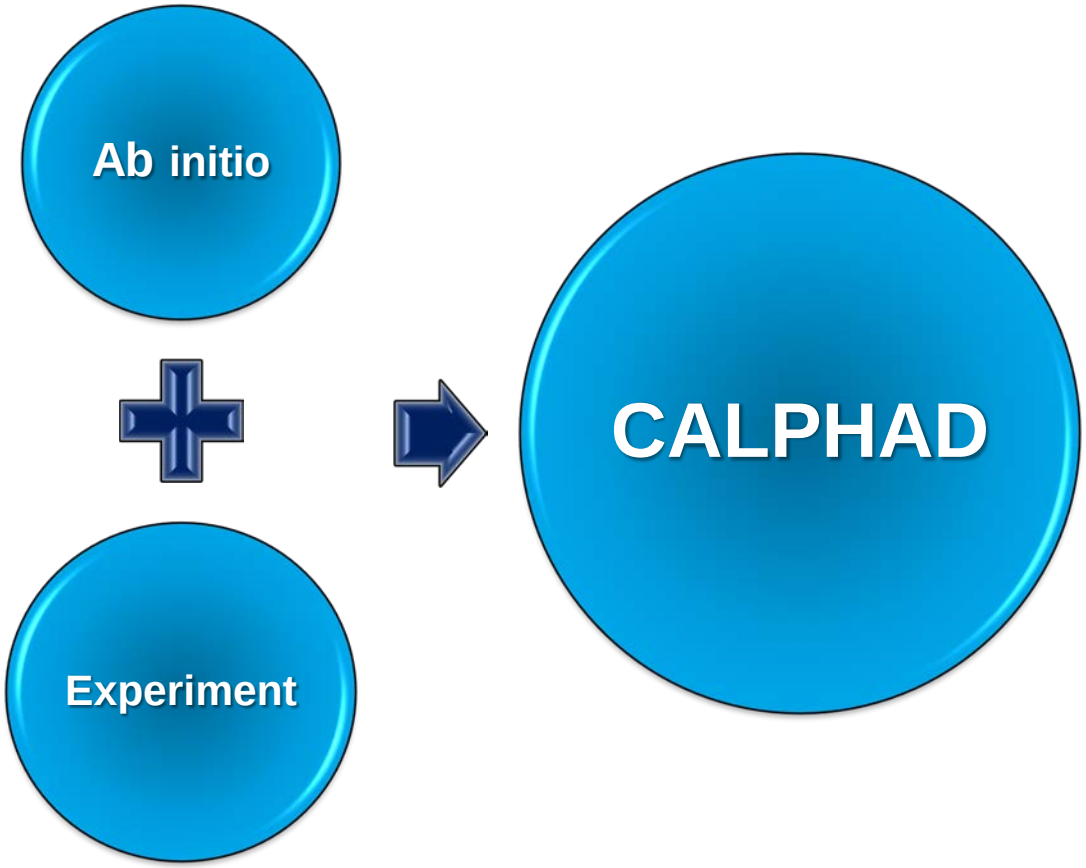


# Ni-V *ab initio* TDB

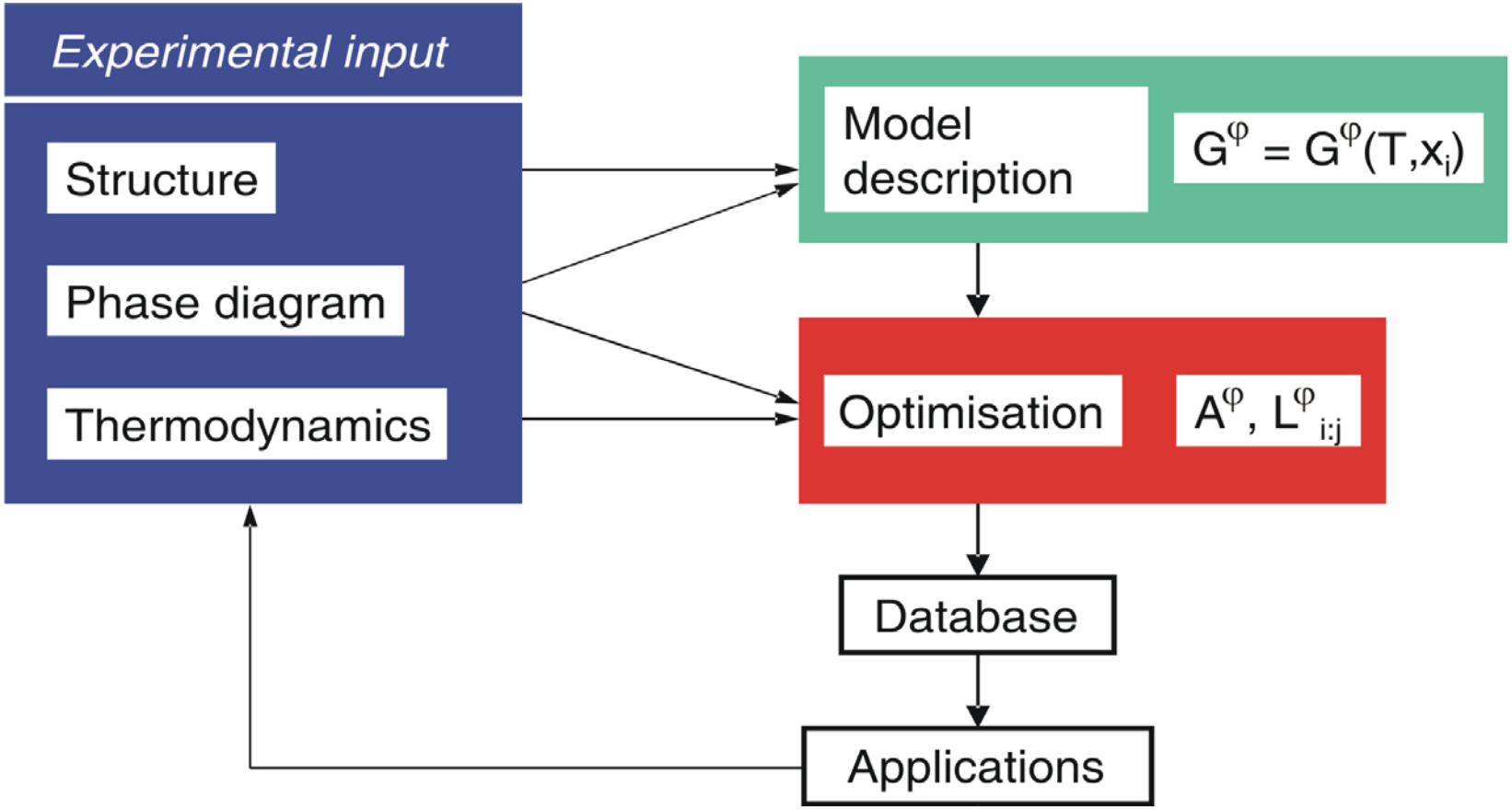


# Calphad modeling

Development of Ni-V binary system

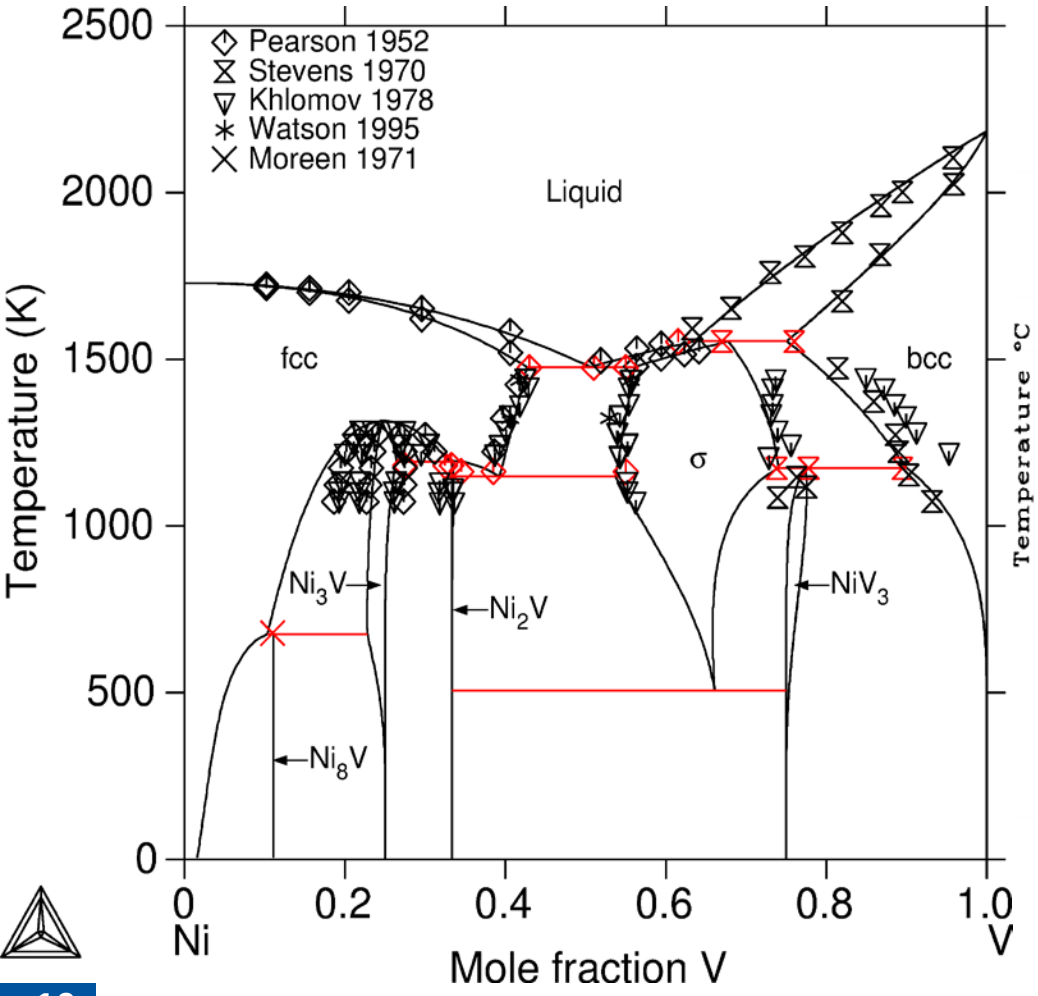


# Calphad method

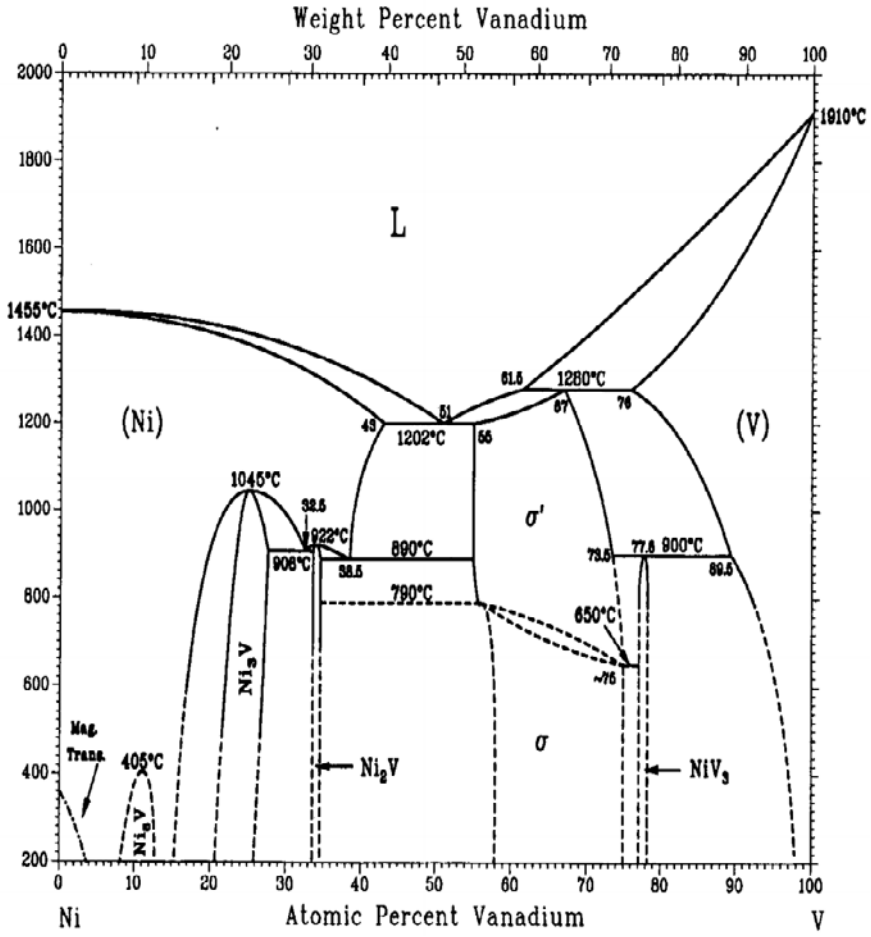


# Ni-V thermodynamic modelling

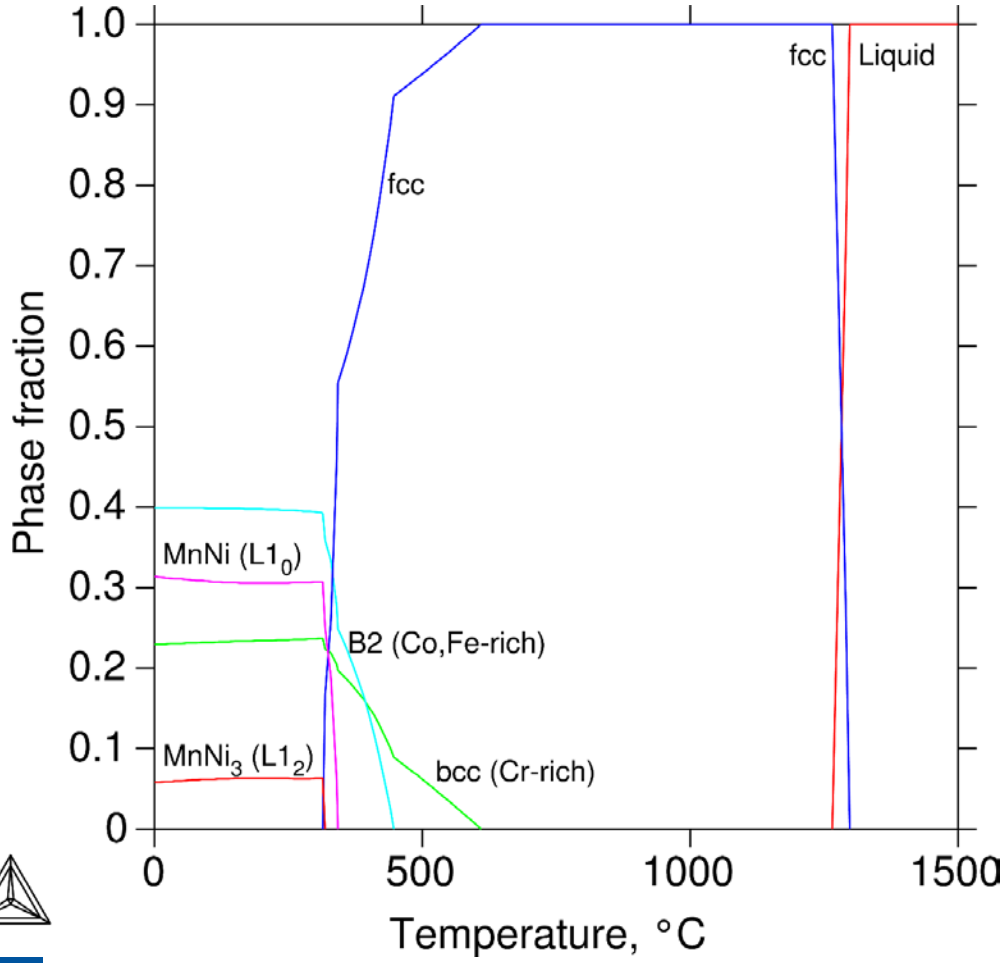
This work




Smith 82



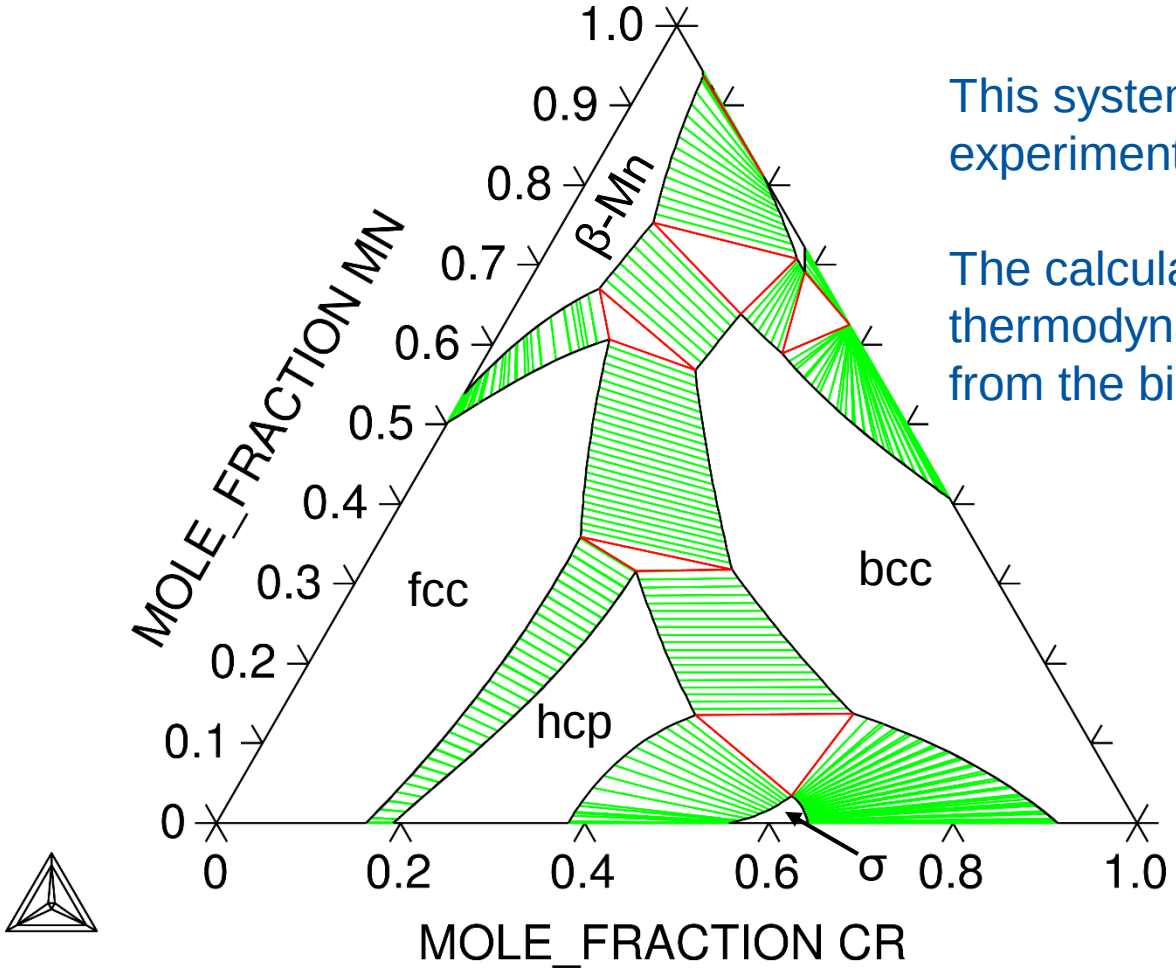
# The CoCrFeMnNi Cantor alloy




Observations by F. Otto et al., Acta Mater., 112 (2016) 40-52:

700 C: Cr-rich σ-phase
500 C: Cr-rich bcc,
Co-Fe-rich B2,
Mn-Ni-rich $L1_0$

# Co-Cr-Mn 800 C isothermal section



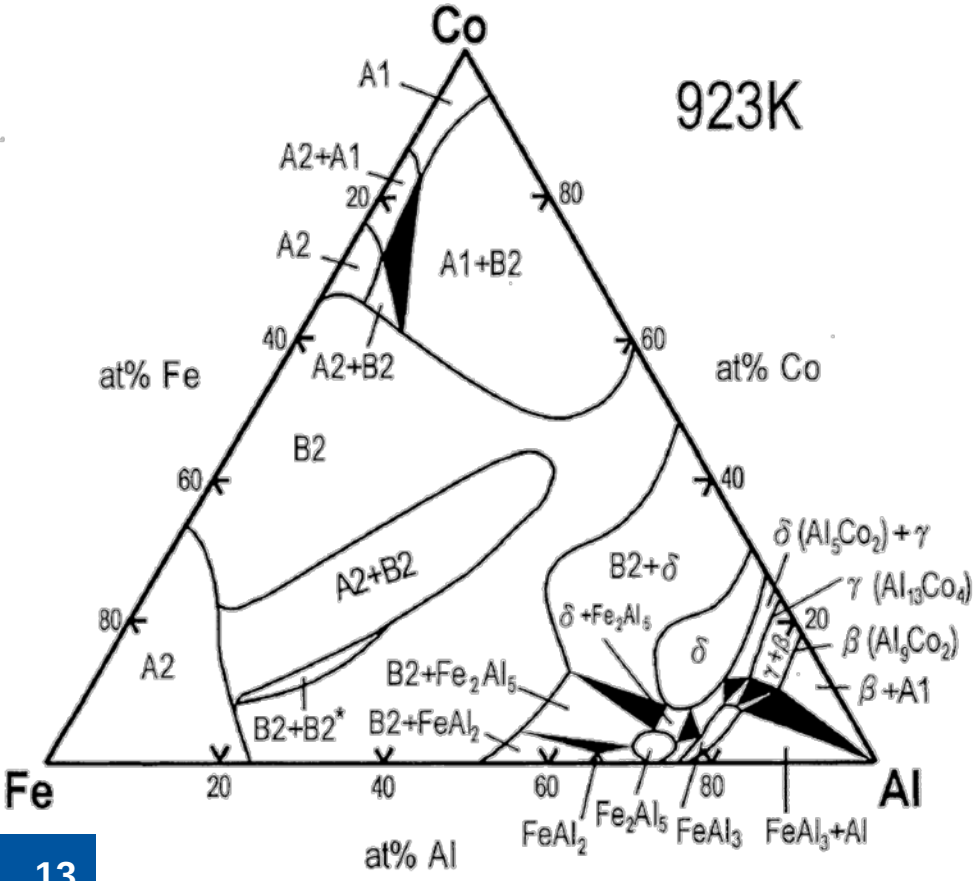

This system has not been experimentally investigated

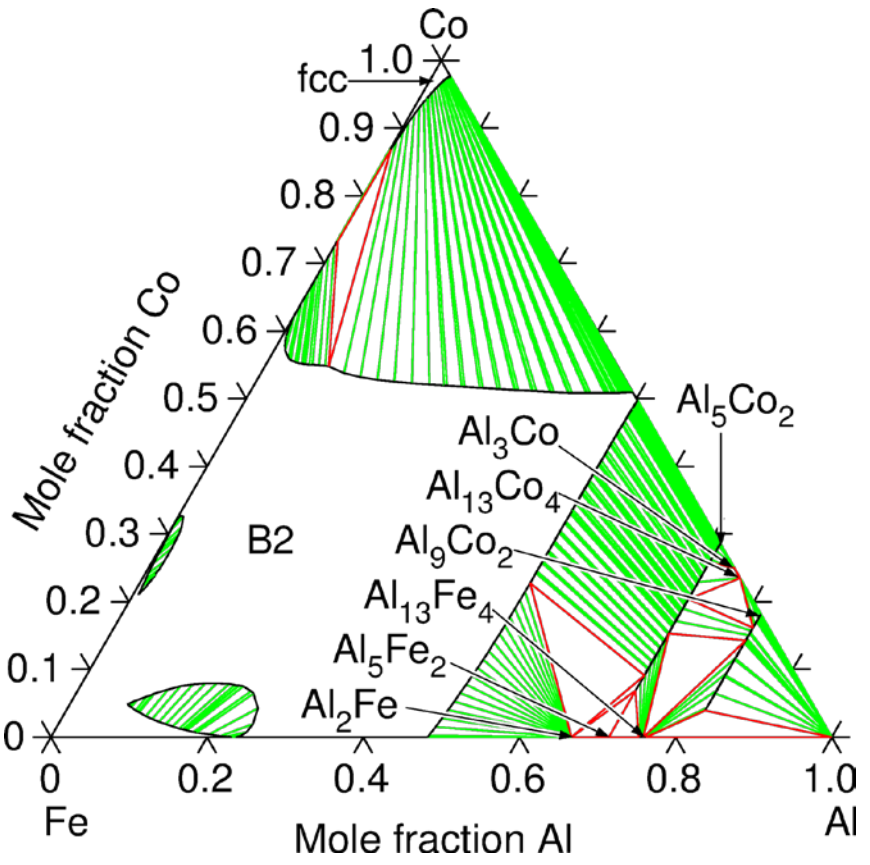
The calculation is a thermodynamic extrapolation from the binaries

# Al-Co-Fe 650 C isothermal section

Experimental work from
T. Kozakai et al., Z. Metallkd.,
90 (1999) 261-66

- Figure out Heusler phases
- Ternary interaction parameters



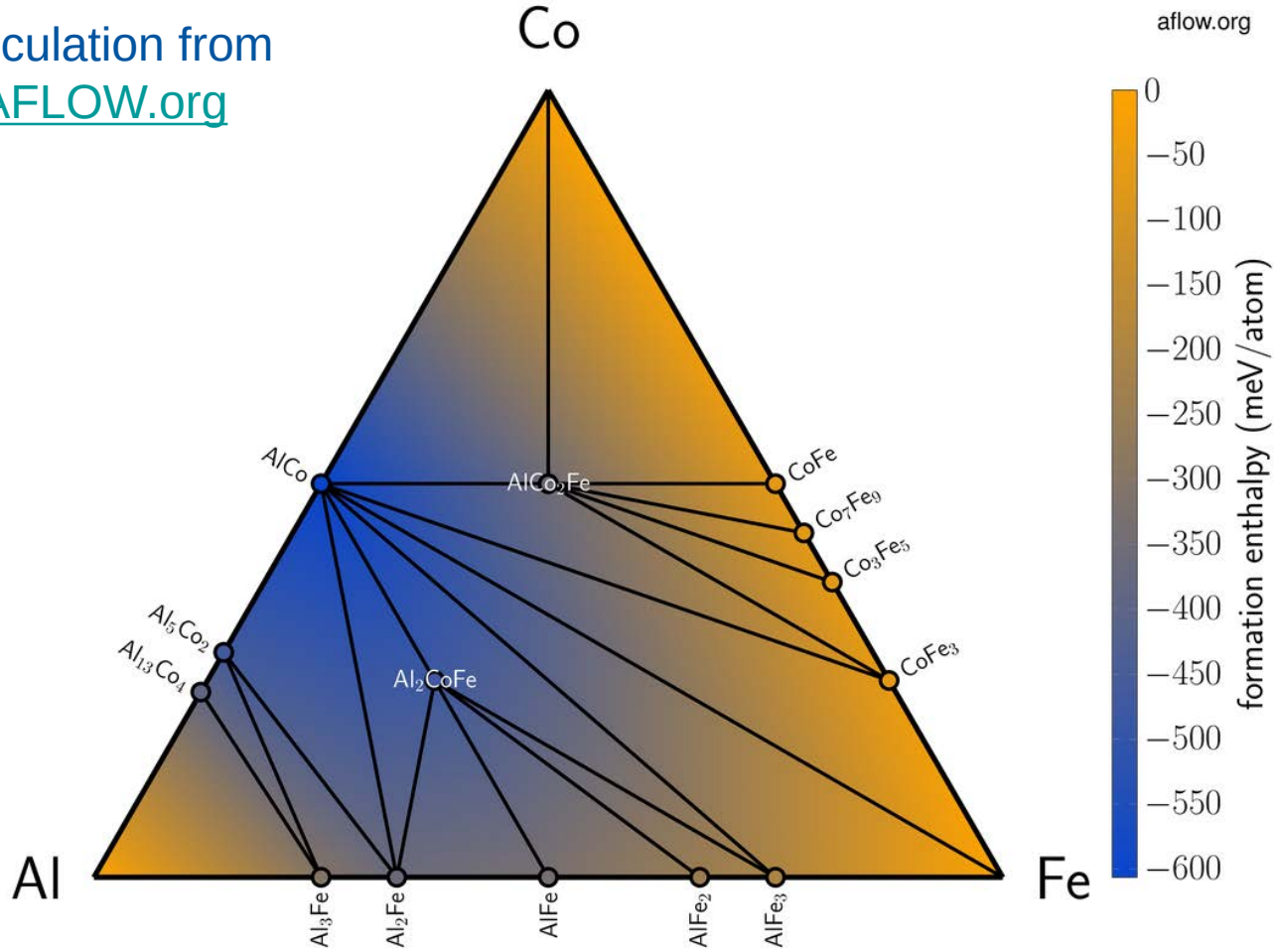
# Crystallographic info. of Al-Co-Fe

| Phase label | Prototype | Pearson symbol | Space group | Strukturbericht |
|---|---|---|---|---|
| $Al_5Co_2$ | $Co_2Al_5$ | *hP28* | *P6$_3$/mmc* (194) | *D8$_{11}$* |
| $Al_{13}Co_4$ | $Co_4Al_{13}$ | *mC100* | *C2/m* (012) | - |
| $Al_9Co_2$ | $Co_2Al_9$ | *mP22* | *P2$_1$/a* (007) | - |
| AlCo | CsCl | *cP2* | *Pm-3m* (221) | *B2* |
| AlFe | CsCl | *cP2* | *Pm-3m* (221) | *B2* |
| $AlFe_3$ | $Fe_3Al$ | *cF16* | *Fm-3m* (225) | *D0$_3$* |
| $Al_2Fe$ | $FeAl_2$ | *aP18* | *P1* (001) | - |
| $Al_{13}Fe_4$ | $Fe_4Al_{13}$ | *mC102* | *C2/m* (012) | - |
| $Al_5Fe_2$ | $Fe_2Al_5$ | *oC24* | *Cmcm* (061) | - |
| $Al_2CoFe$ | $AlCu_2Mn$ | *cF16* | *Fm-3m(225)* | *L2$_1$* |
| $AlCo_2Fe$ | $AlCu_2Mn$ | *cF16* | *Fm-3m(225)* | *L2$_1$* |

Heusler Phases

# Al-Co-Fe *ab initio* calculation

Ab initio Calculation from
http://www.AFLOW.org

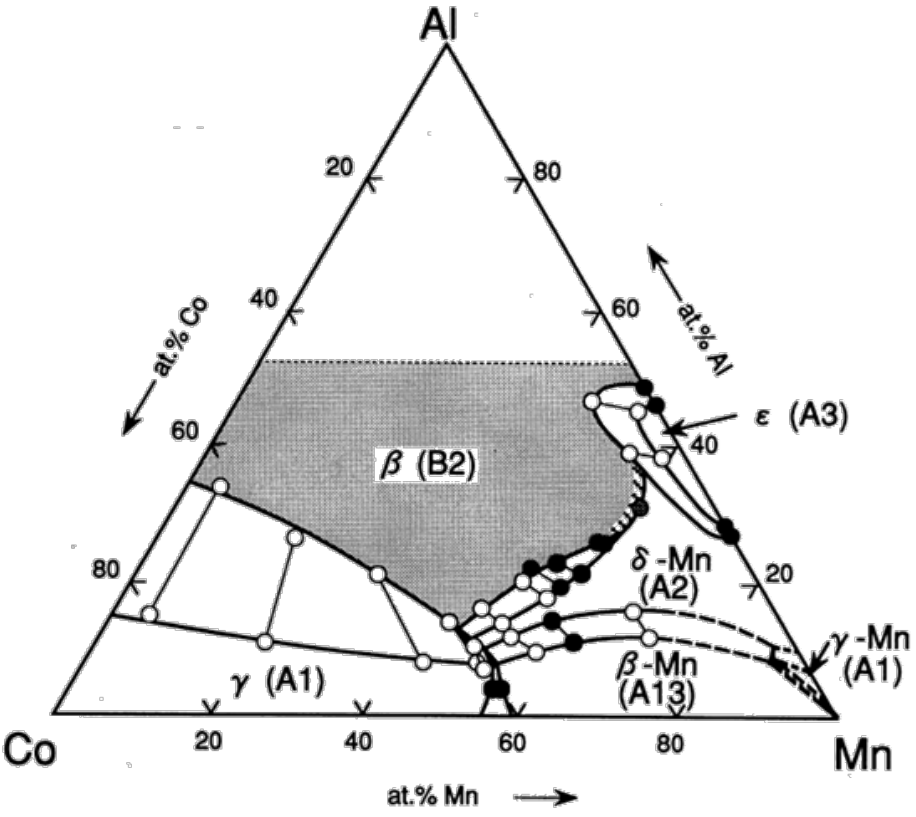


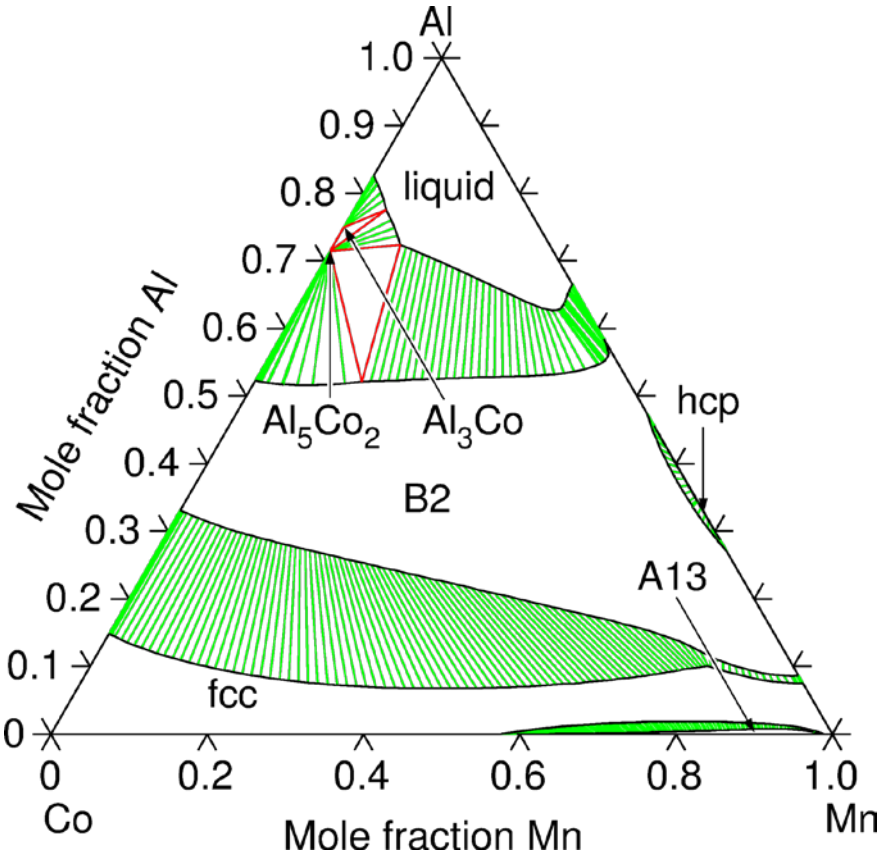
# Future Work

# Al-Co-Mn 1100 C Isothermal section

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

The calculation is a thermodynamic extrapolation from the binaries

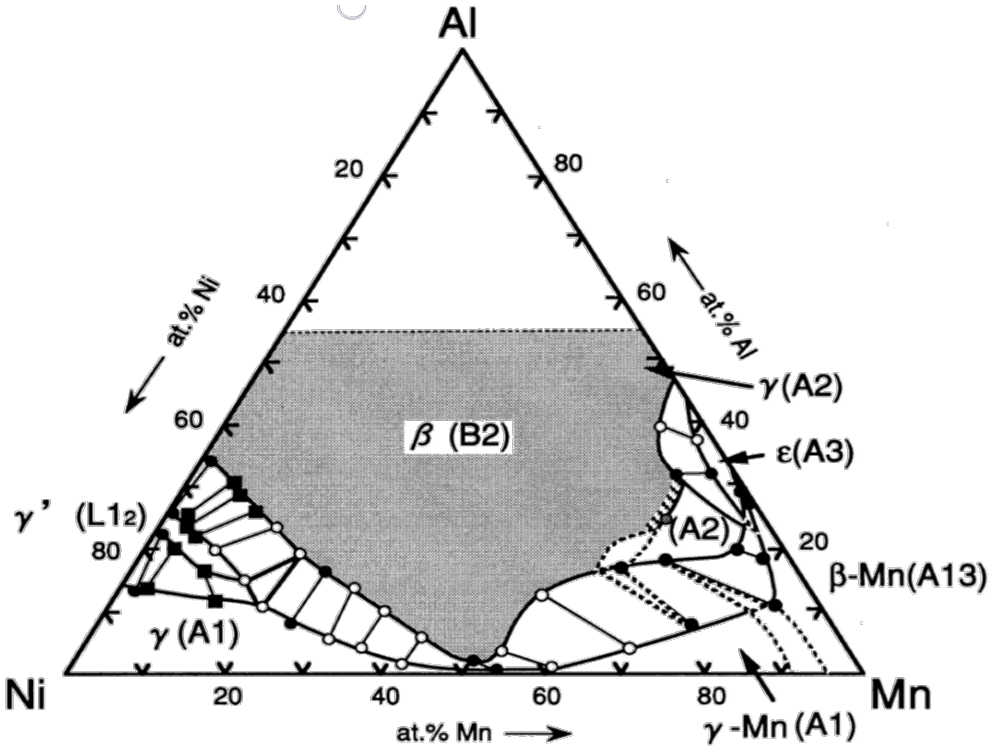


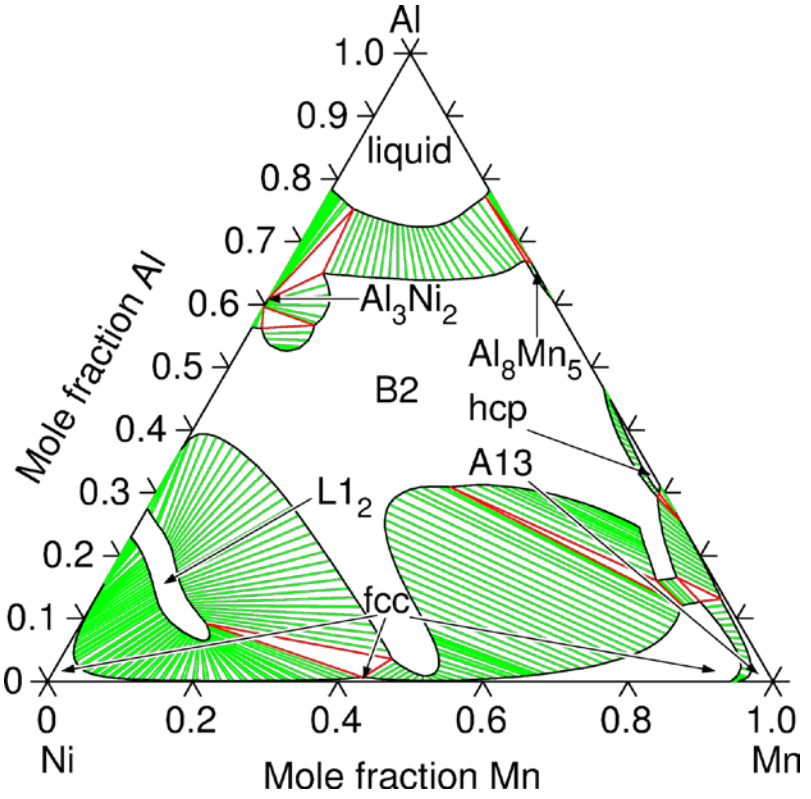



# Al-Mn-Ni 1000 C Isothermal section

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

The calculation is a thermodynamic extrapolation from the binaries



# *Thank you for your attention!*

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