Thermodynamic modeling for High Entropy Alloys (HEA)

Compositionally Complex Alloy – High Entropy Alloys (CCA - HEA)

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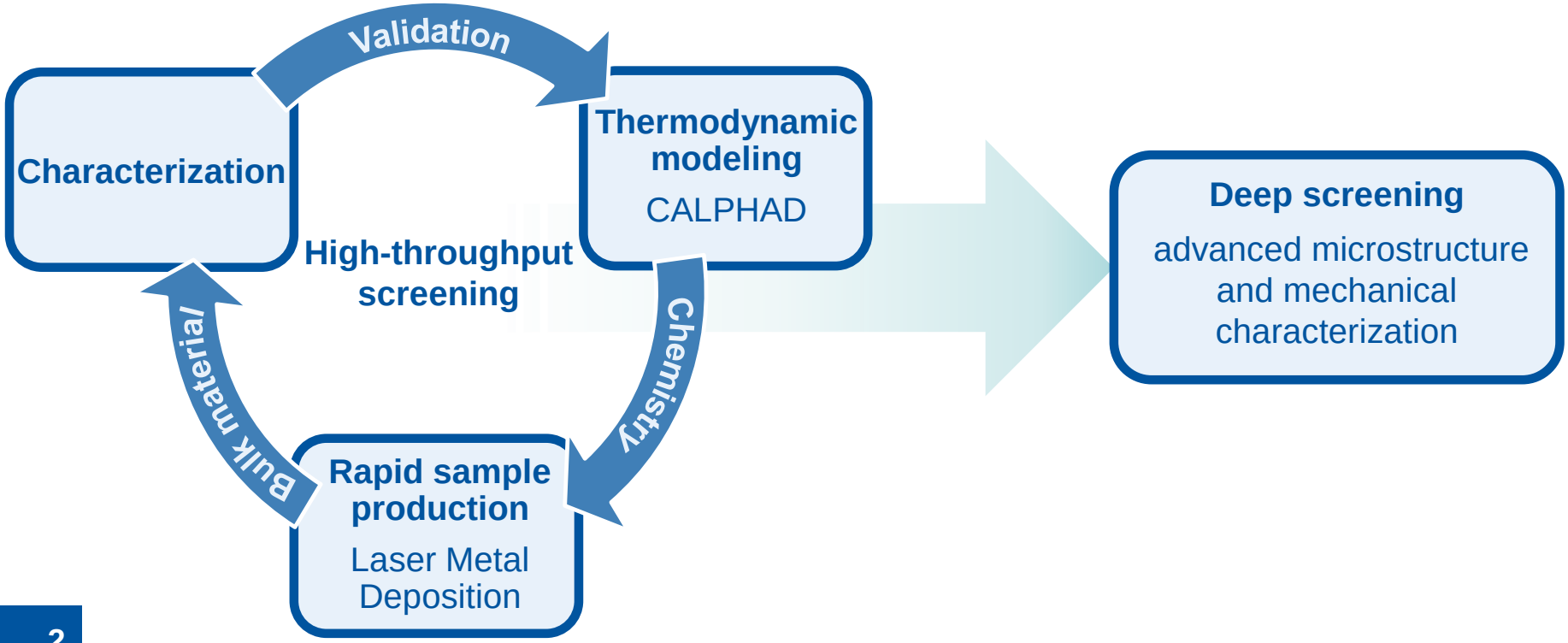
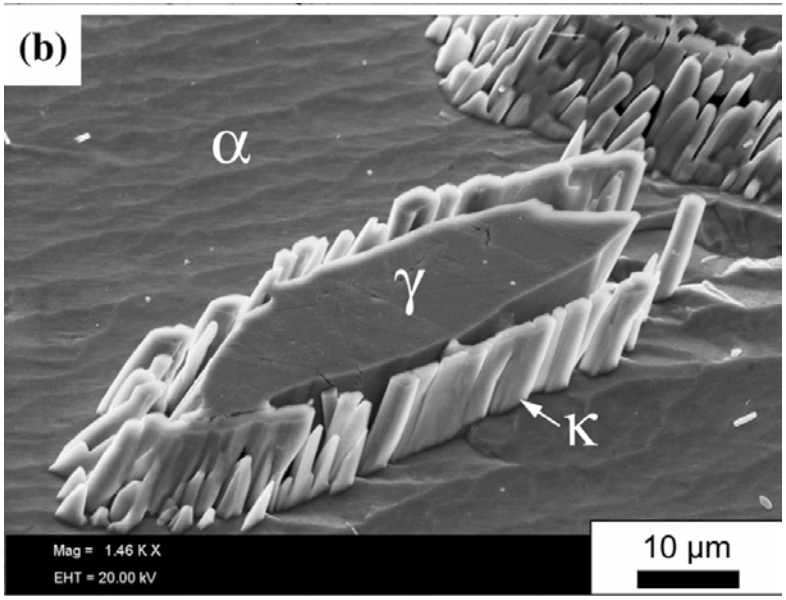
Subgroup-meeting on Modelling and Simulation, 11.10.2018

Goals

- Alloy selection with 7 components
  - → Elements: Fe-Cr-Co-Mn-Ni-Al-C
  - → All possible binary and ternary systems
- Not sufficient experimental data for HEA/CCA



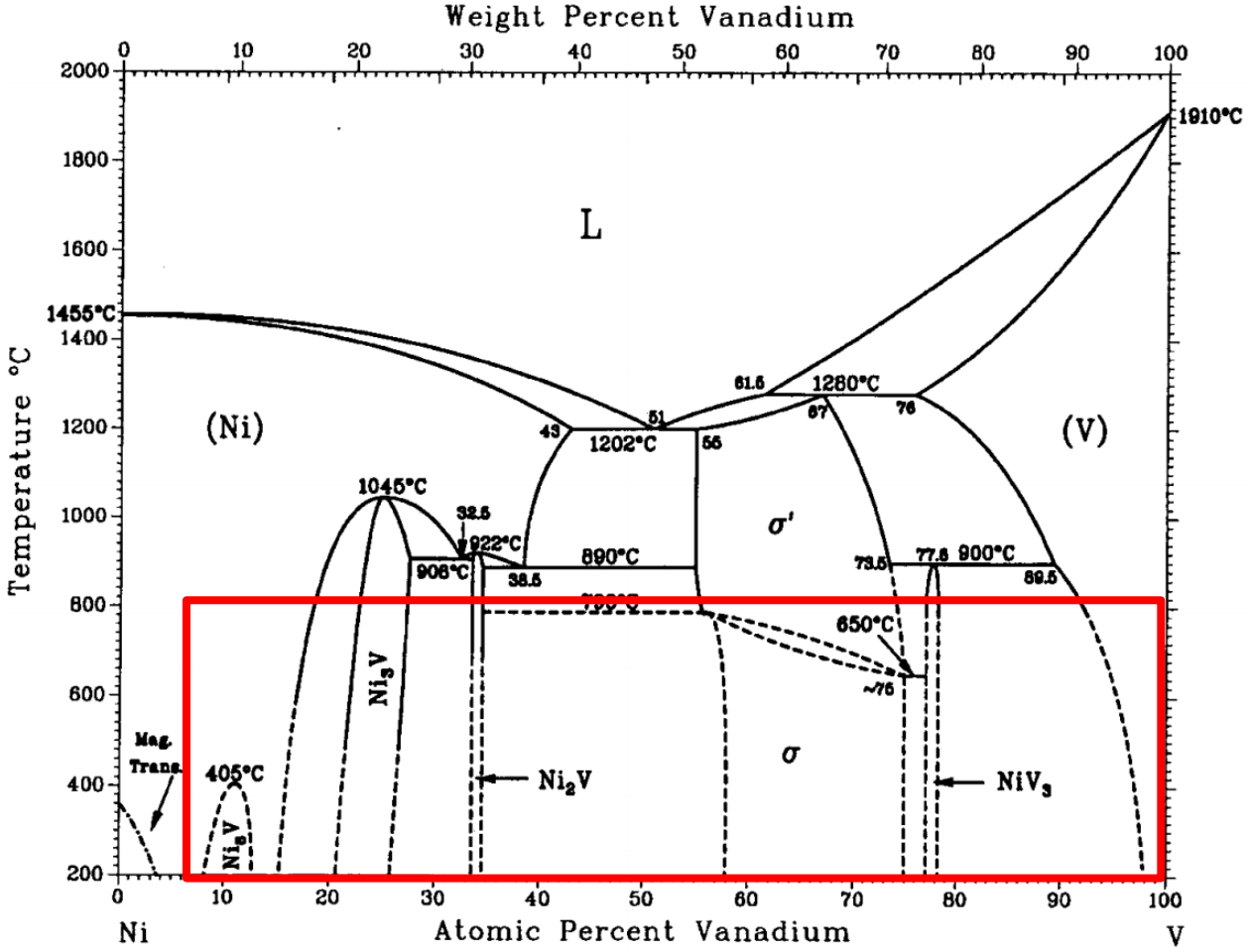
- Finding new alloys with exceptional mechanical properties
  - → Advancing from HEA to CCAs
- Development of database for CCAs
  - → 21 binary systems included
  - → 28 of 35 ternary systems included
  - → Thermodynamic modelling of Al-Co-Fe, Al-Co-Mn, Al-Mn-Ni
- Calphad prediction of precipitates (e.g. 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.

Experimental assessment of Ni-V :

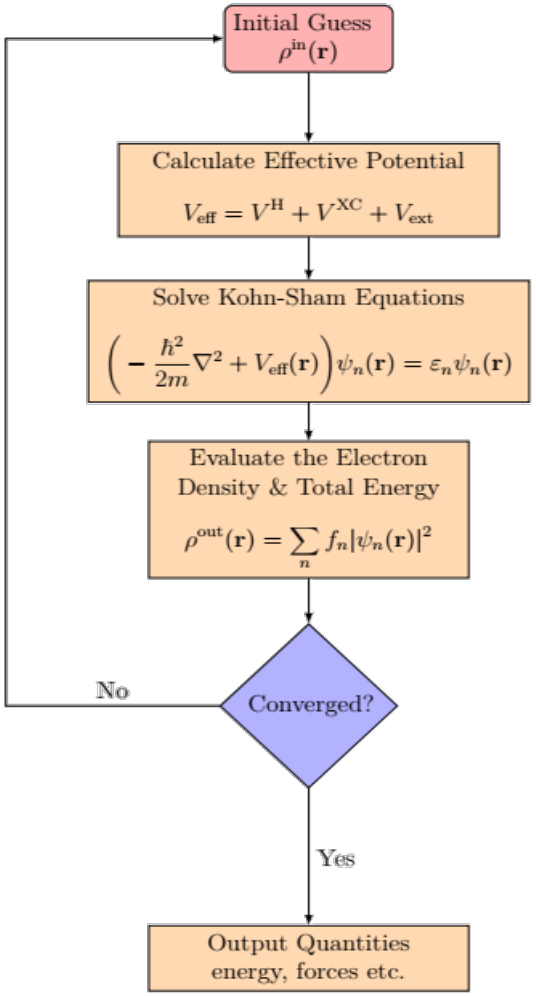


Crystallographic information of Ni-V system

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		

Atomistic modelling

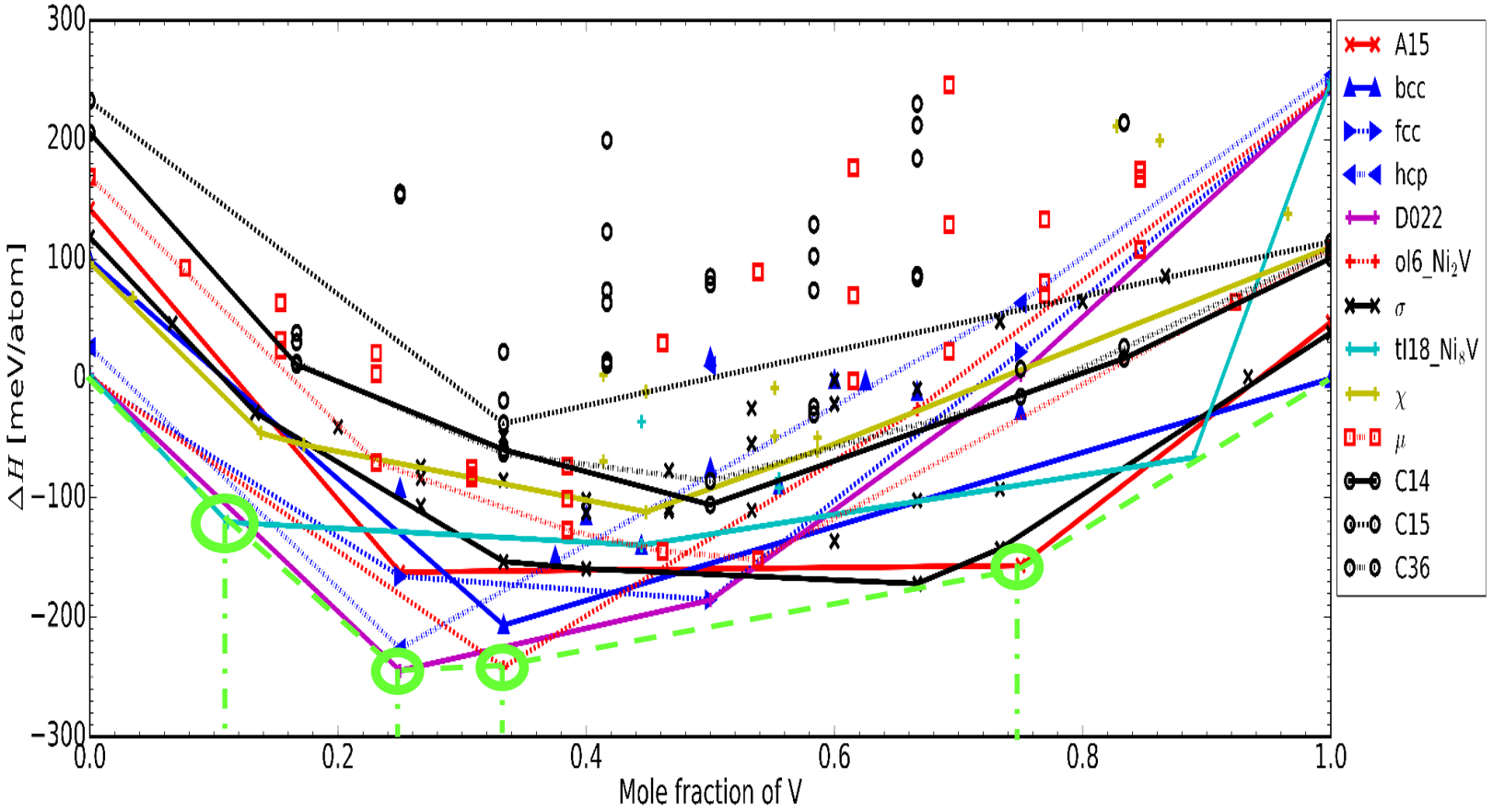
- Flowchart for the self-consistent loop of Kohn-Sham equations



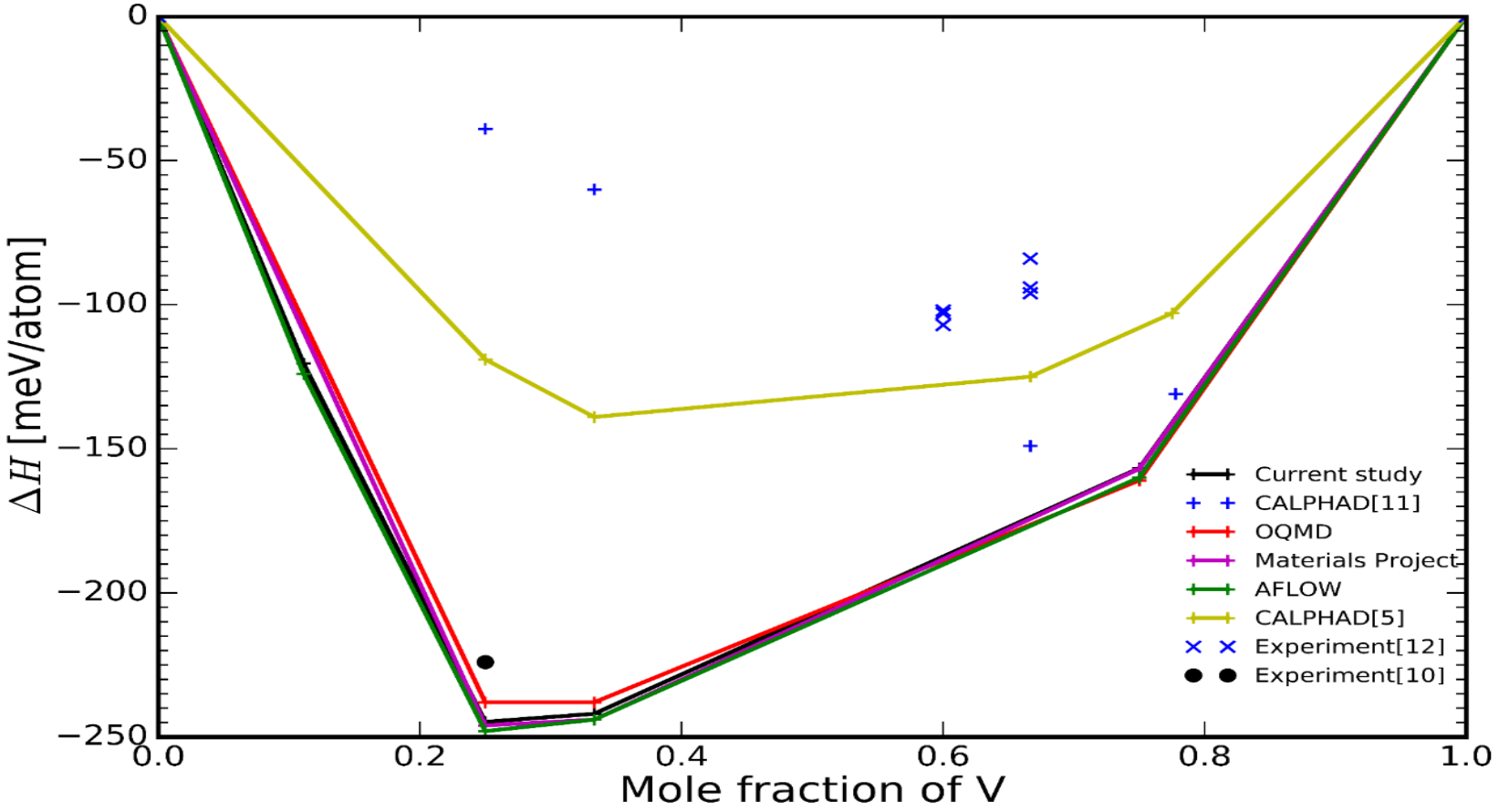
- Ab initio calculation:

  - → GGA-PBE
  - → MP k-point density of 0.02 Å^3
  - → T=0 K
  - → ENCUT=500 eV
  - → EDIFF=1e-6

Calculation of all experimentally reported + TCP + Ordered phases

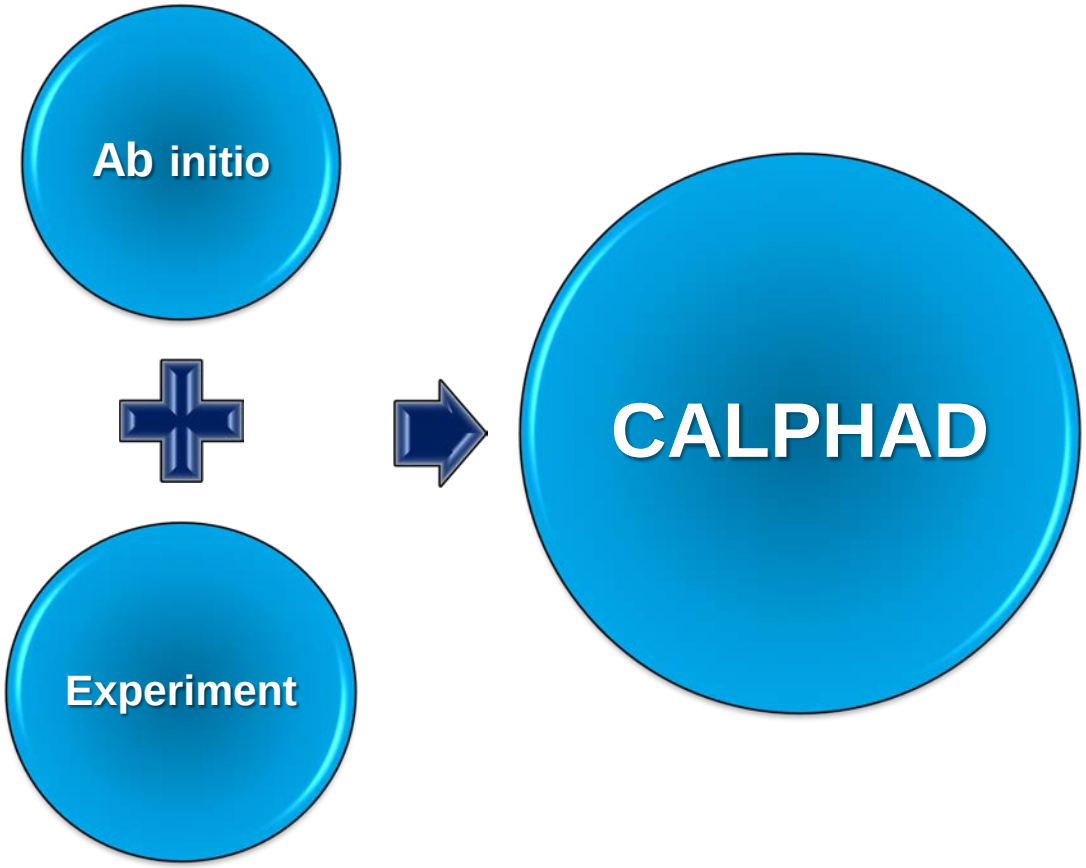


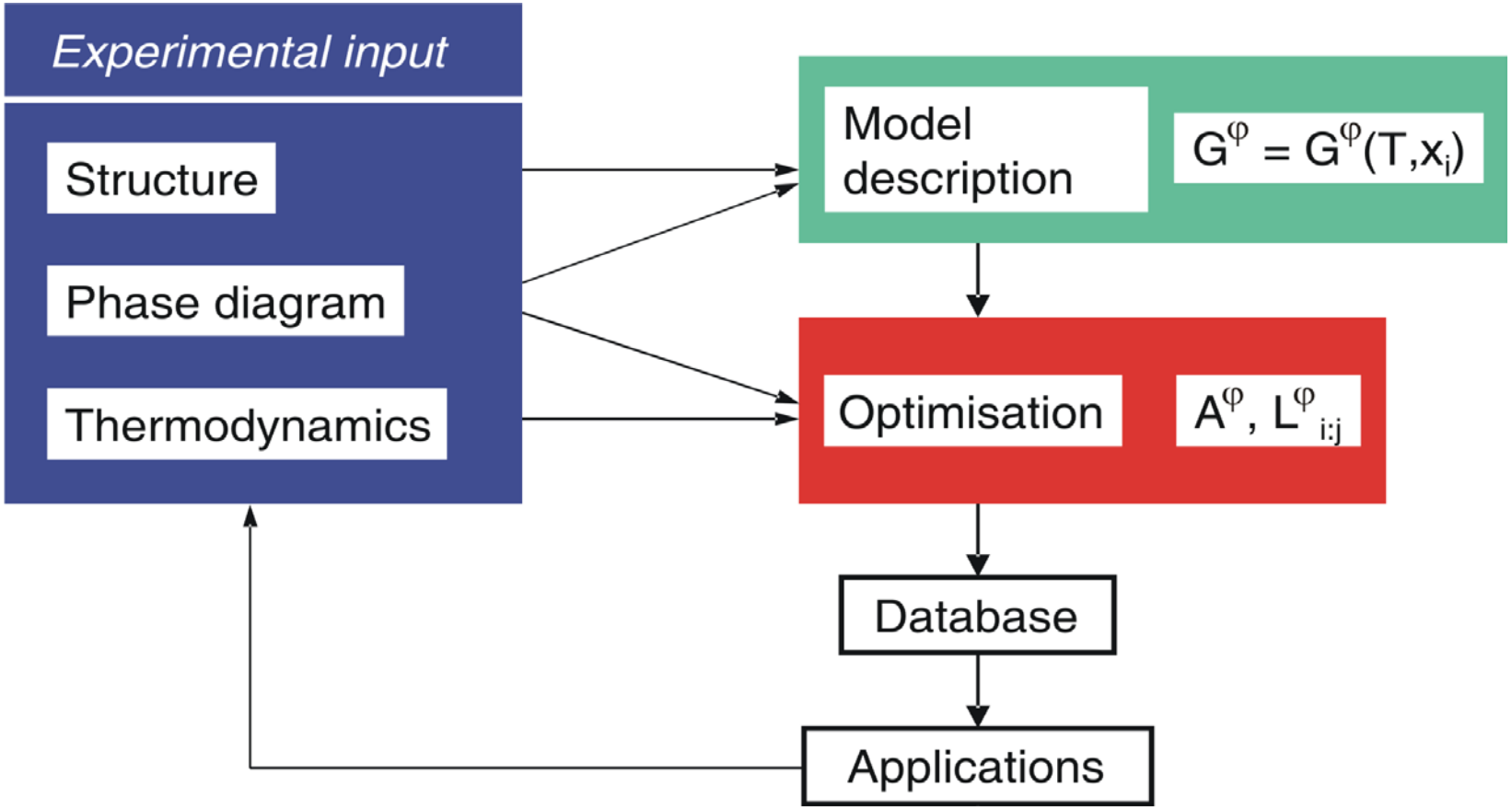
Comparison with different databases



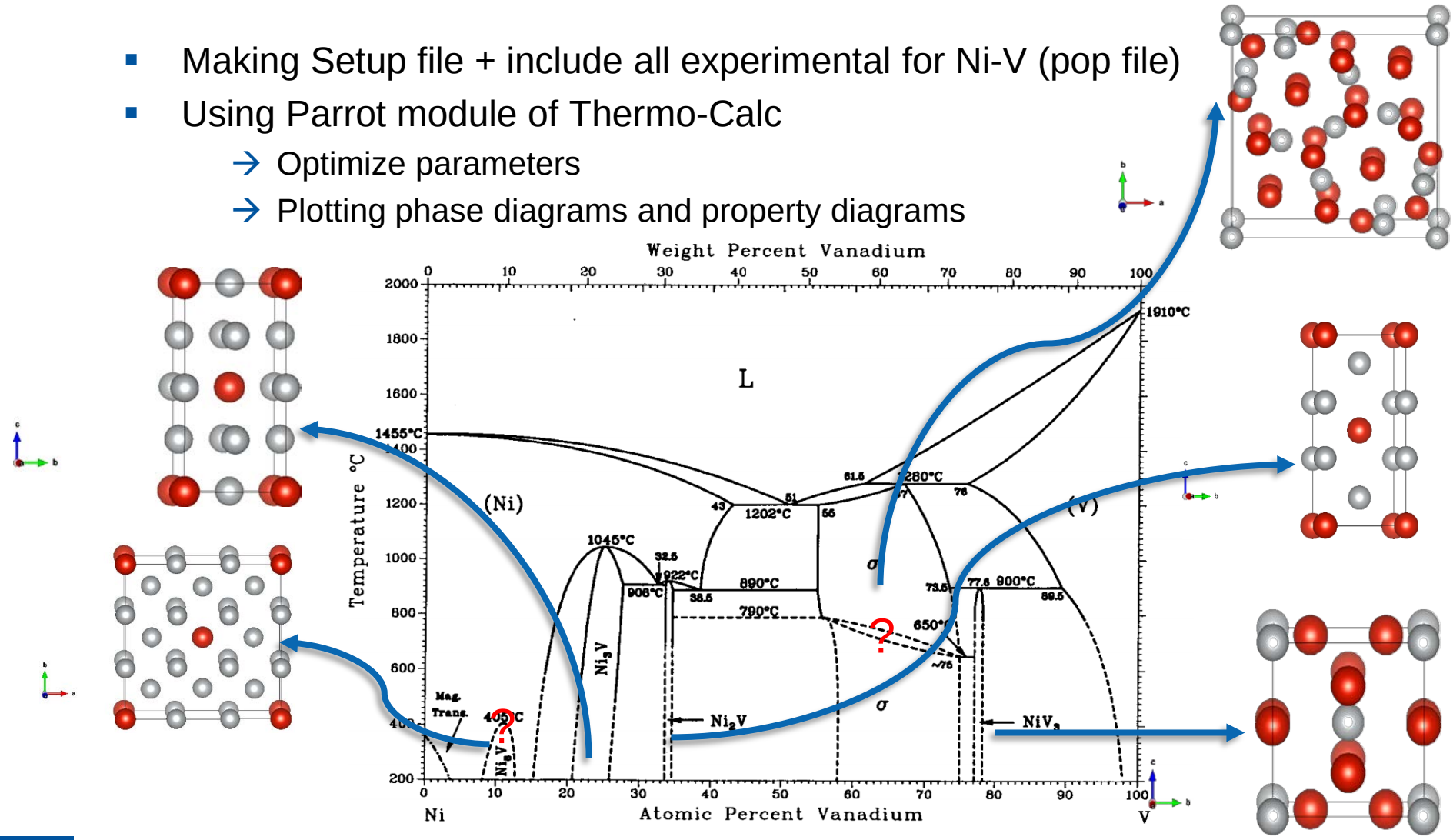
Calphad modeling

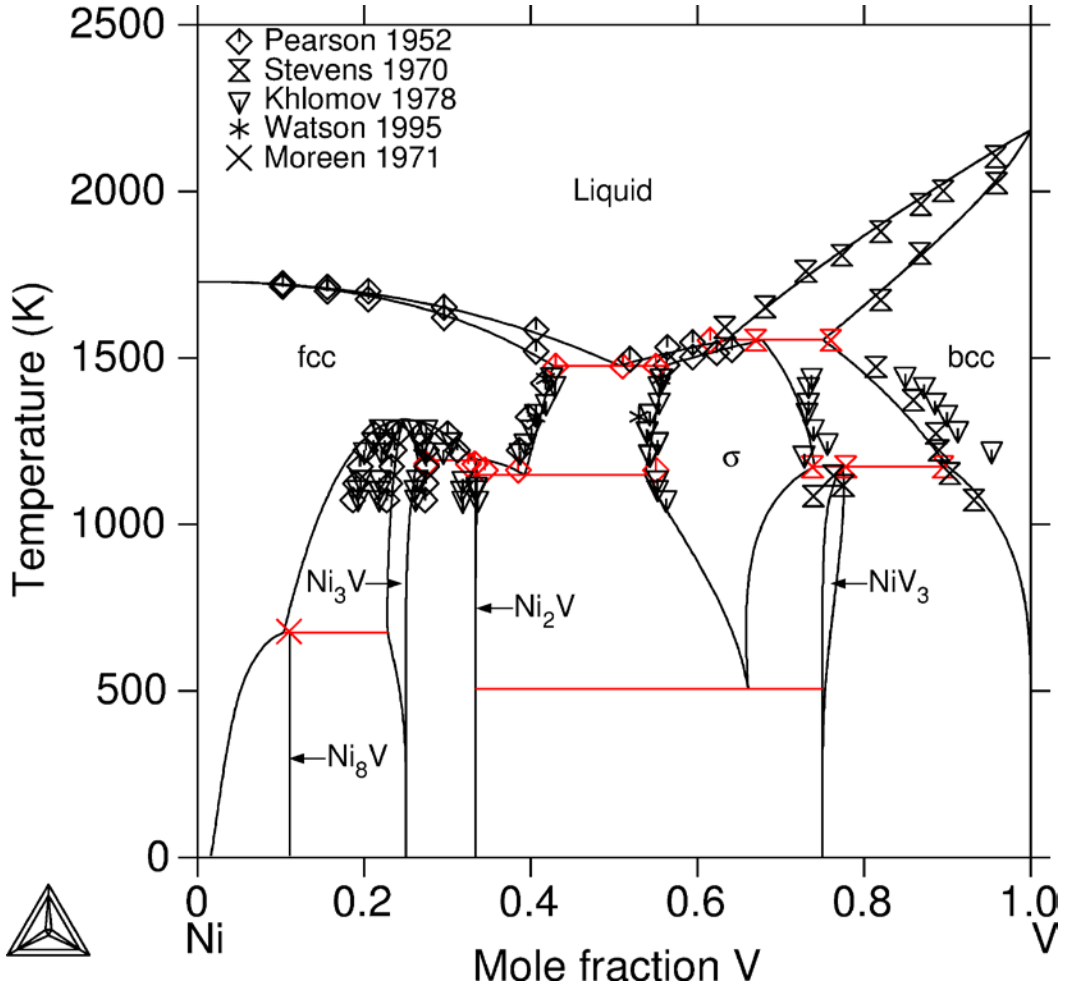
Development of Ni-V binary system




Experimental input
Structure
Phase diagram
Thermodynamics
Model description
$G^{\varphi} = G^{\varphi}(T,x_i)$
Optimisation
A^{φ}, $L^{\varphi}_{i:j}$
Database
Applications

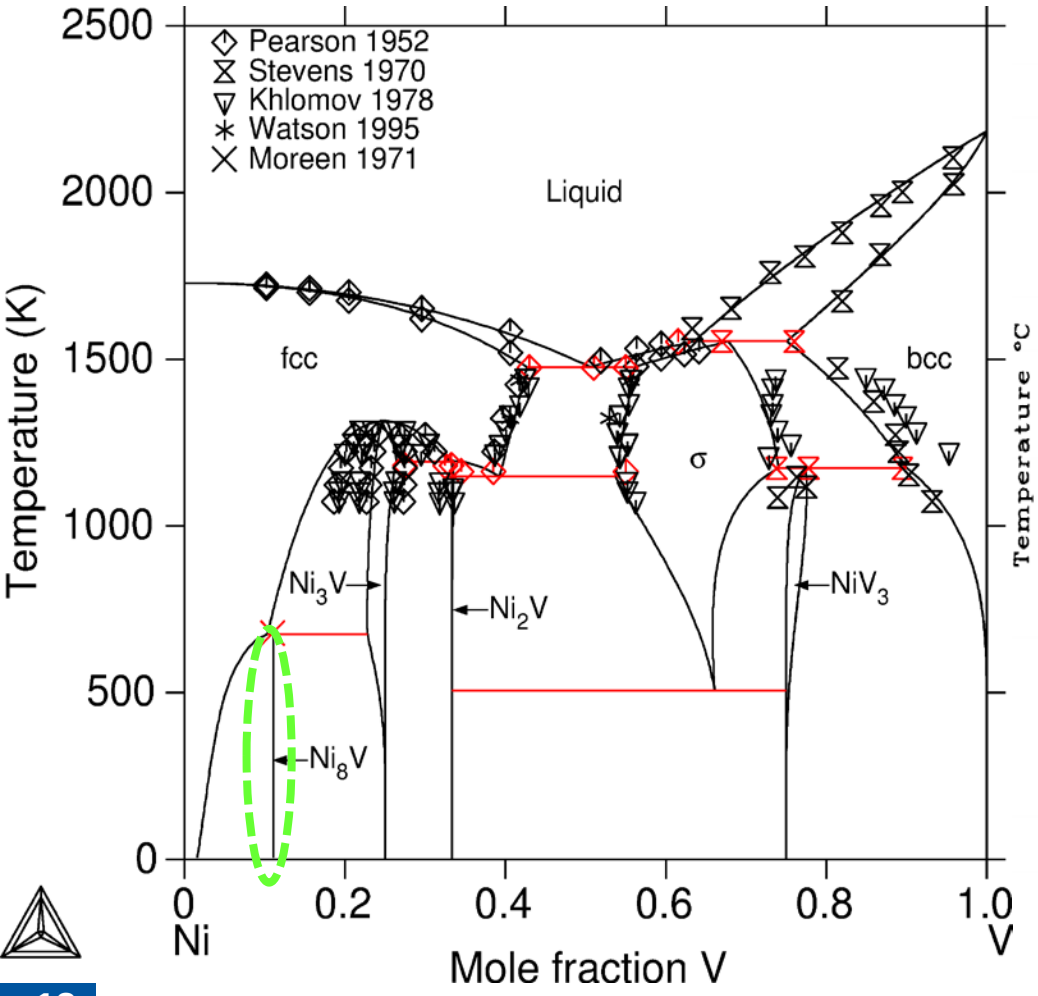
- Making Setup file + include all experimental for Ni-V (pop file)
- Using Parrot module of Thermo-Calc
  - → Optimize parameters
  - → Plotting phase diagrams and property diagrams

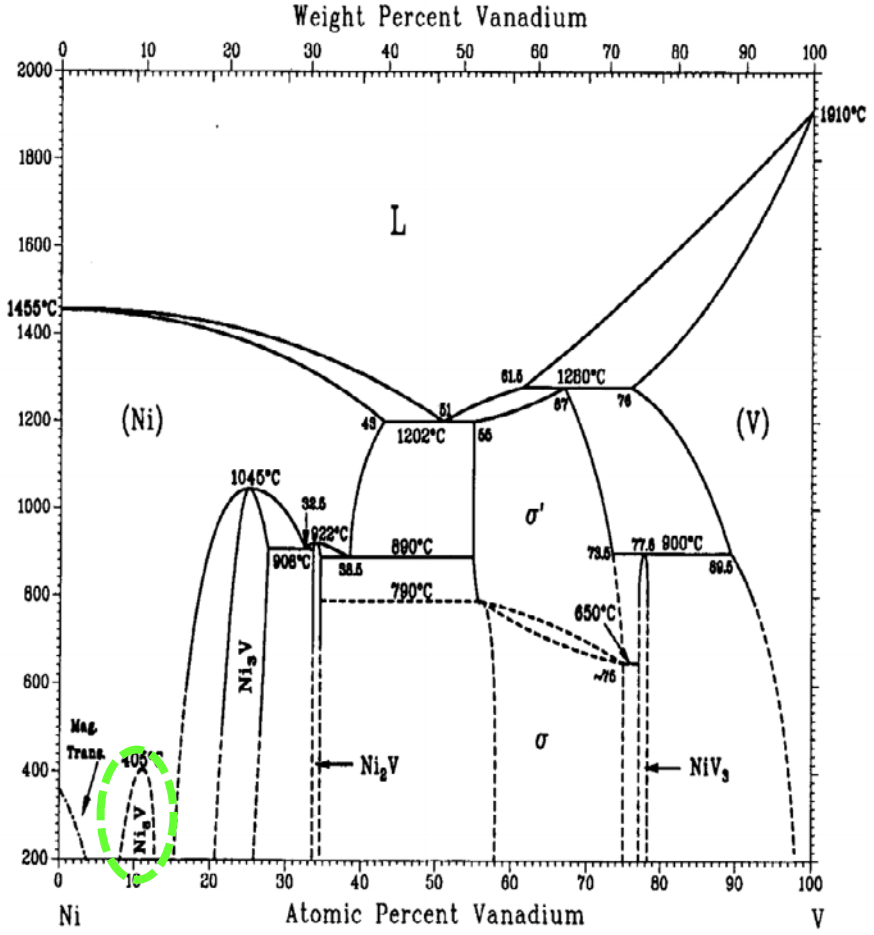



Pearson 1952
Stevens 1970
Khlomov 1978
Watson 1995
Moreen 1971
Liquid
fcc
bcc
σ
Ni3V
Ni2V
NiV3
Ni8V
Temperature (K)
2500
2000
1500
1000
500
0
0
0.2
0.4
0.6
0.8
1.0
Ni
V
Mole fraction V

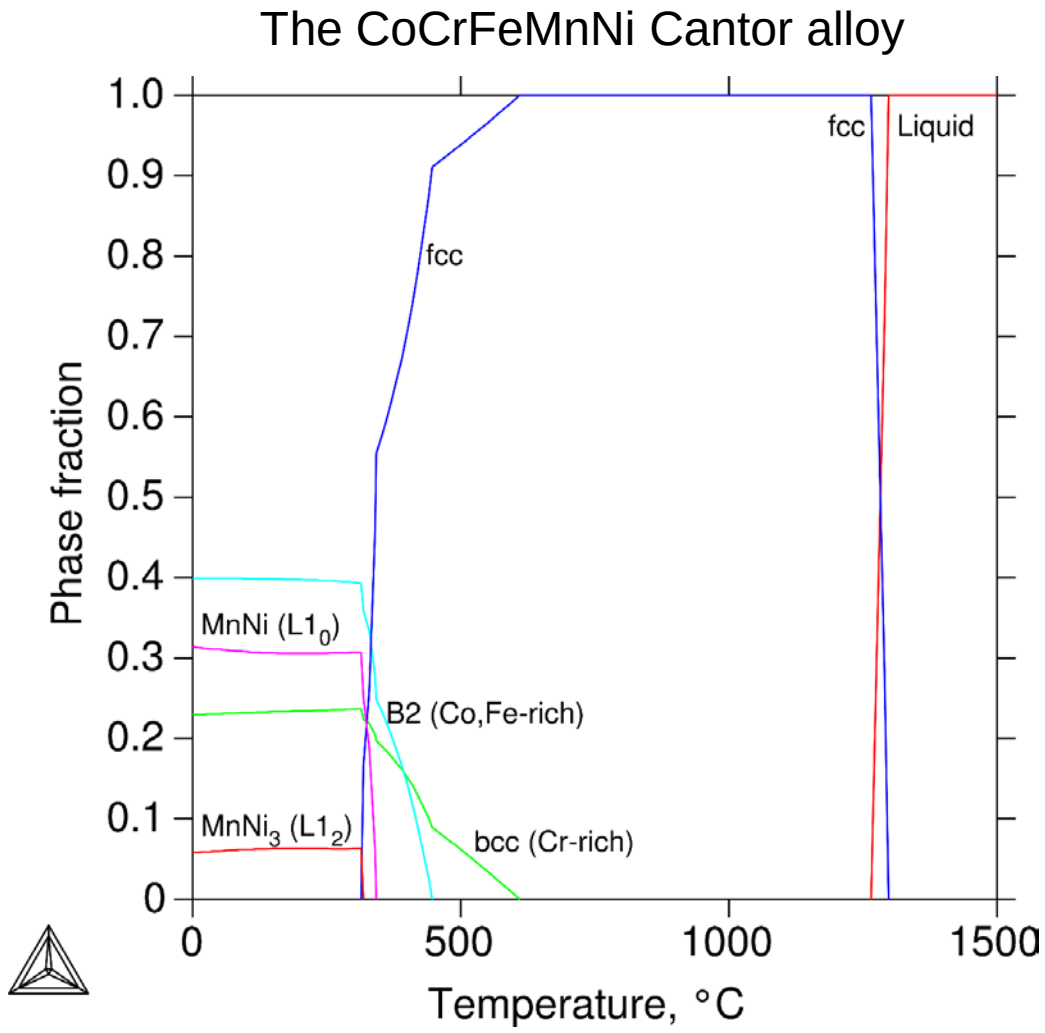
This work

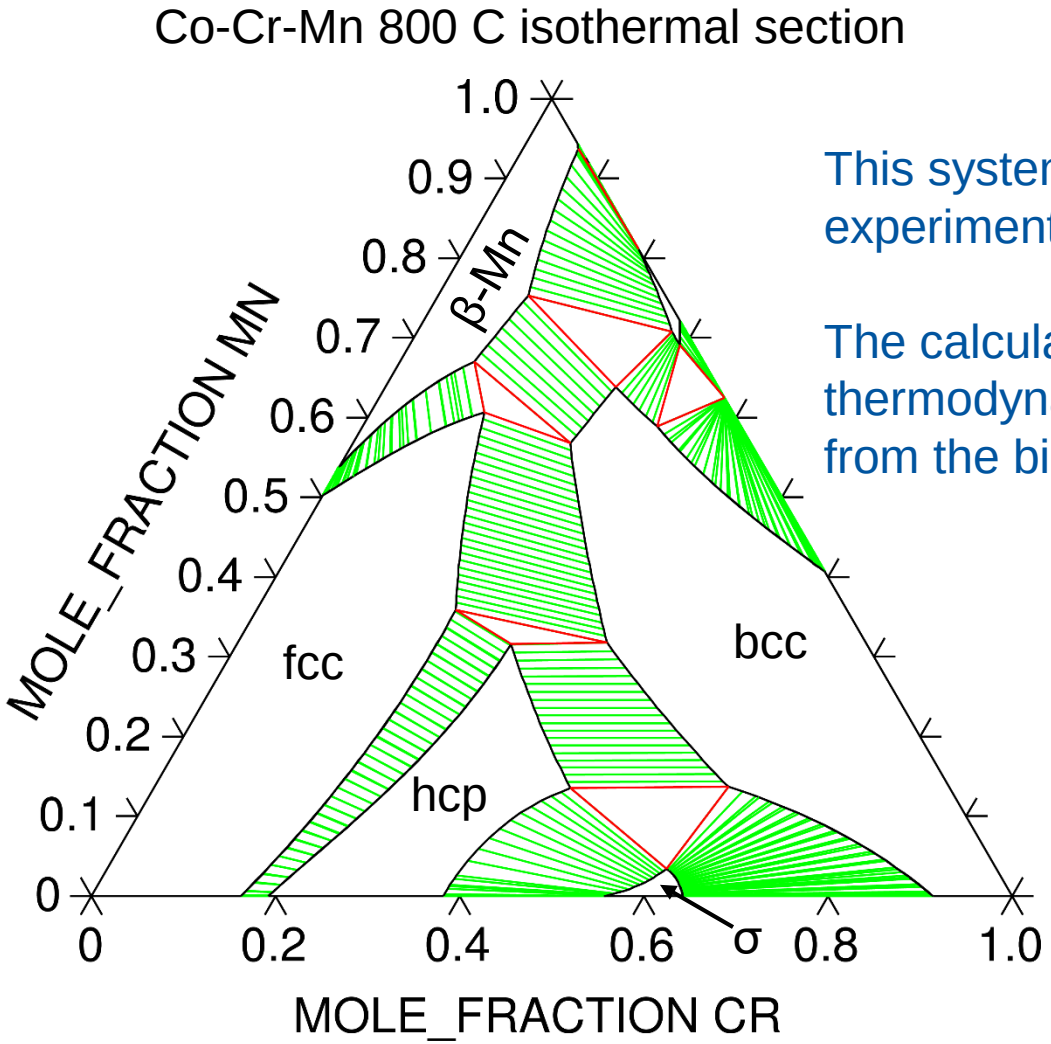
Smith 82





Future work


The CoCrFeMnNi Cantor alloy
Phase fraction
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
500
1000
1500
Temperature, °C
fcc
Liquid
fcc
MnNi (L1$_0$)
B2 (Co,Fe-rich)
MnNi$_3$ (L1$_2$)
bcc (Cr-rich)

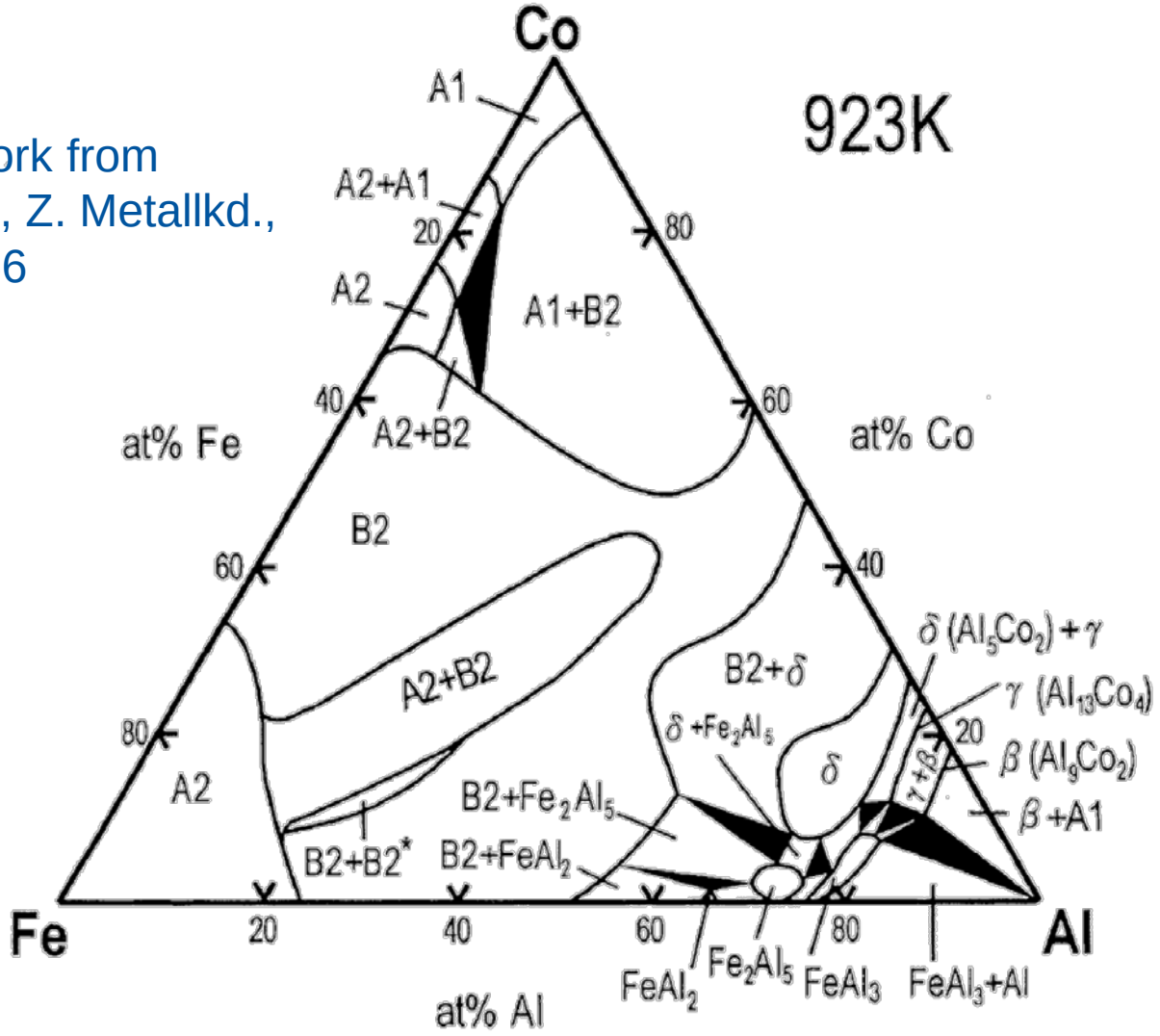


This system has not been experimentally investigated

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



Thank you for your attention!

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