Calphad modelling and databases for fcc-based MPEAs

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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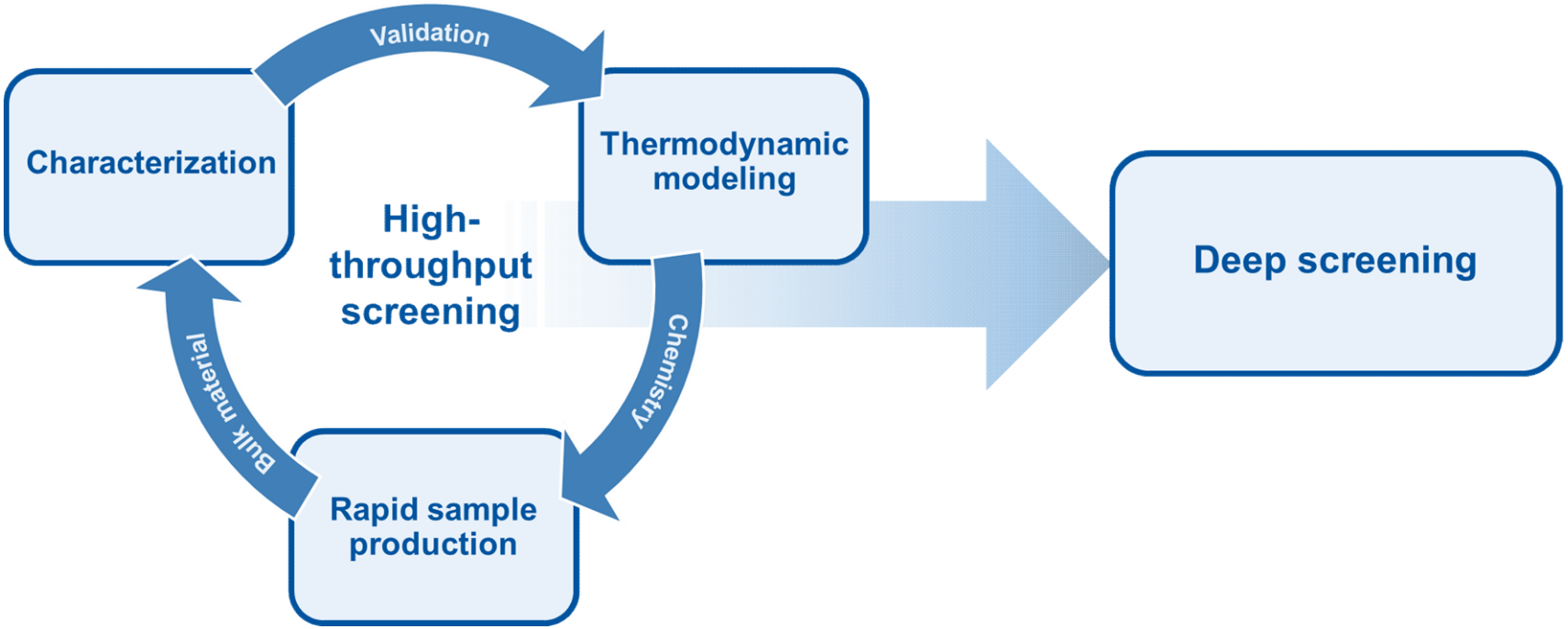
Outline

- Research topics in this project
- Calphad database for Co-Cr-Fe-Mn-Ni+Al,C
- A few comments on the Cantor alloy (CoCrFeMnNi)
- Ternary systems
- Alloy selection
- Conclusion

General strategy (complete project)



Research topics (work program)

- Database development
  - → Calphad database for Co-Cr-Fe-Mn-Ni-Al-C (a preliminary database has been constructed)
- Modelling of individual ternary systems
  - → Al-Co-Fe, Al-Co-Mn, Al-Mn-Ni
- Calphad calculations for selection of alloys and heat treatment
  - → Alloy selection
  - → Limits of fcc single phase region

General strategy, databases

Binary systems

+

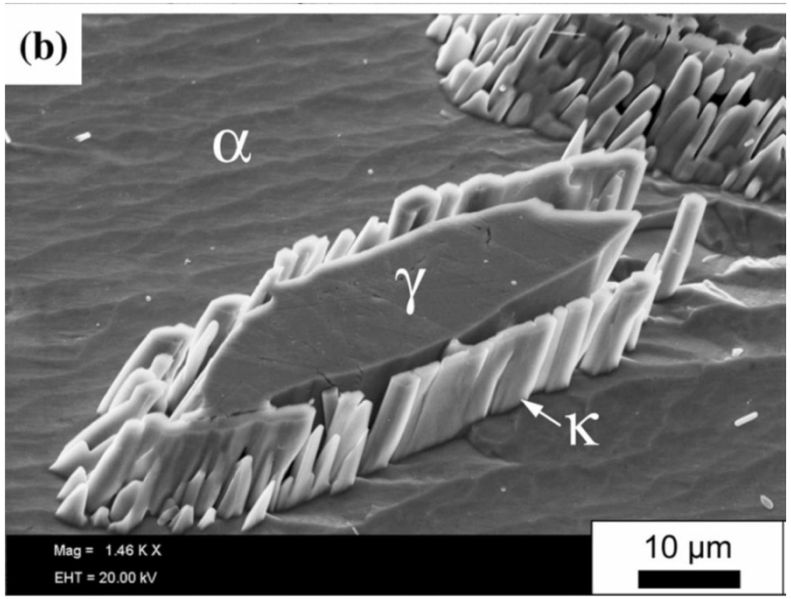
(Important)
Ternary systems

+

Extrapolations

=

Real alloys
(several elements)

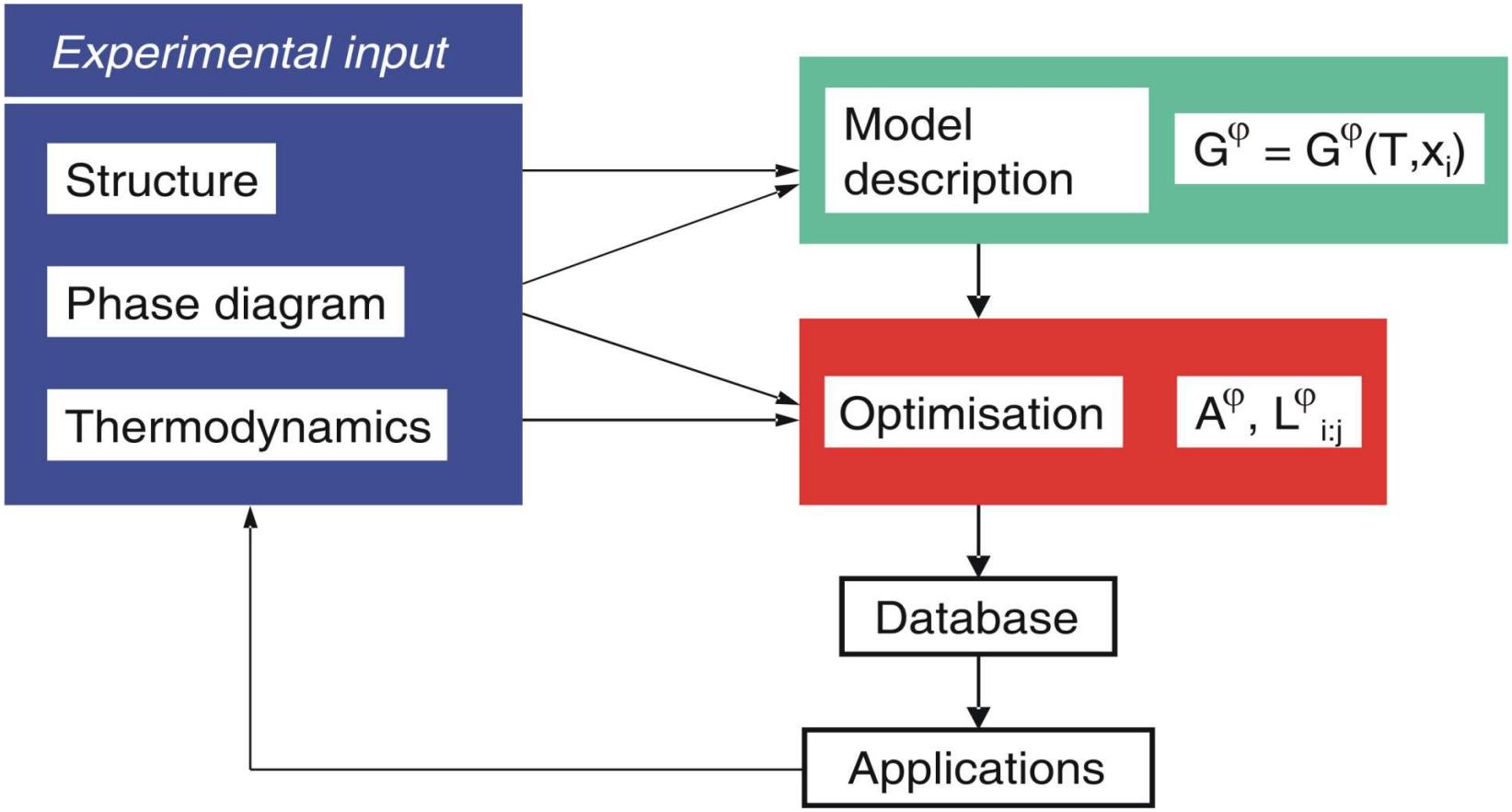


Fe-2%Mn-8%Al-0.2%C, cooling 10K/s from 1400 C, quenched from 870 C.

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 Calphad method

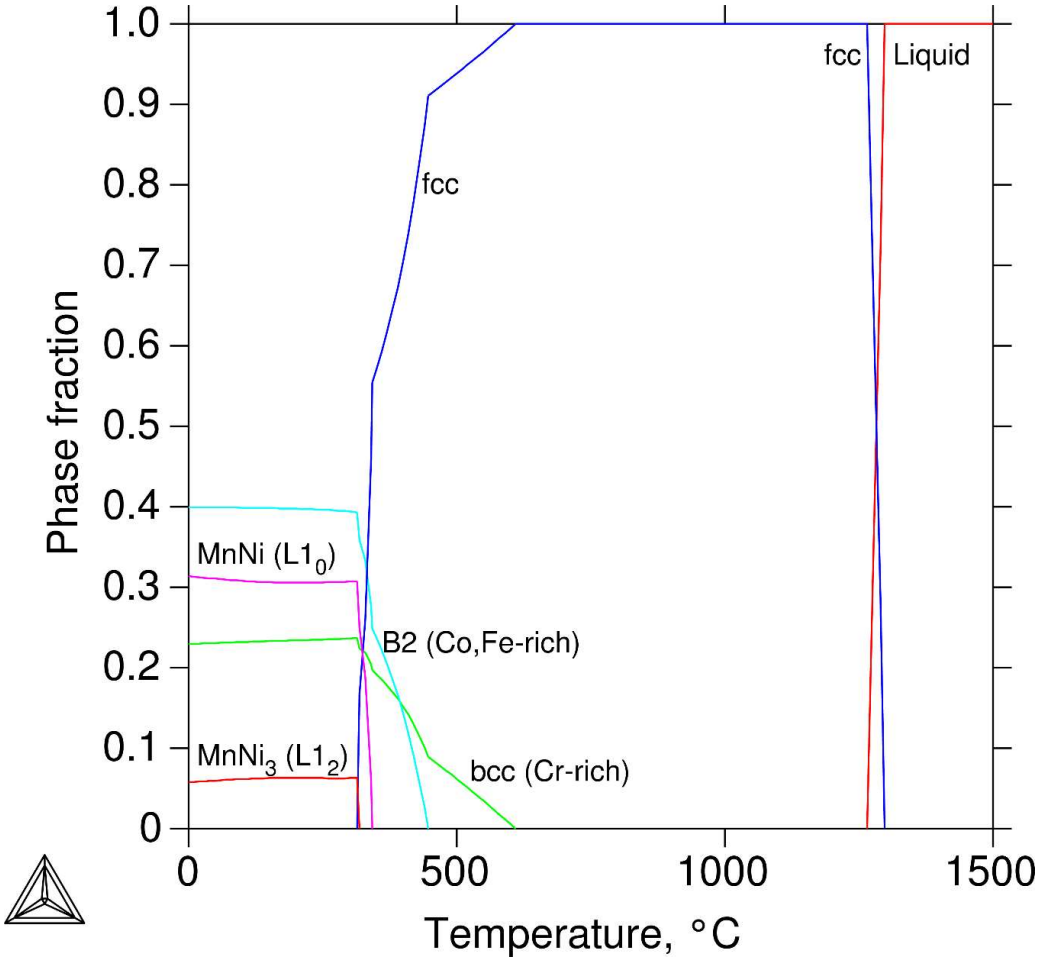


Thermodynamic database

- Elements: Co-Cr-Fe-Mn-Ni-Al-C
- All 21 binary systems included
- 28 ternary systems of 35 possible are included, but several are based on very scant experimental information
- The ternary systems Al-Co-Fe, Al-Co-Mn, Al-Cr-Fe, Al-Cr-Mn, Al-Mn-Ni, Co-Mn-C and Mn-Ni-C are not yet modelled

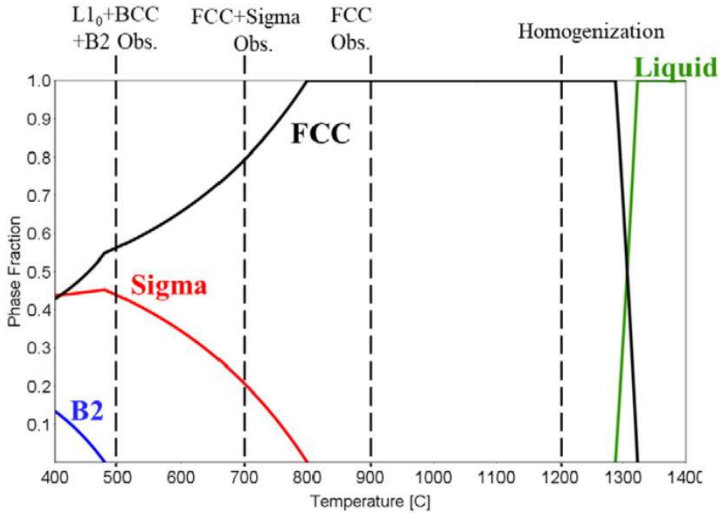
  → Systems in green are planned for modelling within this project

The CoCrFeMnNi Cantor alloy



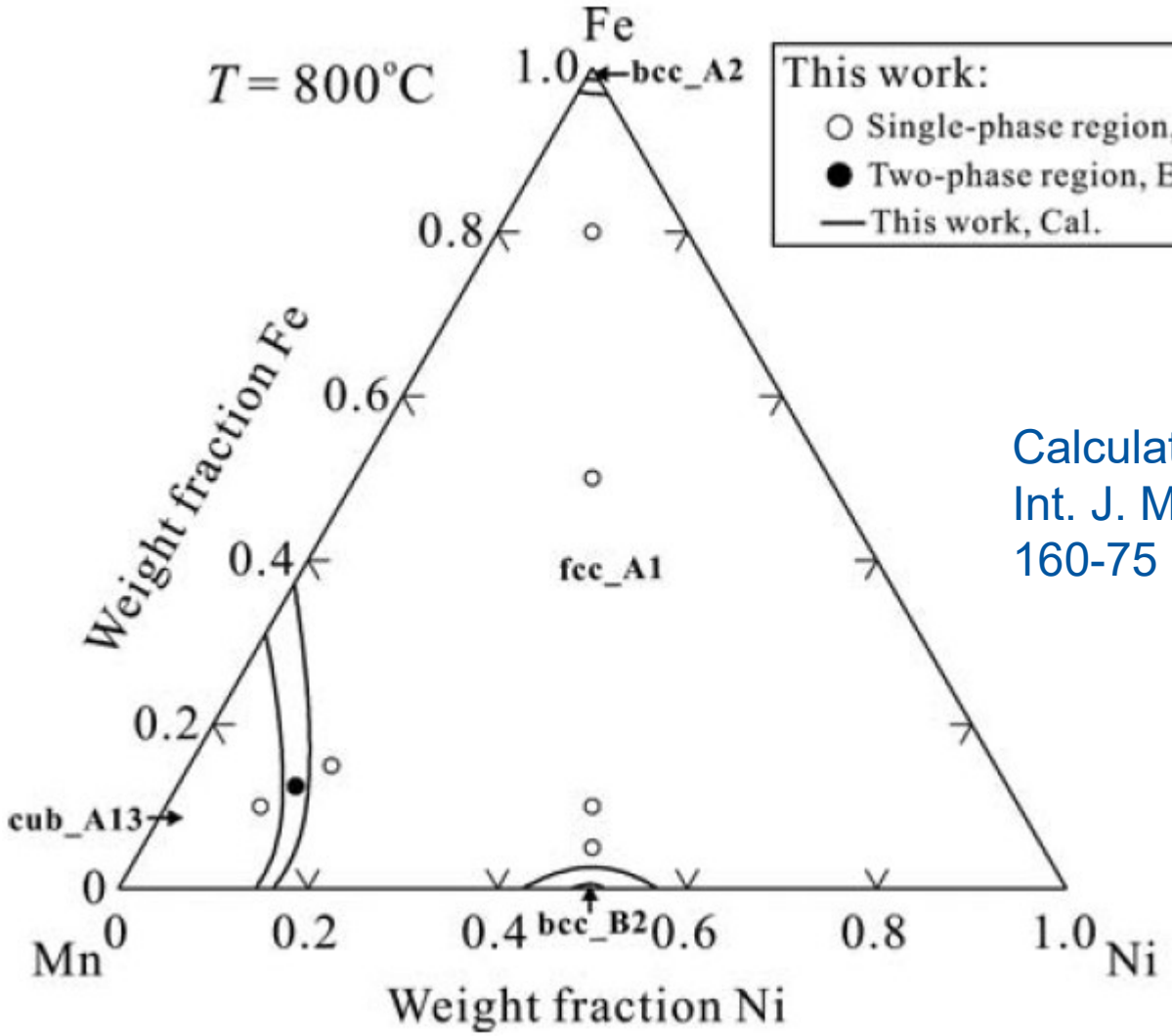
Observations by F. Otto et al., Acta Mater., 112 (2016) 40-52:

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



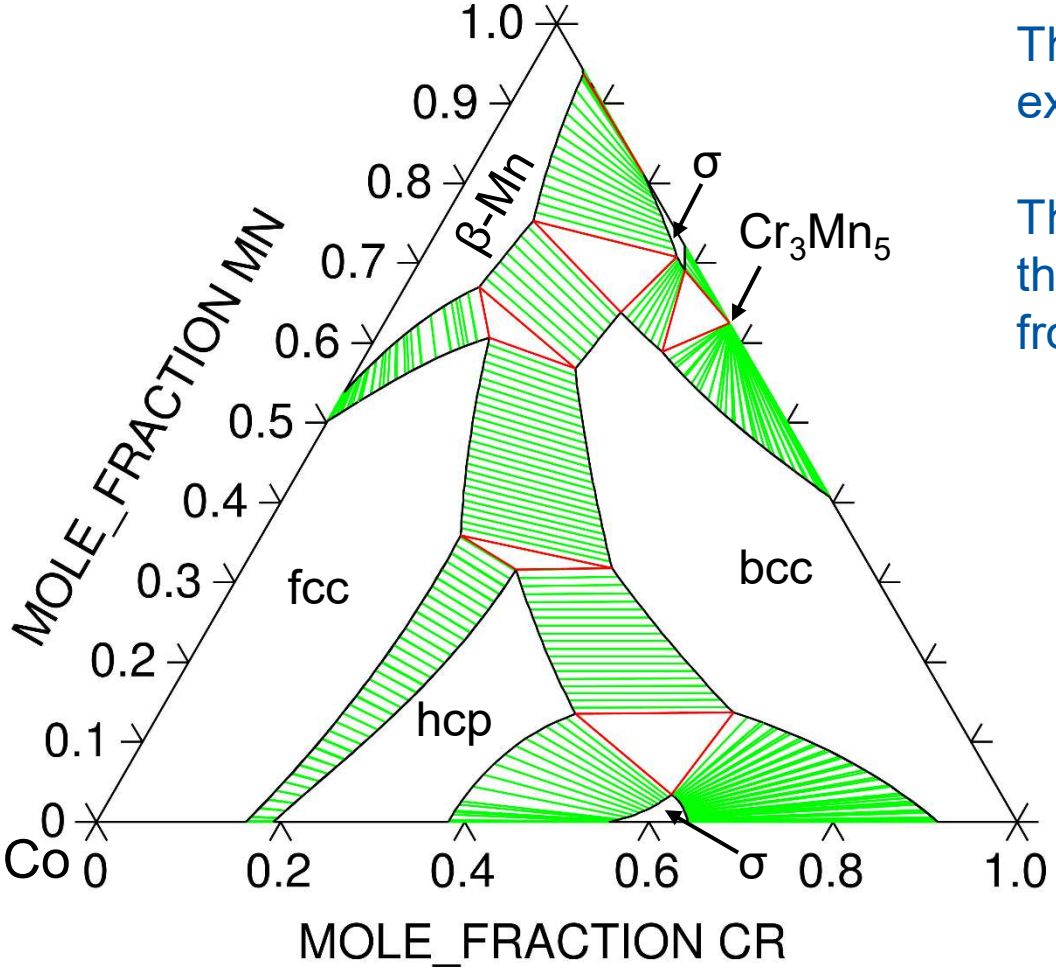
Calculation with TCHEA2 by J.E. Saal et al., Scripta Mater., 146 (2018) 5-8

Fe-Mn-Ni 800 C isothermal section



Calculation from L. Zhang et al., Int. J. Mater. Res., 100 (2009) 160-75

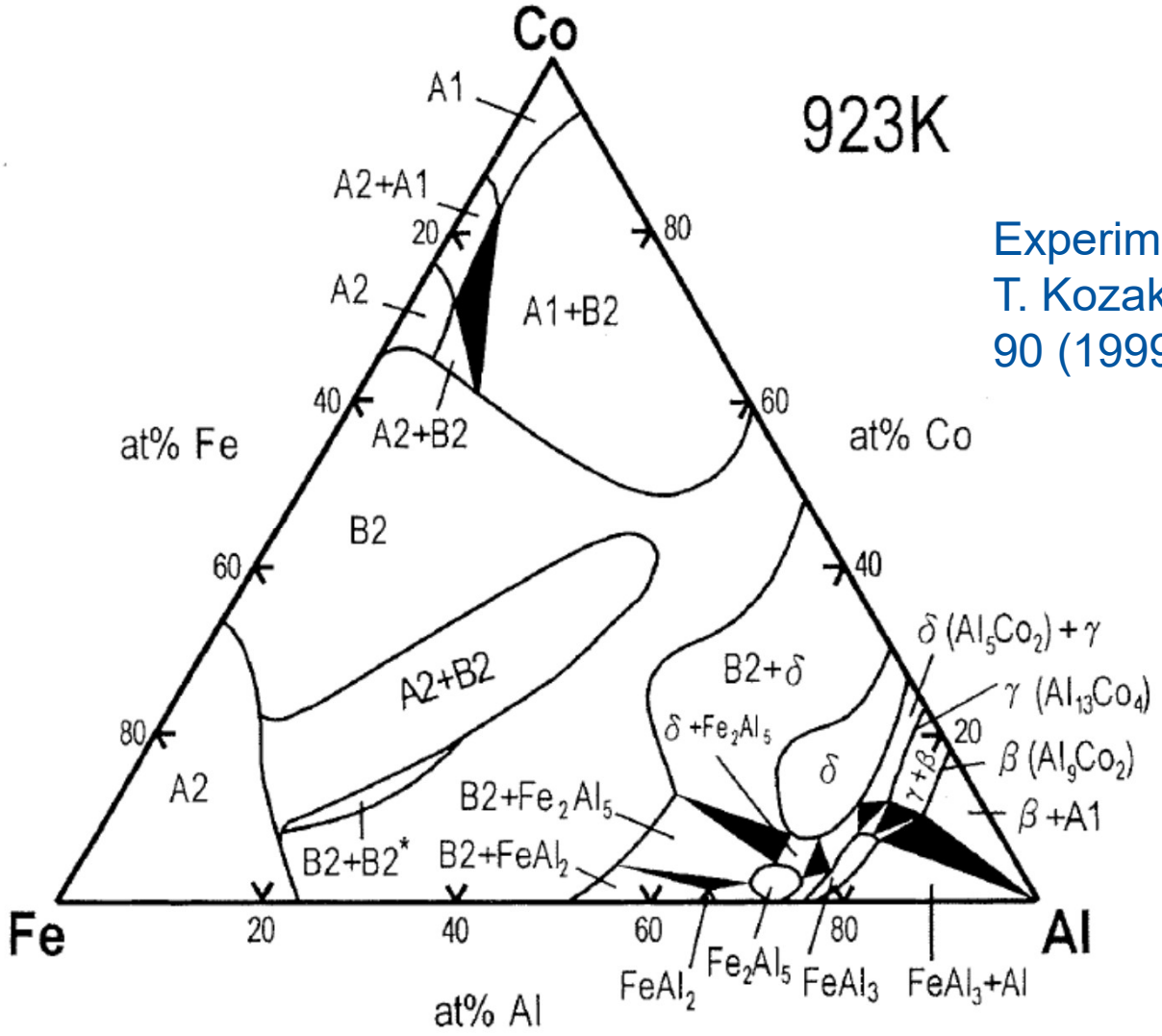
Co-Cr-Mn 800 C isothermal section



This system has not been experimentally investigated

The calculation is a thermodynamic extrapolation from the binaries

Al-Co-Fe 650 C isothermal section

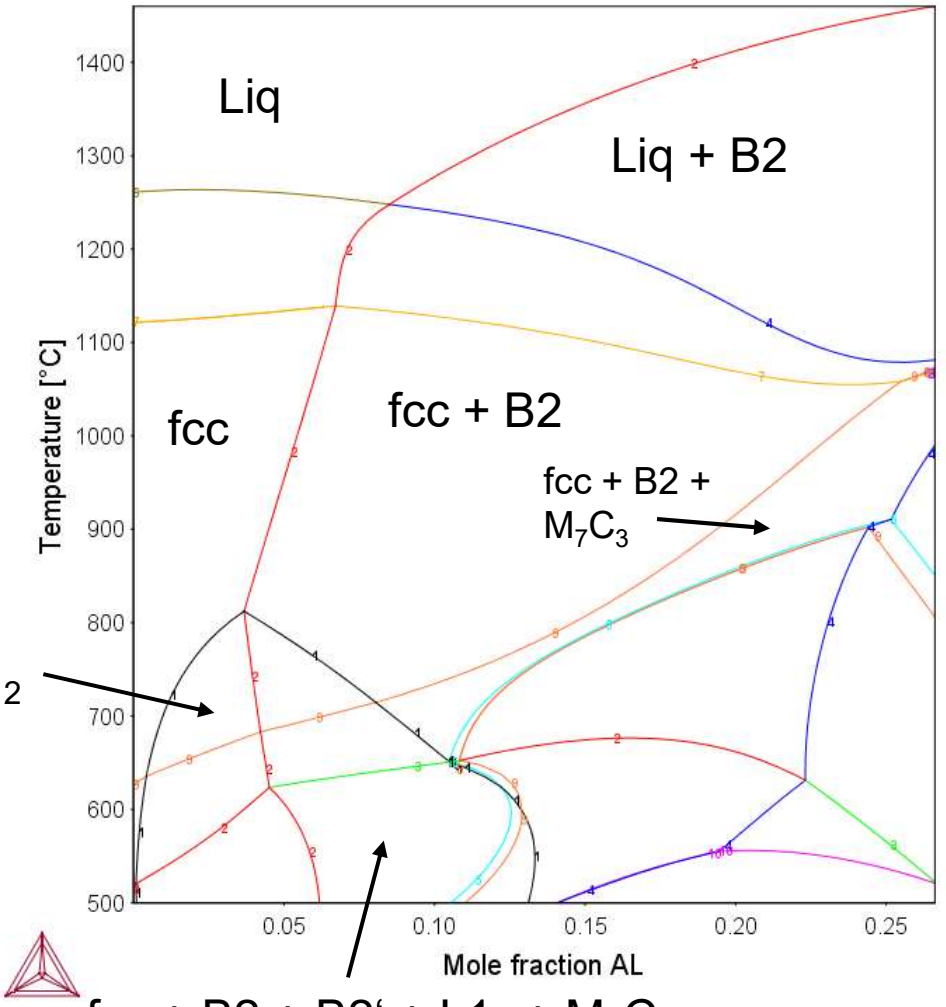


Experimental work from
T. Kozakai et al., Z. Metallkd., 90 (1999) 261-66

Alloy selection

CoFeMnNi-Al
with 0.6 wt.% C

B2 is “NiAl” at high T
(closer to “MnNi” at low T)
B2’ is “CoFe”
$L1_2$ is “Ni3Al”
M_7C_3 is Mn-rich



Conclusion

- Construction of Calphad databases for MPEAs is challenging
  - → All elements are equally important: All ternaries needed
  - → Many ordered phases at low temperature: Difficult to model (and sometimes to calculate)
- We have a preliminary database for Co-Cr-Fe-Mn-Ni-Al-C
- There is a great potential to find precipitation hardening and other multiphase alloys within this system
- However, many of these alloys will be brittle
- Alloy selection and processing is highly non-trivial

Thank you for your attention!

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