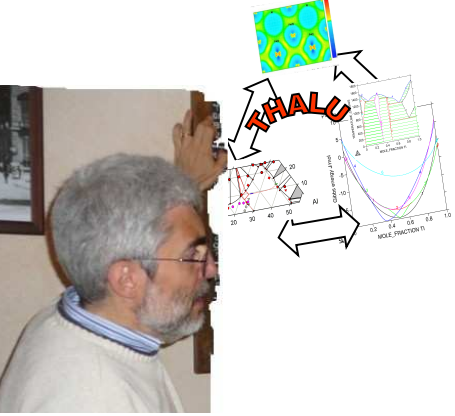


Gabriele Cacciamani
Dipartimento di Chimica e Chimica Industriale, via Dodecaneso 31, I-16146 Genova, Italy



Suzana G. Fries
SGF Scientific Consultancy Aachen, Germany



Jozefien De Keyzer
MTM, KULeuven, Kasteelpark Arenber 44, B-3001 Heverlee,Belgium



Nathalie Dupin
Calcul Thermodynamique 3 rue de l'avenir F-63670 Orcet, France



Bo Sundman
CIRIMAT, ENSIACET, F-31077 Toulouse, cedex 4, France

FCC, BCC AND HCP BASED BINARY PHASE DIAGRAMS IN THE AL-FE-NI-TI COST535 SYSTEM AND THEIR EXTRAPOLATION INTO TERNARY : A CALPHAD-FIRST-PRINCIPLES STUDY



Look the mountains below

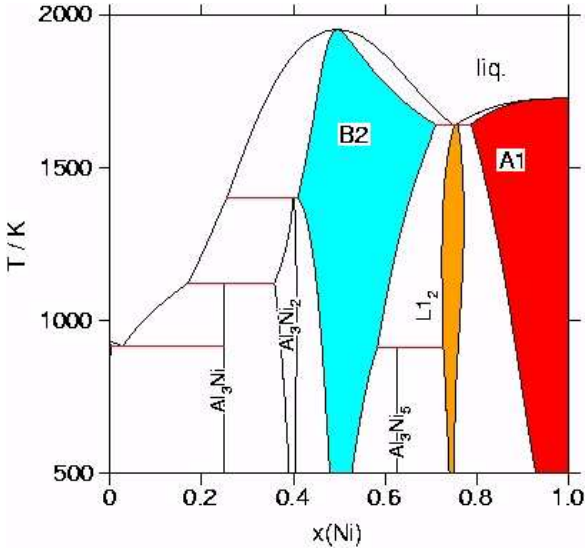


What is under the fog?



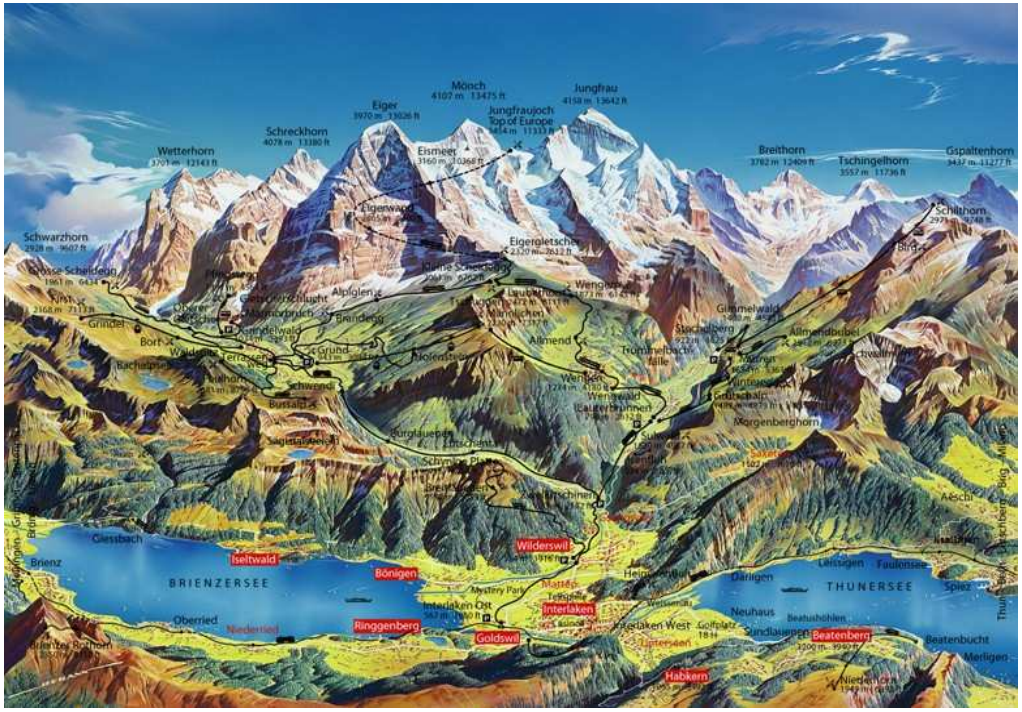
What is behind a phase diagram?

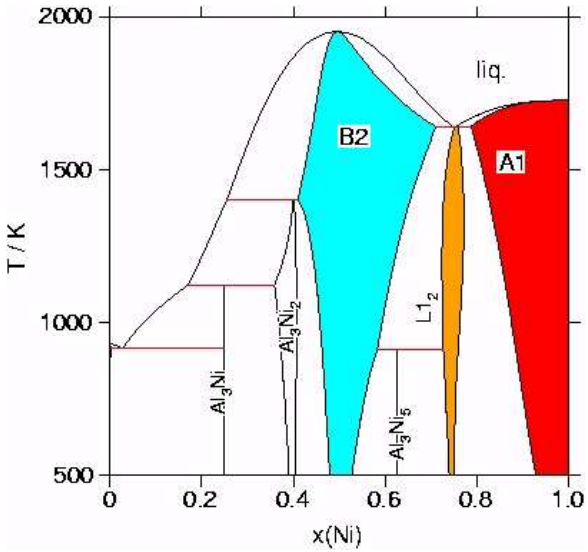


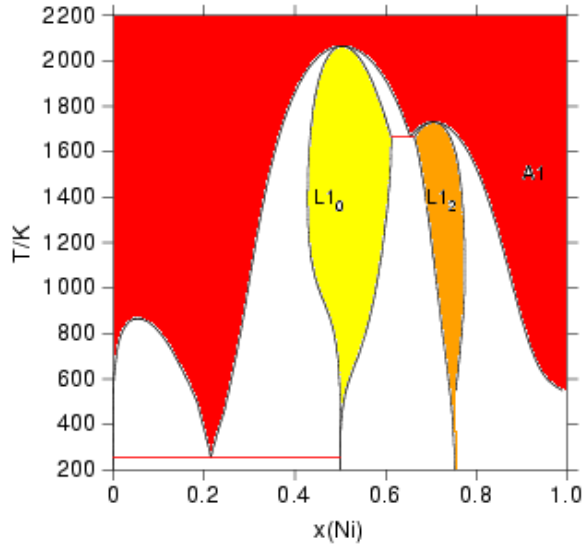


What is behind a phase diagram?



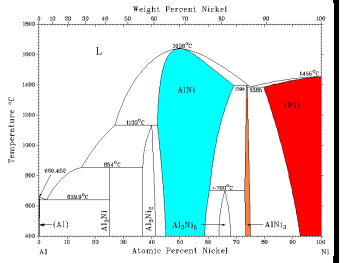
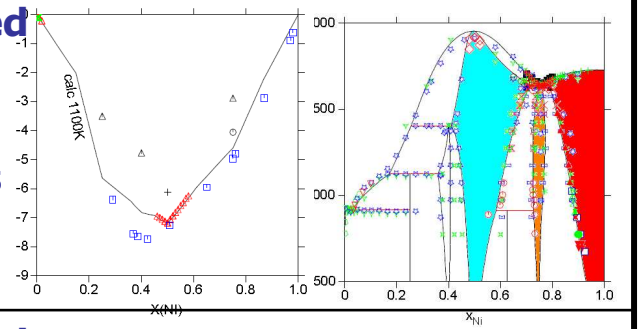
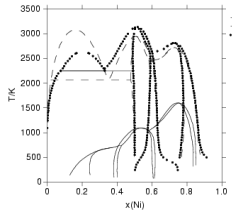
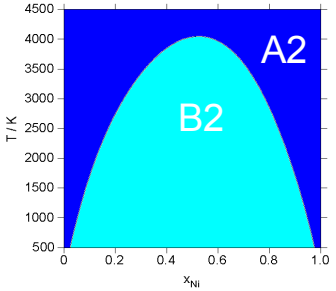
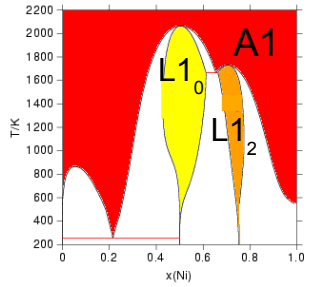




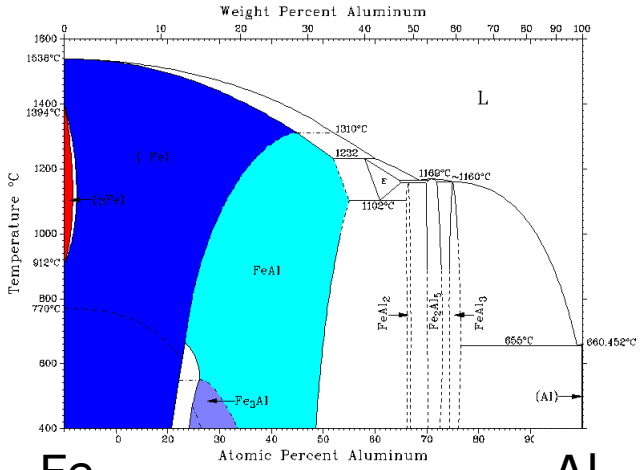


Metastable states (CALPHAD $^{++}$)

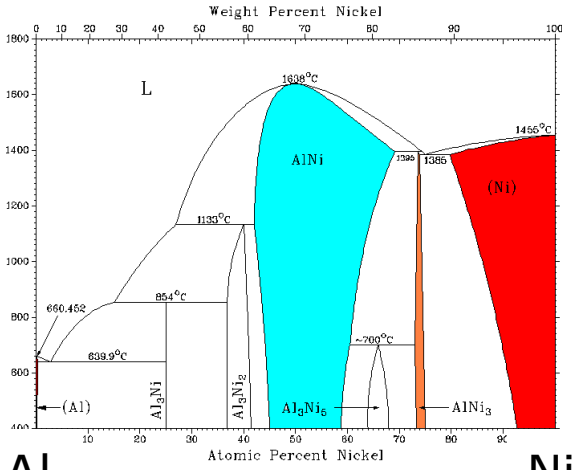
Assessments evolution

Massalki	**Experimental** Phase diagram	Zeroth Critical evaluation		**Drawn** phase diagrams 
Calphad	**Experimental and theoretical** **Phase diagram** Enthalpies Entropies …	**Zeroth Critical evaluation** **Optimiser**	**Modelled Gibbs energy**	**Calculated** phase diagrams enthalpies entropies … 
Calphad ++	**Experimental and theoretical** **Phase diagram** **Enthalpies** **Entropies** Order disorder topology from first principles 	**Zeroth Critical evaluation** **Optimiser**	**Modelled Gibbs energy** Phases modelled by families based in the parent sublattices **fcc** **bcc** **hcp**	**Calculated** phase diagrams enthalpies entropies… metastable regions  

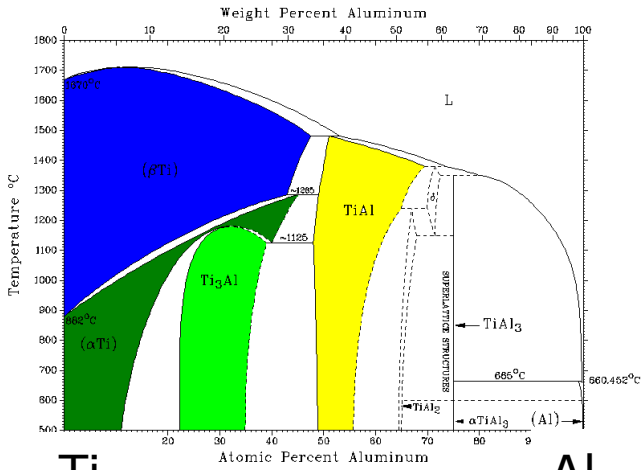
Drawn binary systems



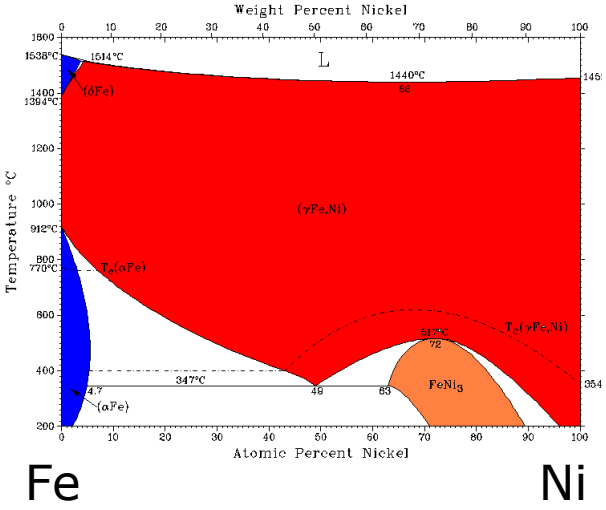
Fe Al



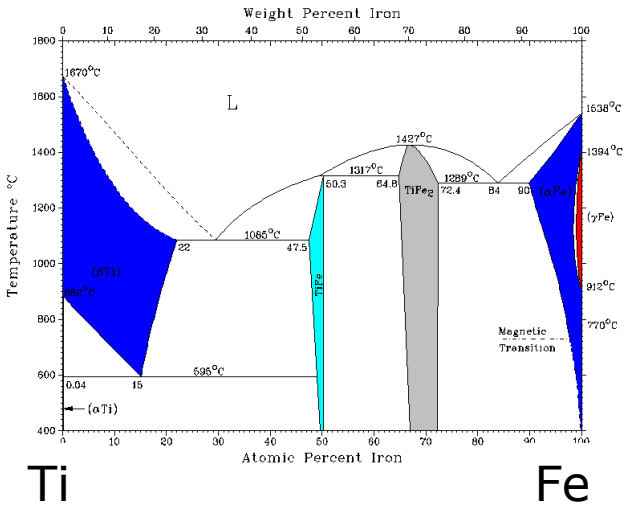
Al Ni



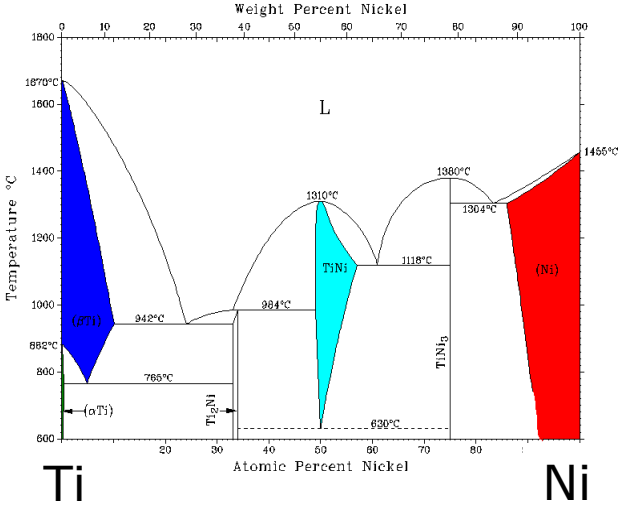
Ti Al



Fe Ni



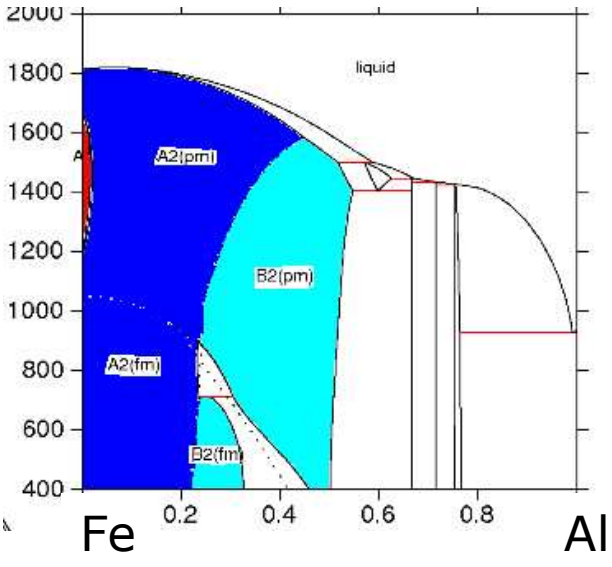
Ti Fe

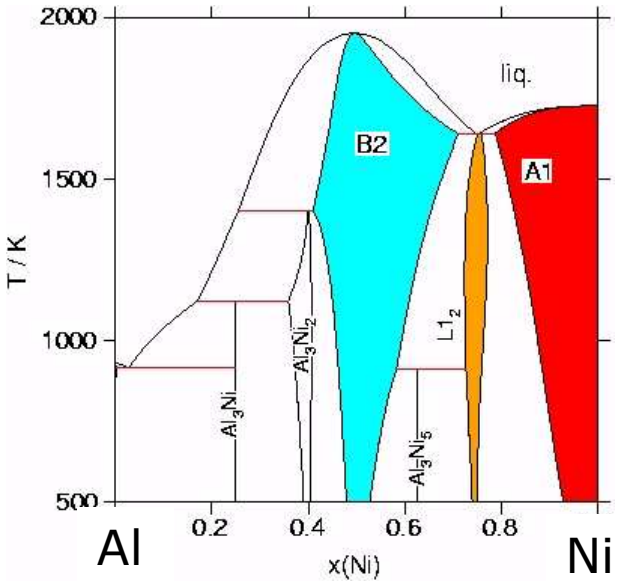


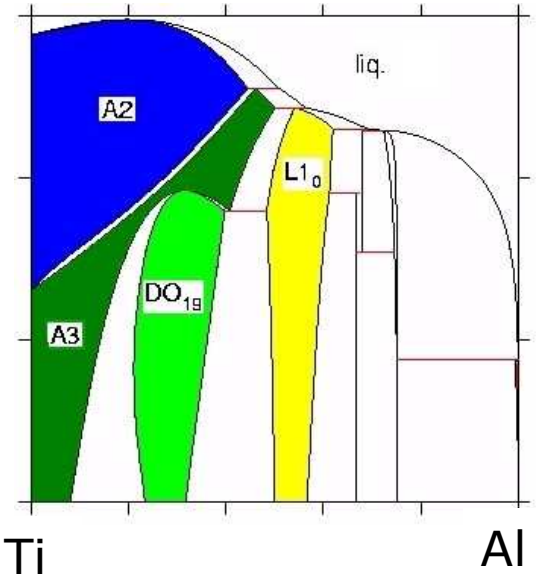
Ti Ni

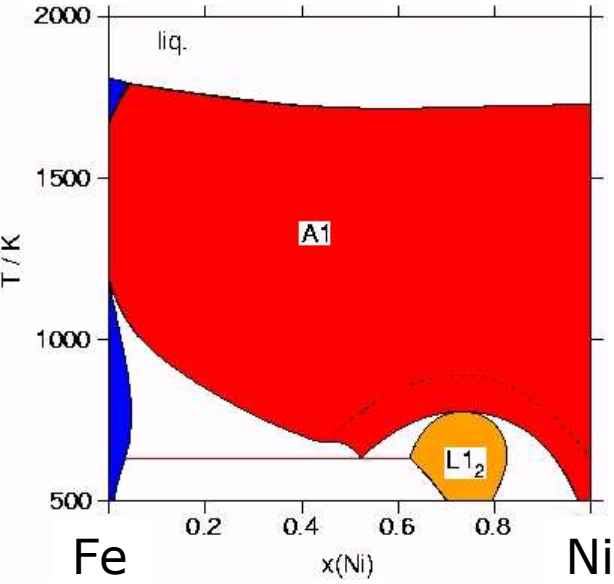
Phases are colored by crystal structure families

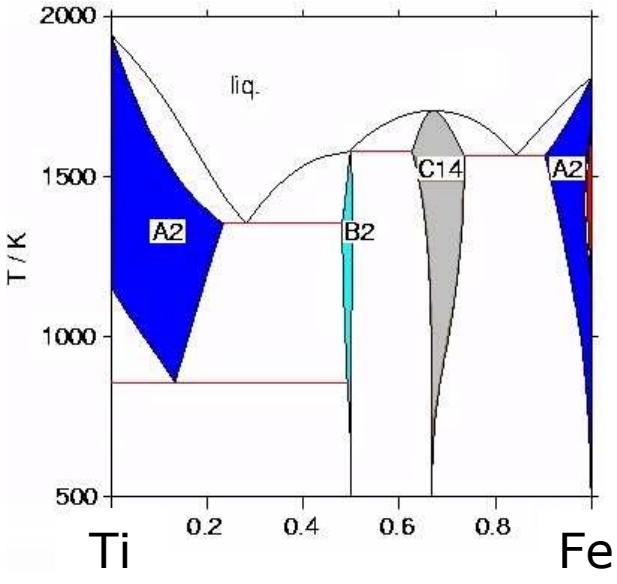
Calculated Binary Systems : Status 2003

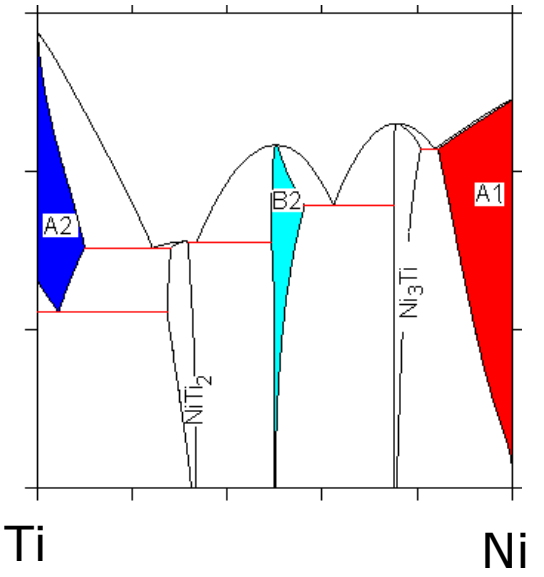




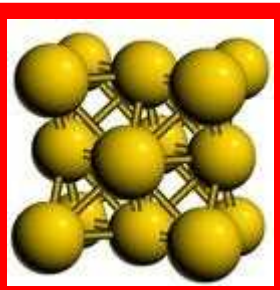


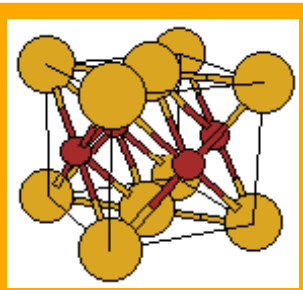


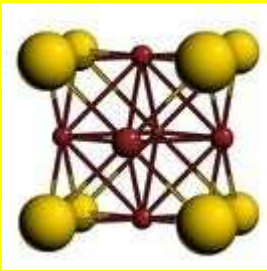


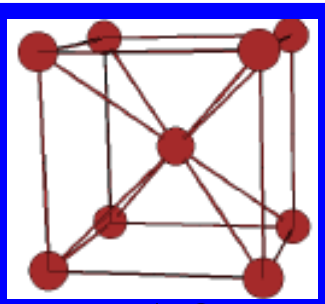


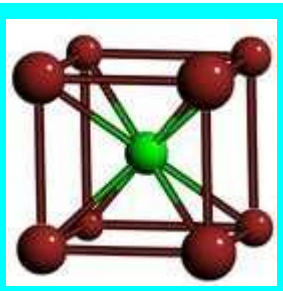
The fcc, bcc and hcp families

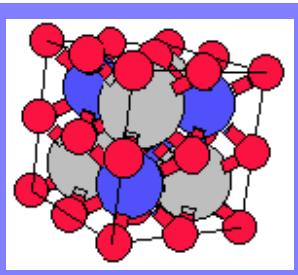

A1

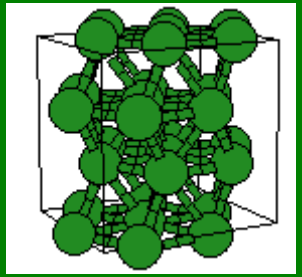

$L1_0$

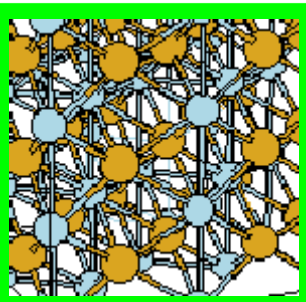

$L1_2$

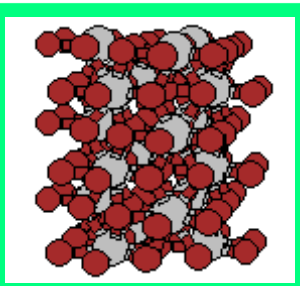

A2


B2


$L2_1$

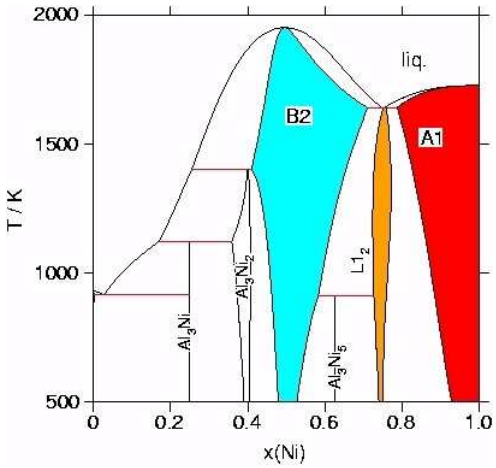

A3


B19

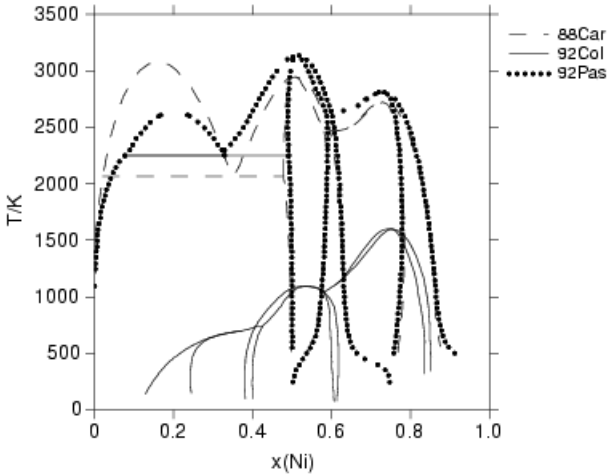

$D0_{19}$

fcc Al-Ni

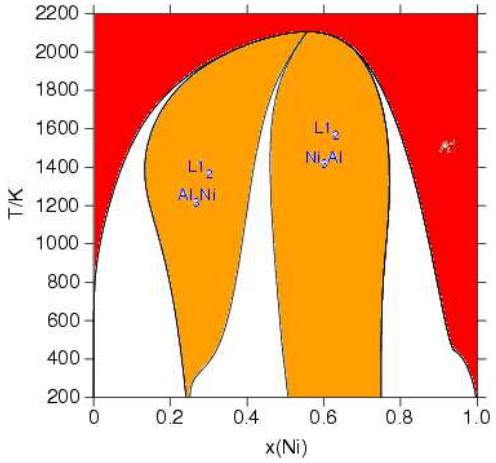
stable Ansara et al.



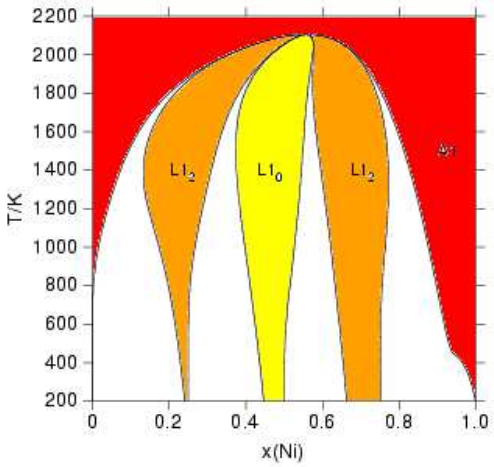
metastable, first-principles



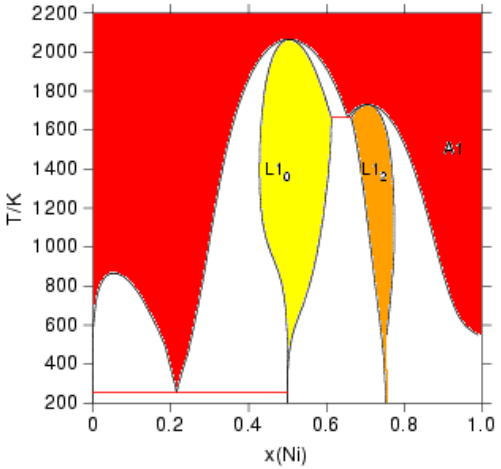
2SL : $(Al,Ni)_3$ (Al,Ni)



4SL : (Al,Ni) (Al,Ni) (Al,Ni) (Al,Ni)



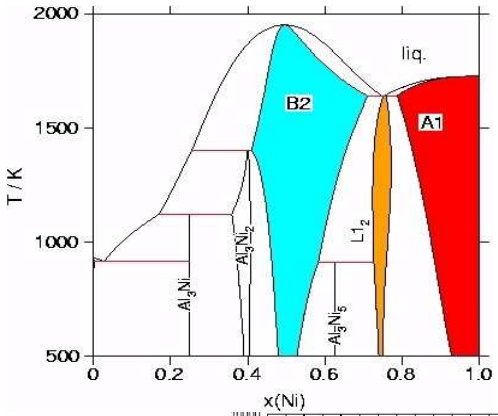
without $L_{Al,Ni:Al,Ni:*:*}$



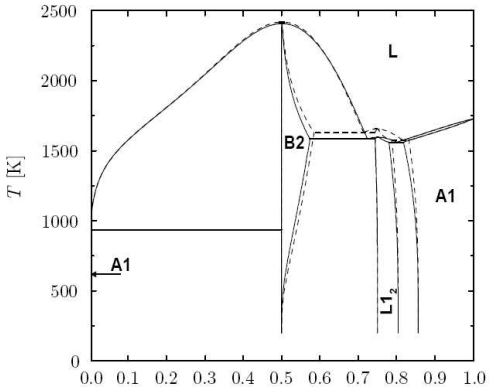
2003, with $L_{Al,Ni:Al,Ni:*:*}$

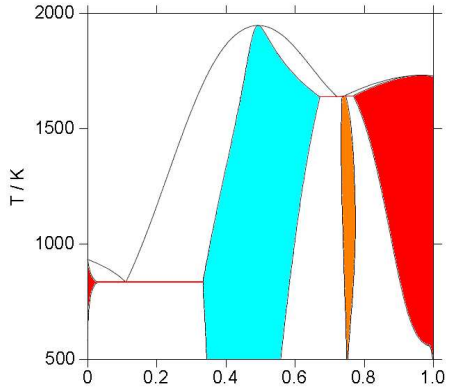
Al-Ni

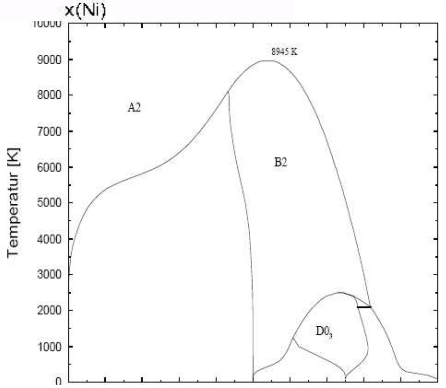
stable Ansara et al.

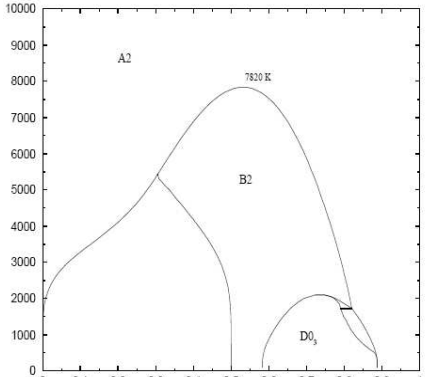


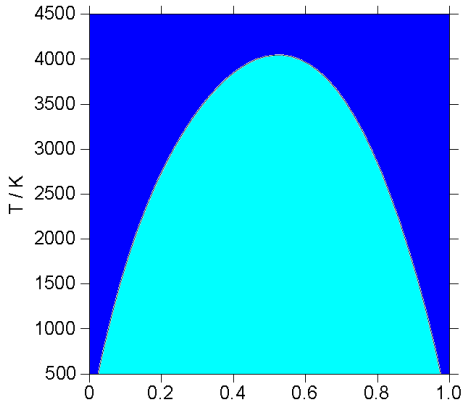
2003 Lechermann

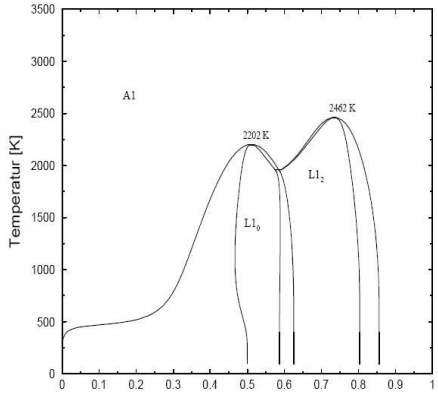


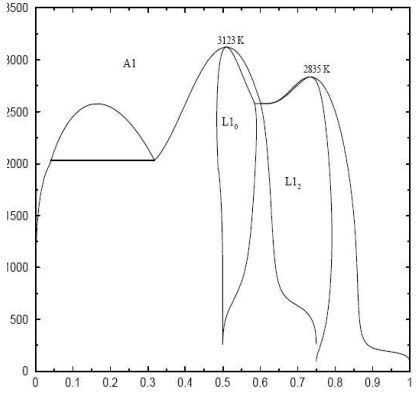


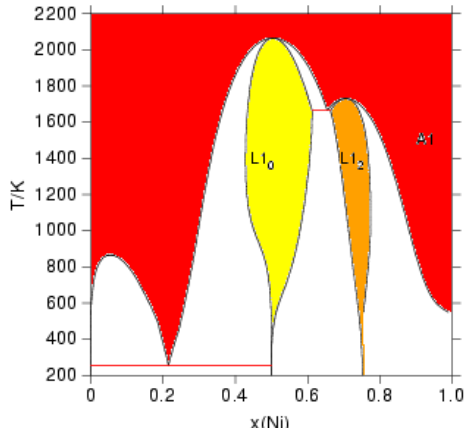






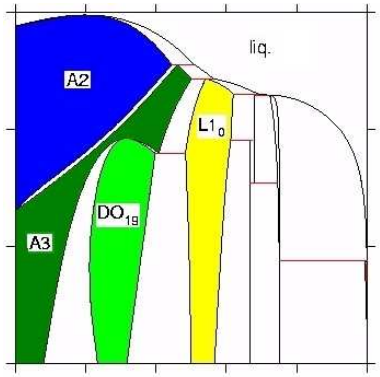




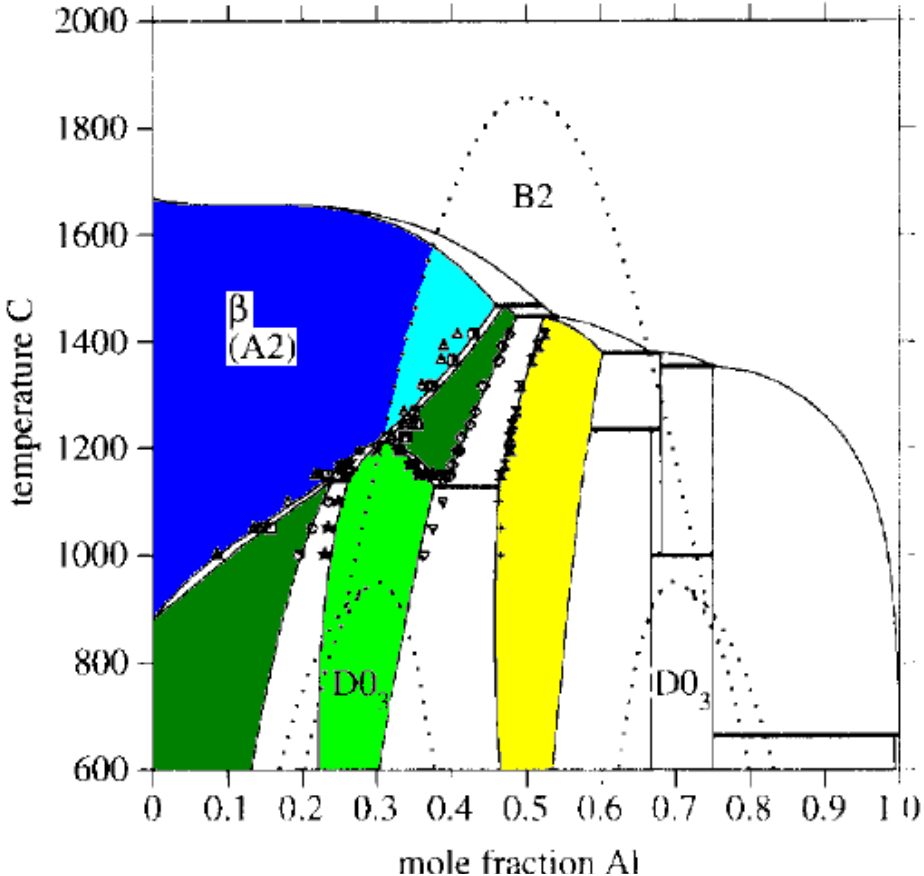


Al-Ti

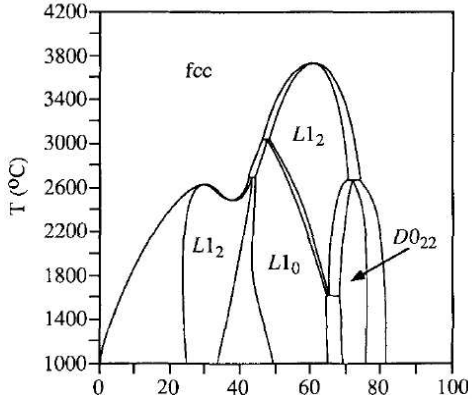
Saunders stable

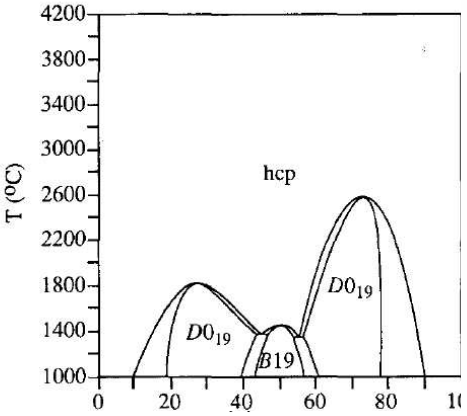


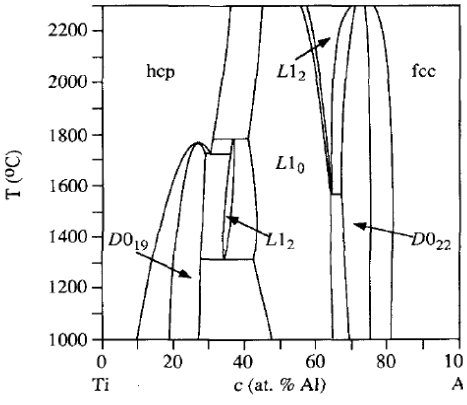
Ohnuma, Schoen



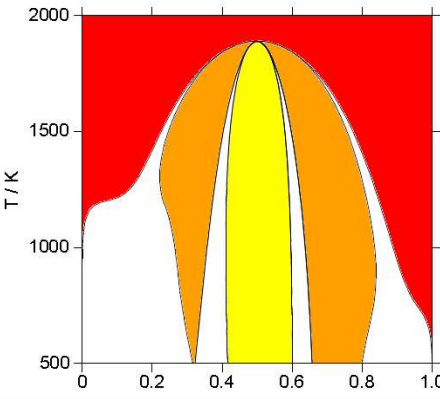
Mark Asta

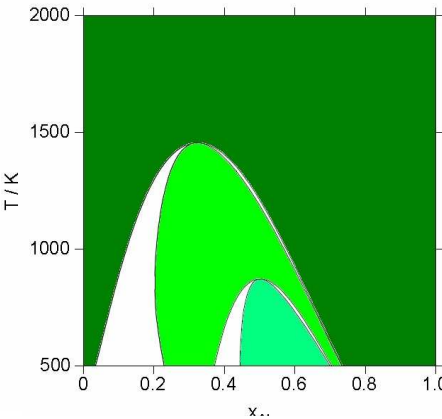


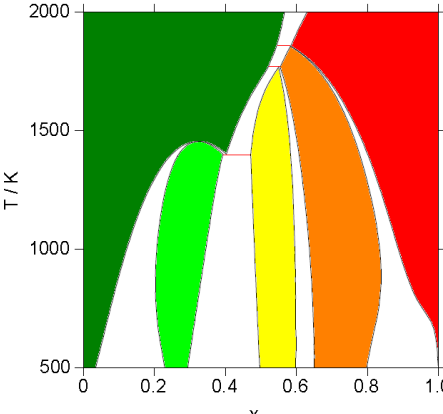




Ohnuma, metastable

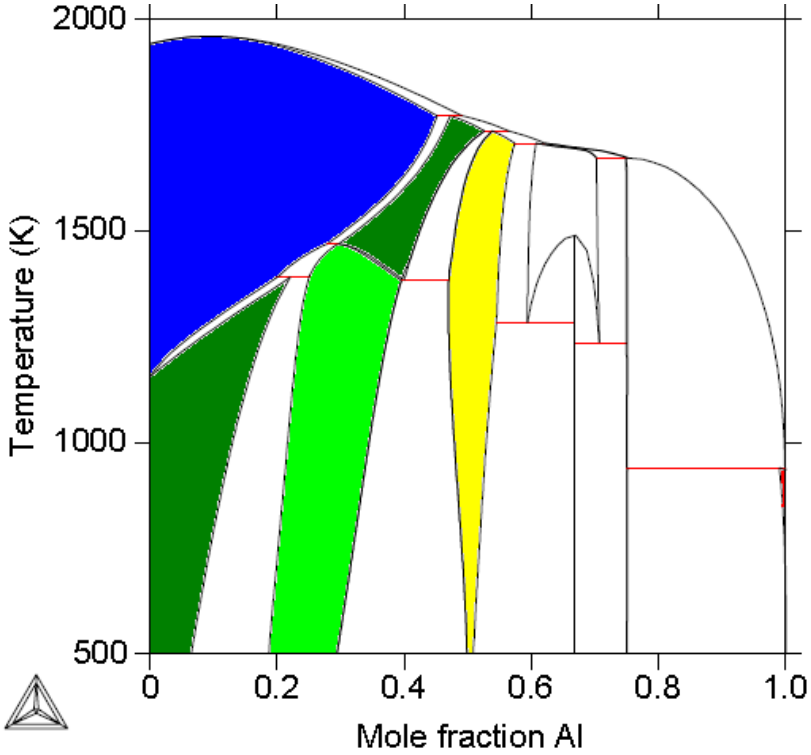


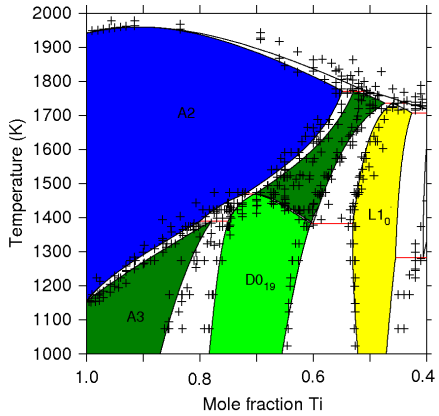


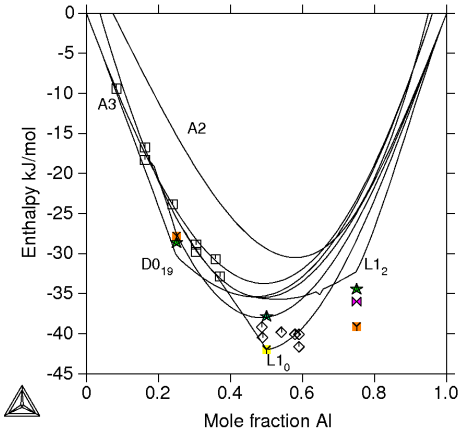


Al-Ti

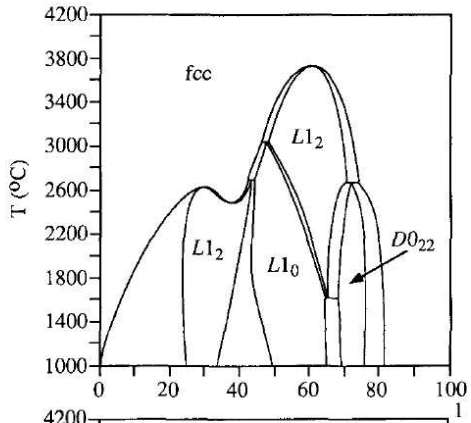
Sundman

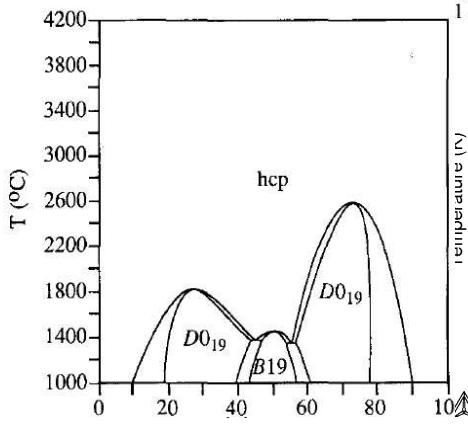


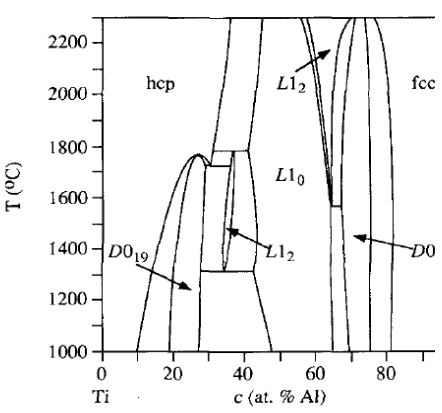




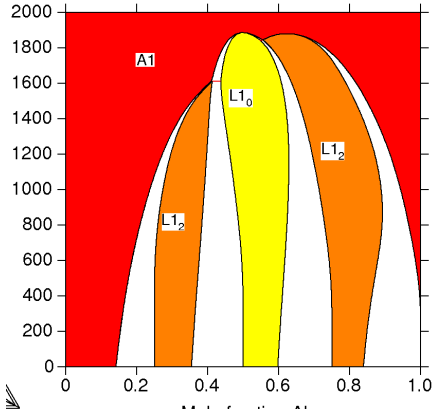
Mark Asta

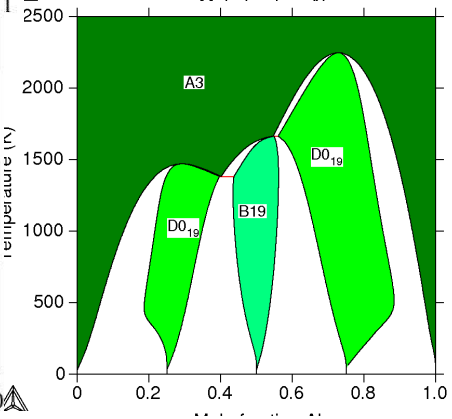


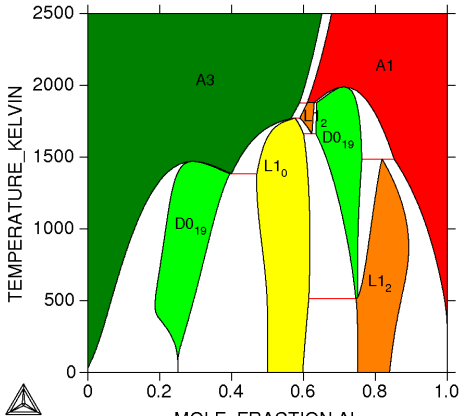




2007,Sundman

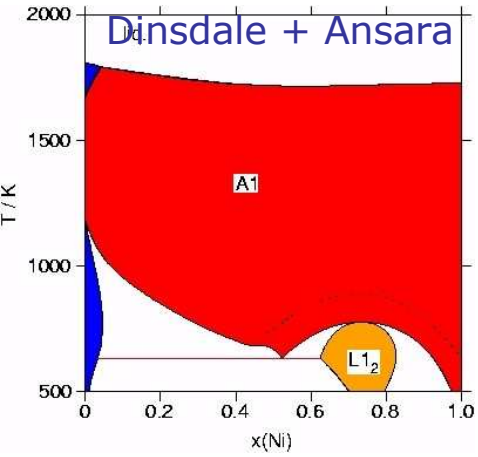




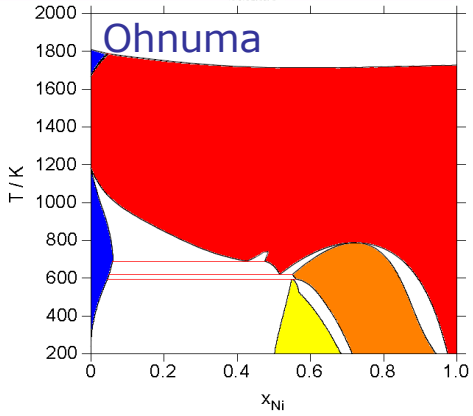


Fe-Ni

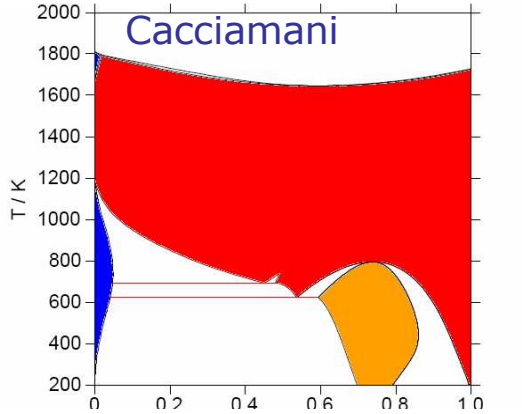
Dinsdale + Ansara



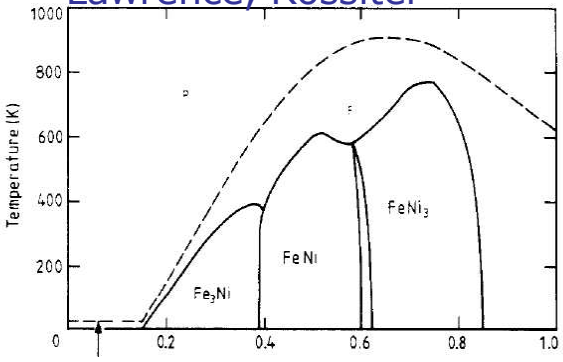
Ohnuma



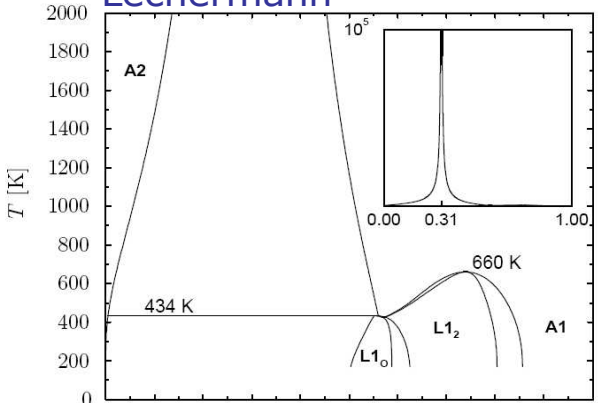
Cacciamani

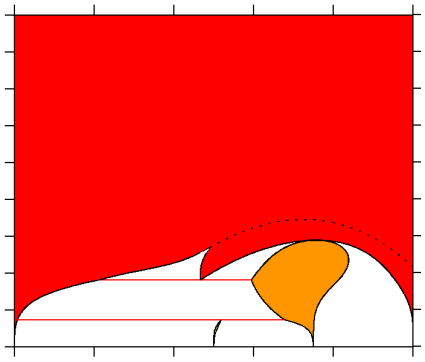


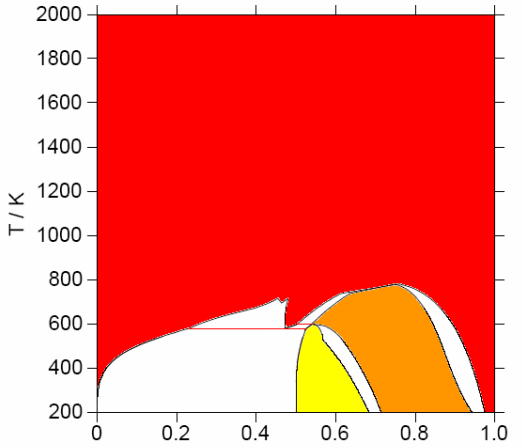
Lawrence, Rossiter

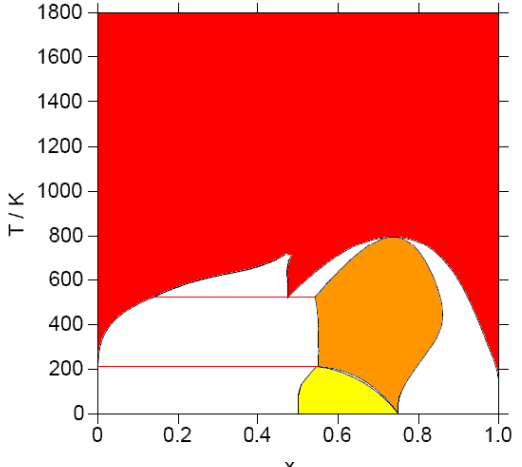


Lechermann



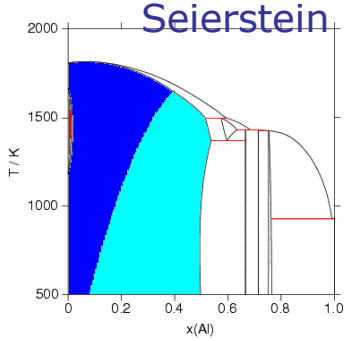




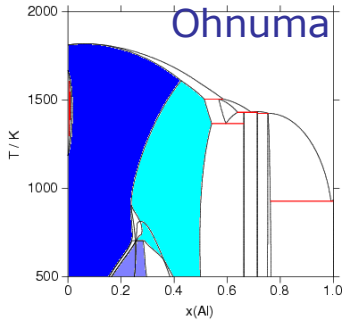


Al-Fe

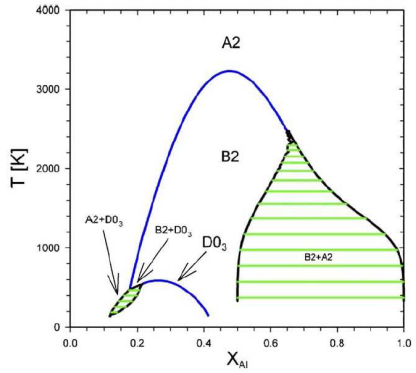
Seierstein

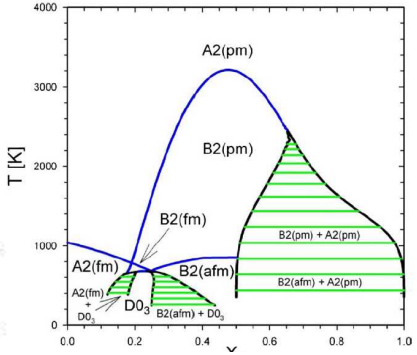


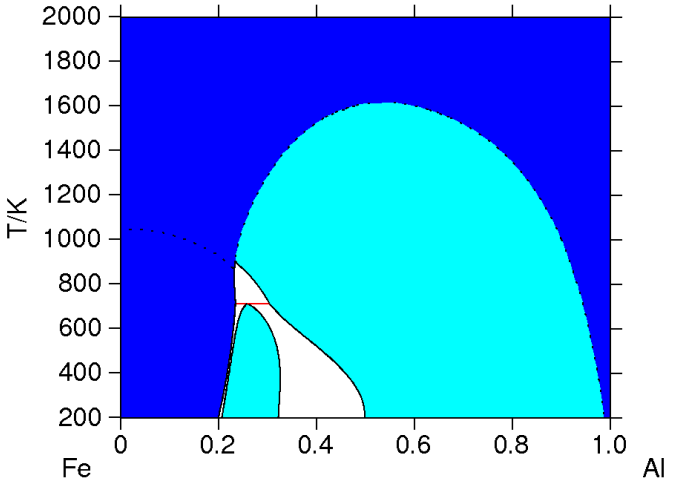
Ohnuma



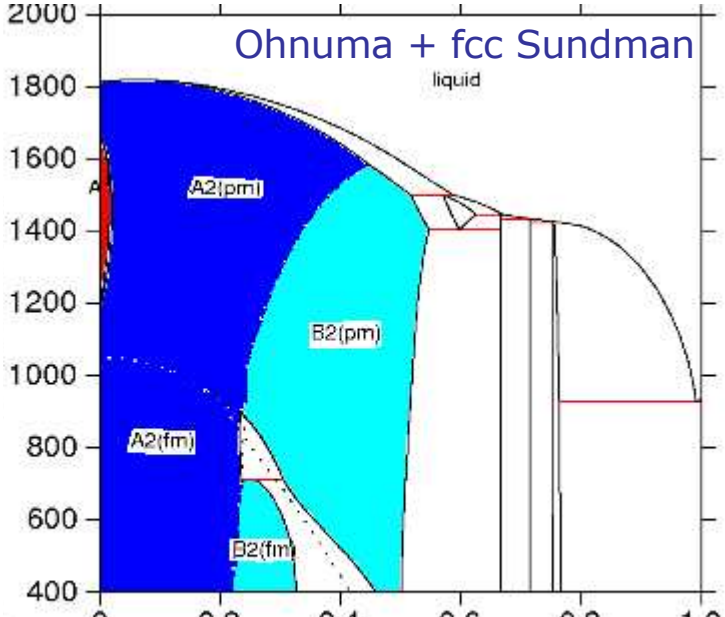
Schoen

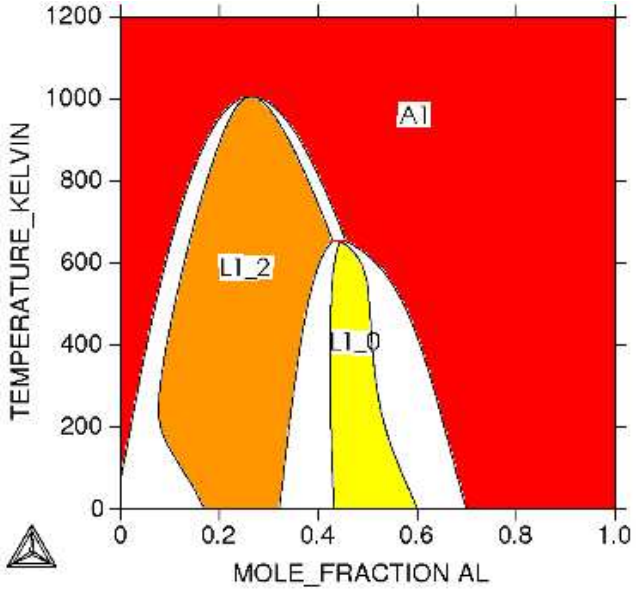






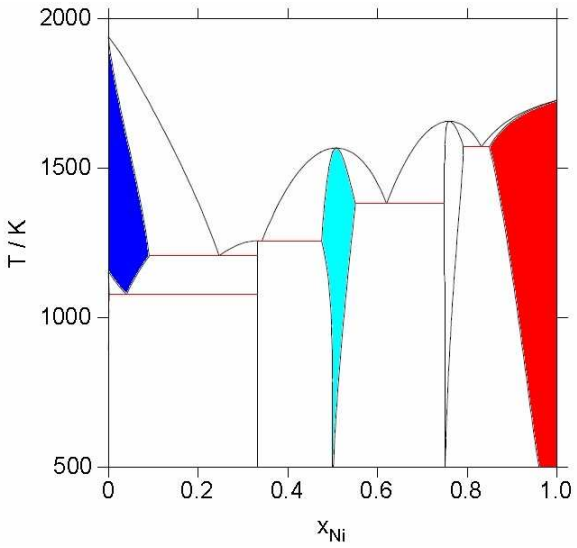
Ohnuma + fcc Sundman

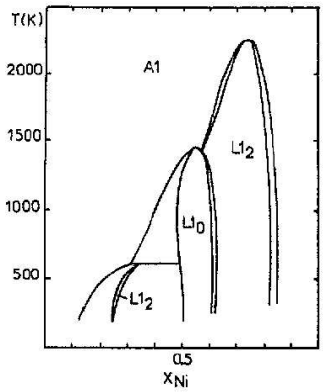




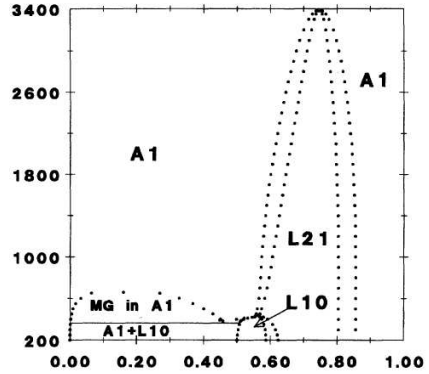
Ni-Ti

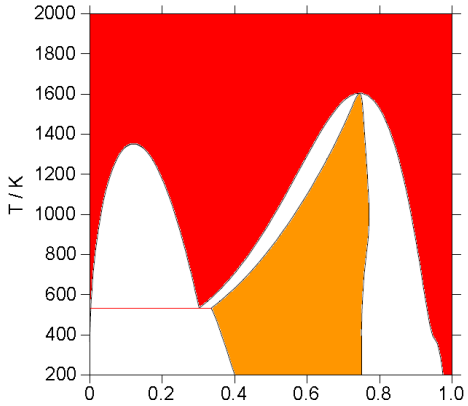
Bellen + Dupin + De Keyzer

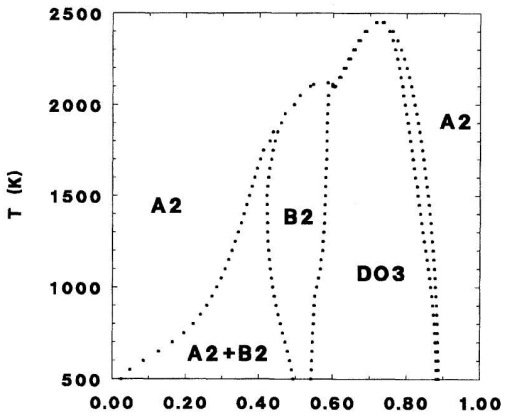


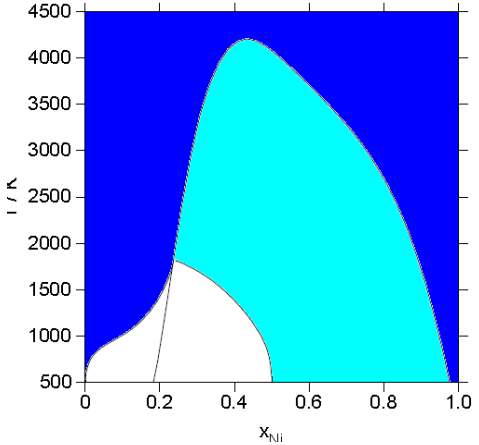


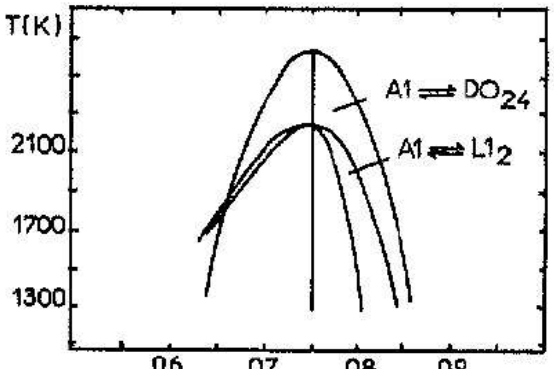
Pasturel, Colinet

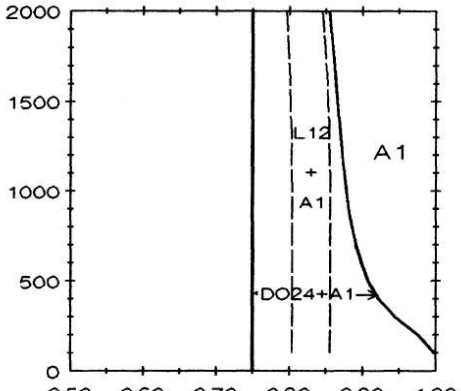


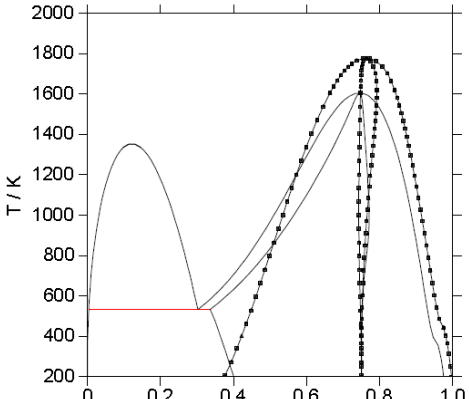






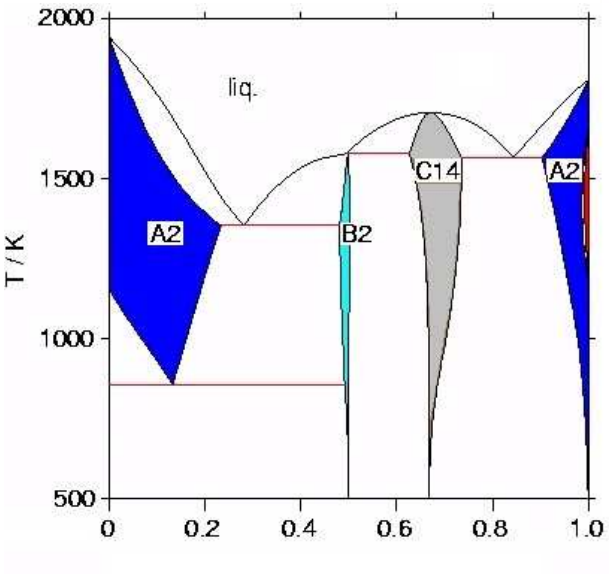




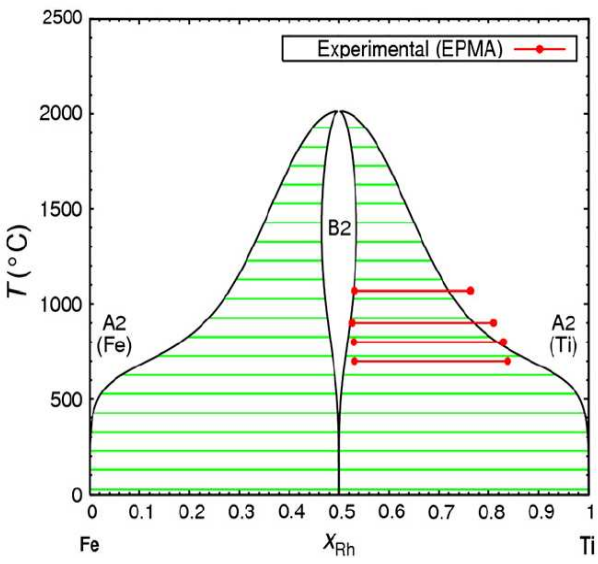


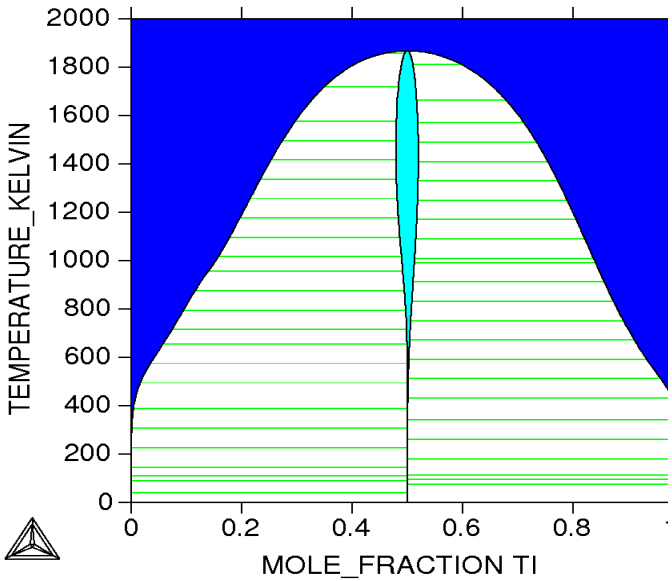
Fe-Ti

Kumar



Schoen





Al-Ti-Nb,Fe-Al-Si, NiAl-NiTi, Fe-FeTi-FeAl

Chaumat, Colinet

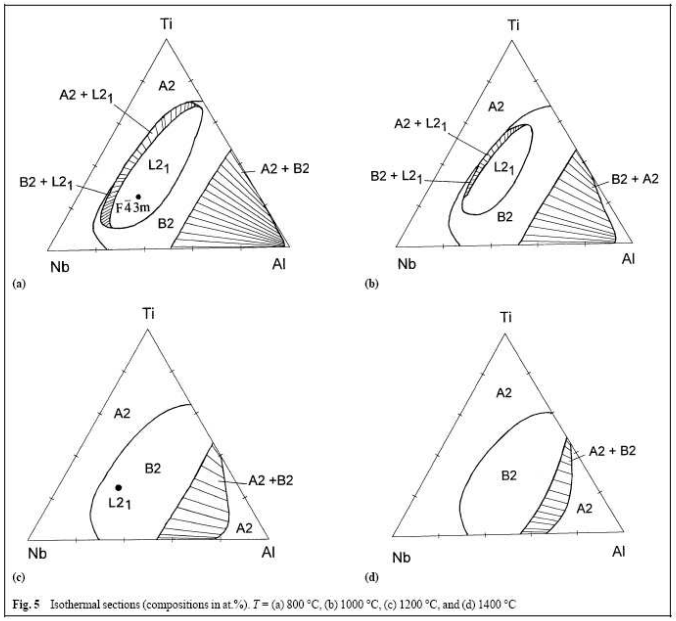
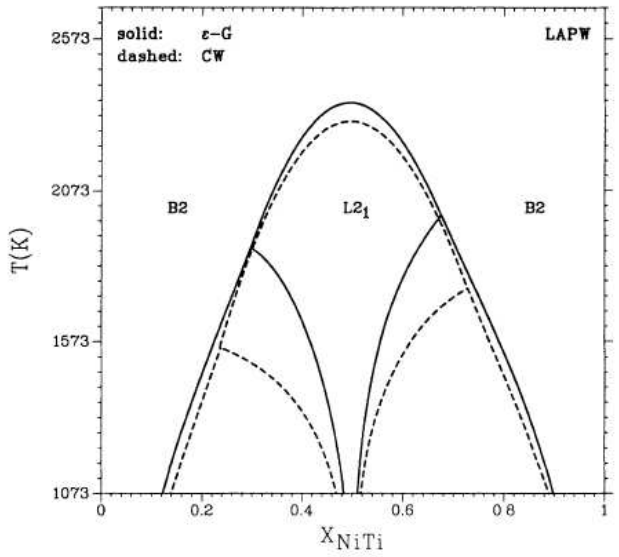


Fig. 5 Isothermal sections (compositions in at.%). T = (a) 800 °C, (b) 1000 °C, (c) 1200 °C, and (d) 1400 °C

Burton, Pasturel



Ohnuma, Schoen

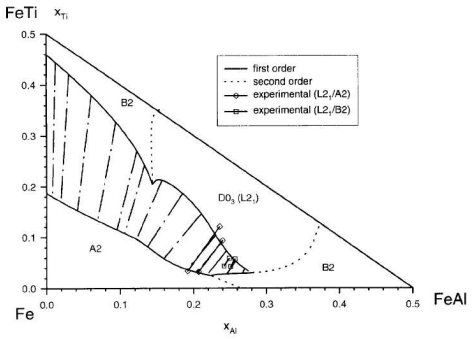


Fig. 15. Calculated isothermal section at 1073 K of the b.c.c. phase equilibria. Symbols: experiments (this work). CVM calculations using the binary interactions in Table 5.

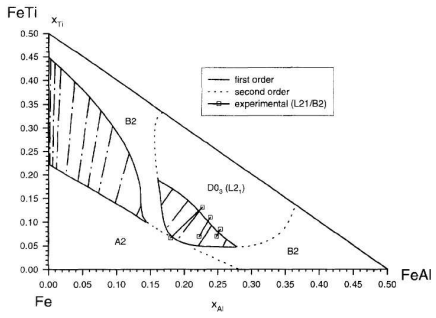


Fig. 14. Calculated isothermal section at 1173 K of the b.c.c. phase equilibria. Symbols: experiments (this work). CVM calculations using the binary interactions in Table 5.

Miyasaki

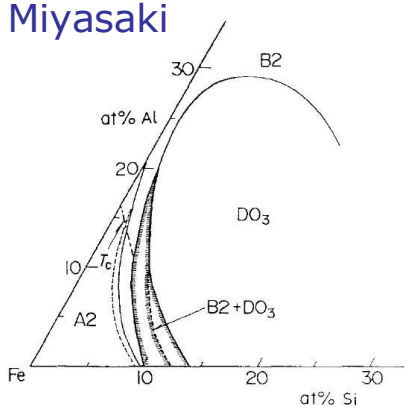


Figure 9 The calculated phase diagrams of both paramagnetic (– – – –) and ferromagnetic ( ) states, respectively, at 873 K, to demonstrate the influence of ferromagnetism on phase separation.

Fe-Ti-Rh, Al-Fe-Ni

Schoen

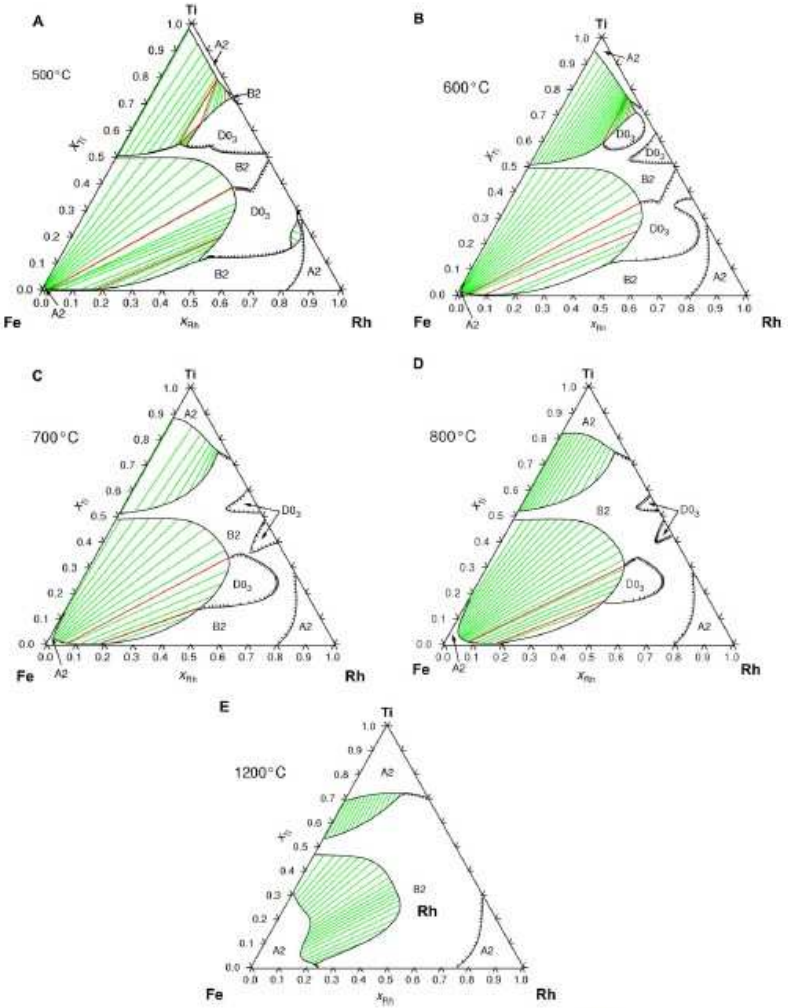
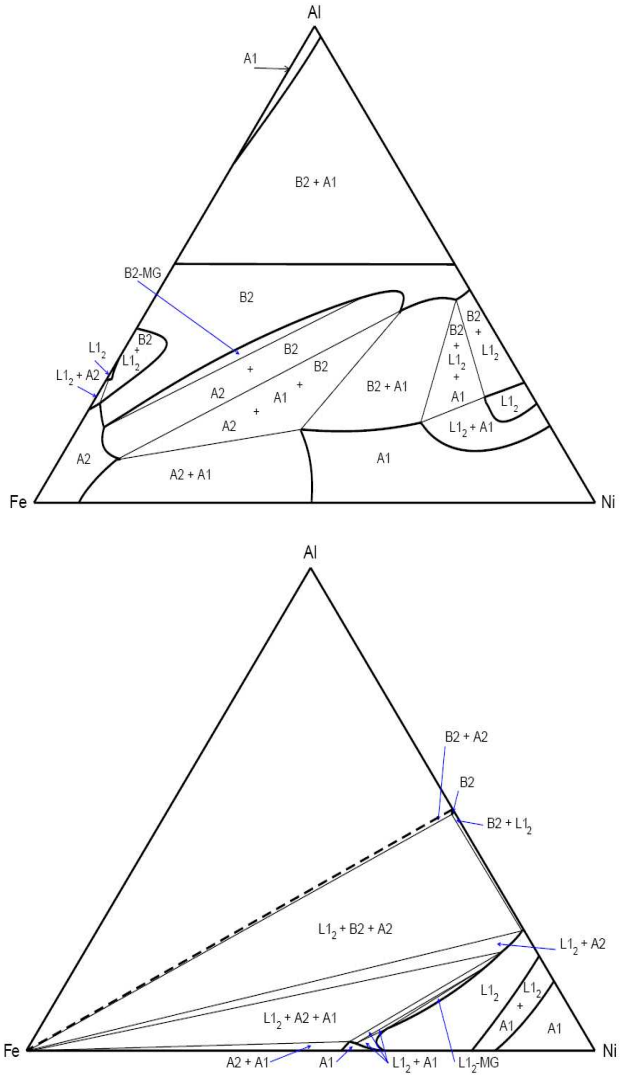


Fig. 9. Isothermal sections of Bcc Fe–Rh–Ti calculated with the CVM in the IT approximation, using the parameters in Table 3. (a) 500 °C, (b) 600 °C, (c) 700 °C, (d) 800 °C, (e) 1200 °C.

Lechermann



Al-Fe-Ni

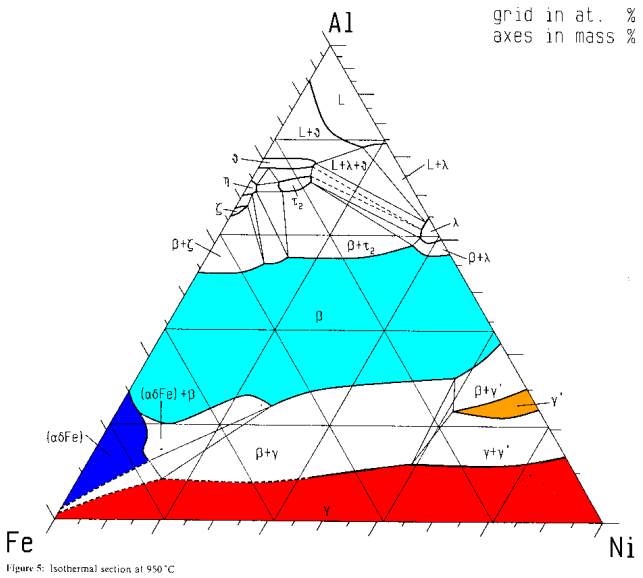
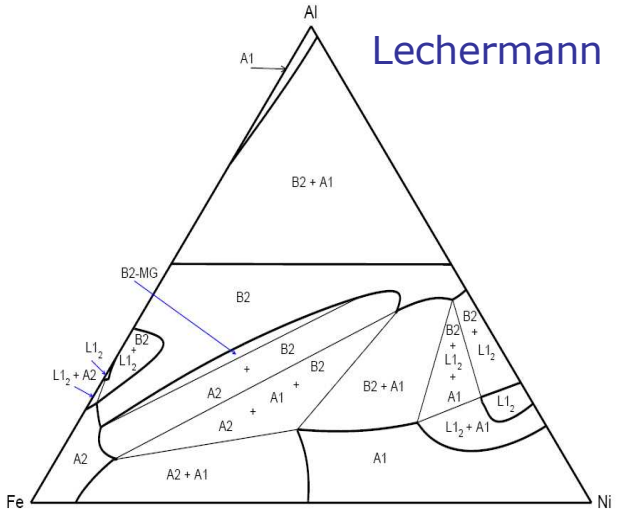
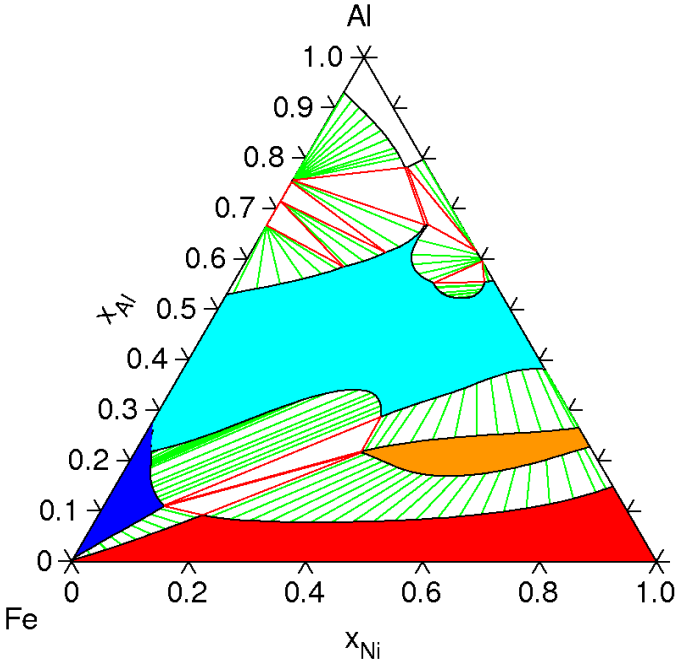
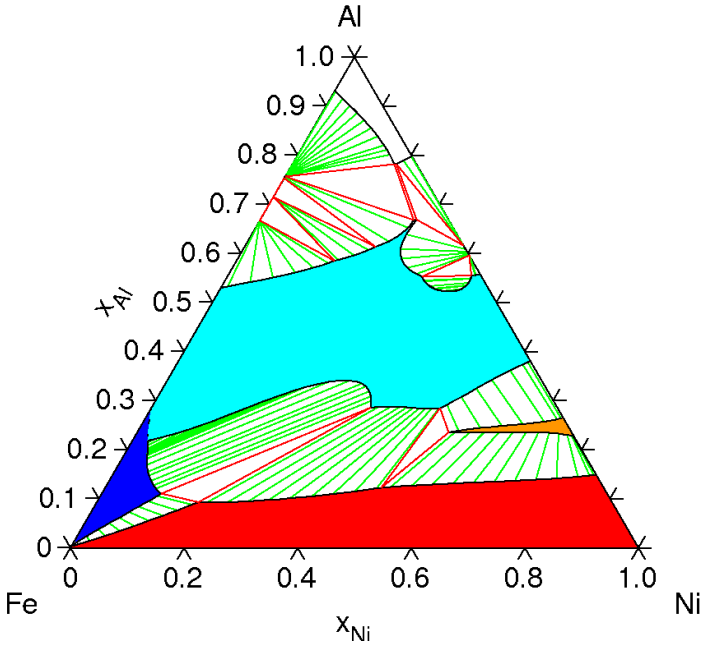


Figure 5: Isothermal section at 950 °C

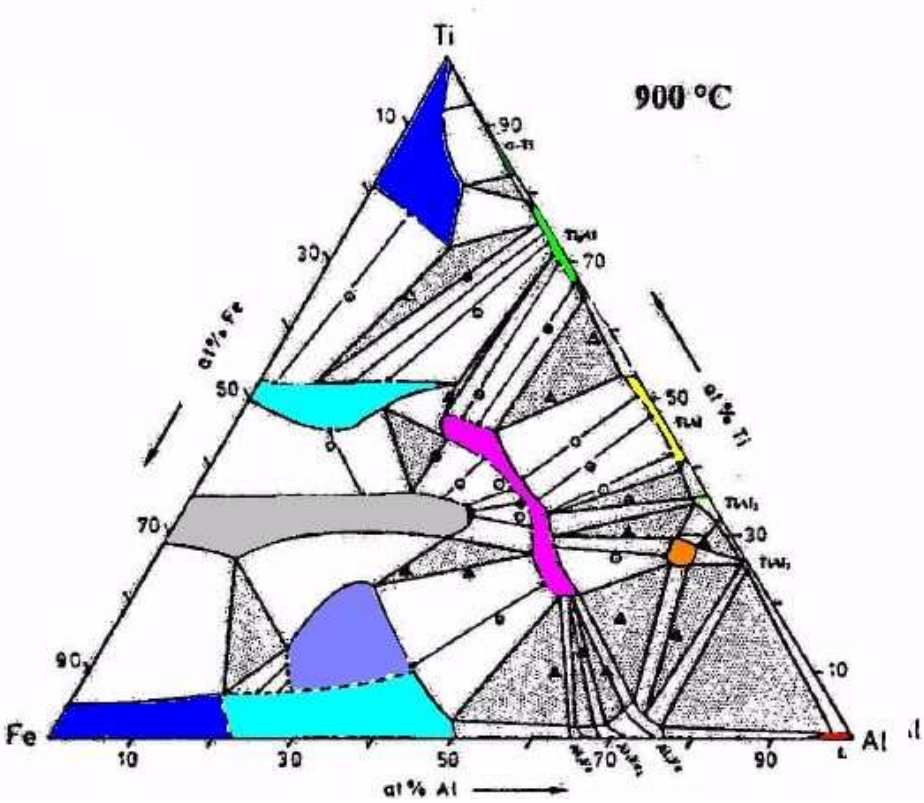


Lechermann

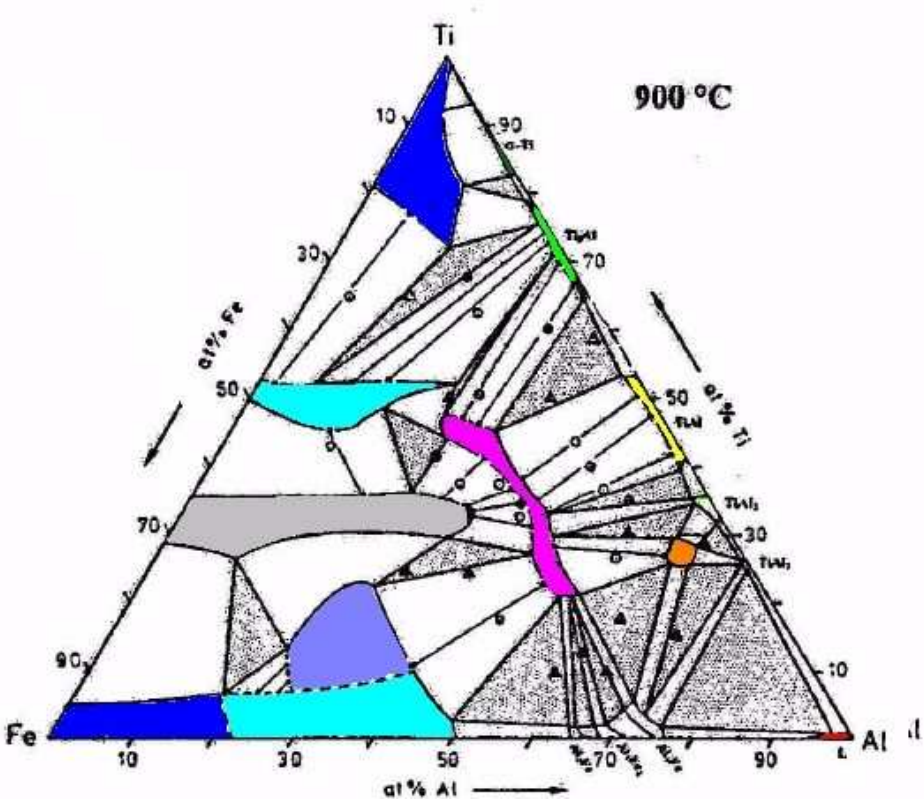


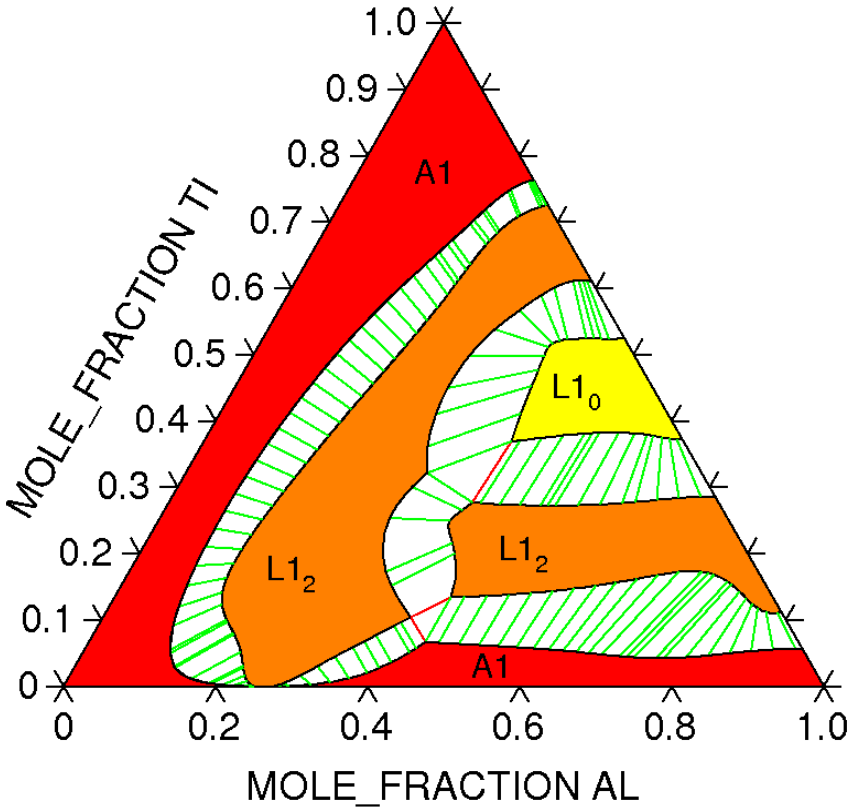


Al-Fe-Ti

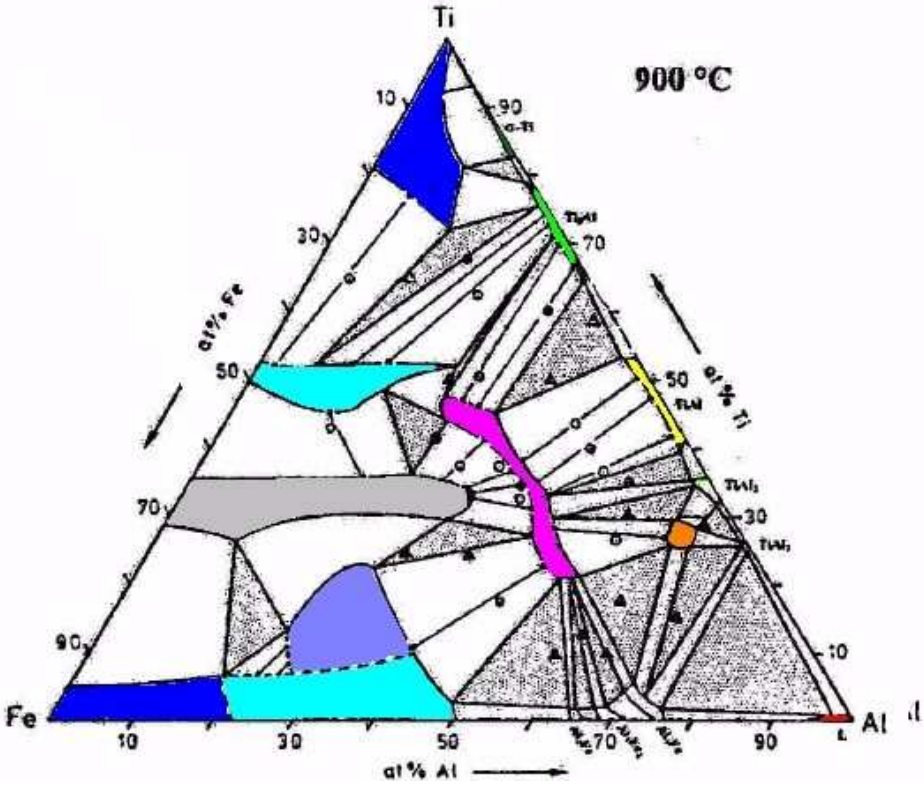

Ti
900 °C
10
90
α-Ti
30
70
at% Fe
50
50
at % Ti
70
30
90
10
Fe
10
30
50
70
90
Al
at % Al

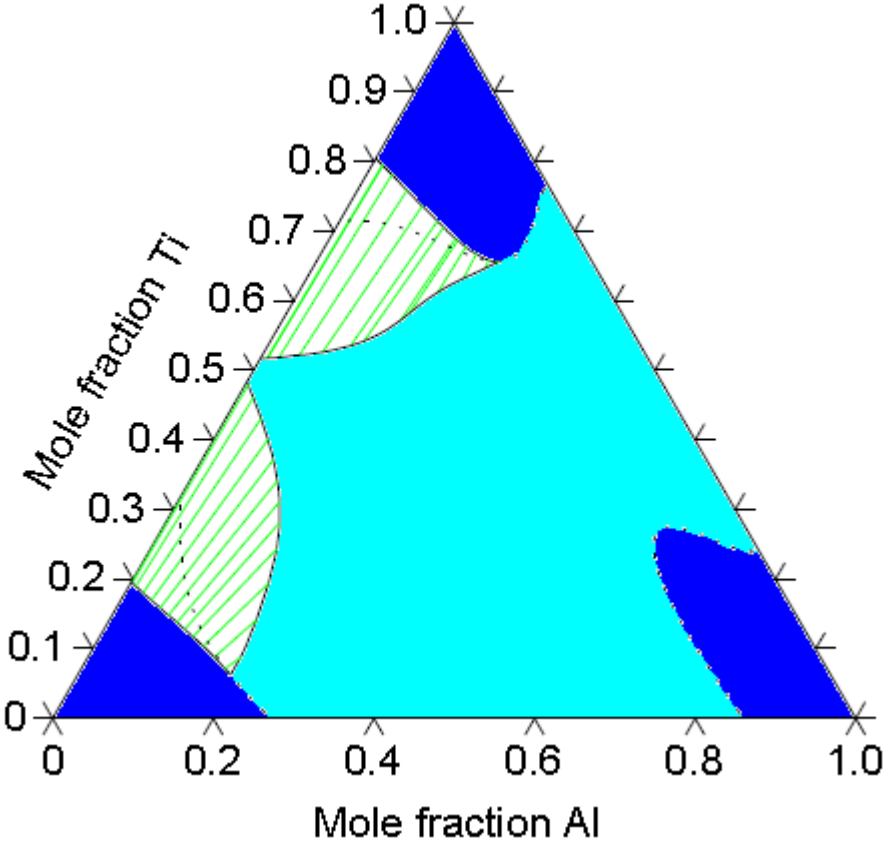
Al-Fe-Ti


Ti
900 °C
Fe
Al
at % Fe
at % Ti
at % Al

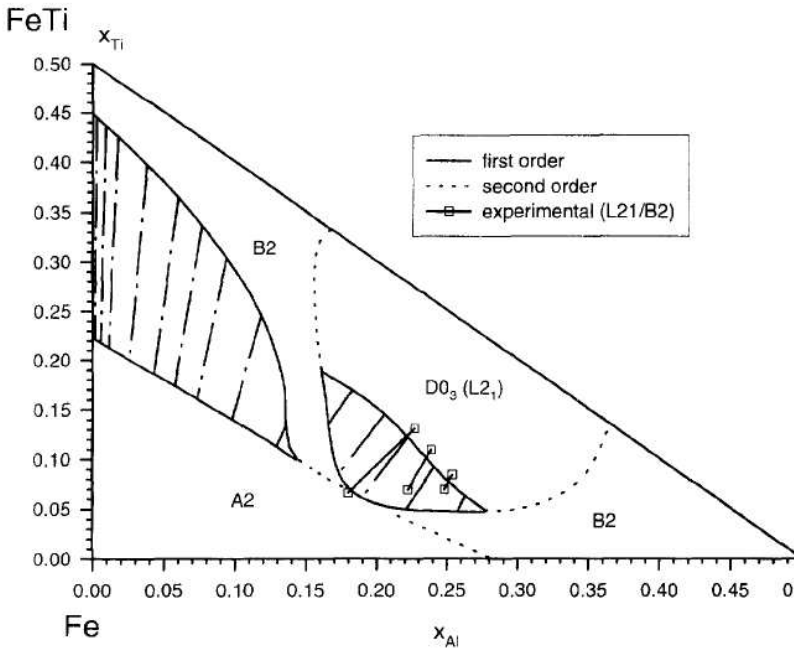

MOLE_FRACTION TI
MOLE_FRACTION AL
A1
L1$_0$
L1$_2$
L1$_2$
A1

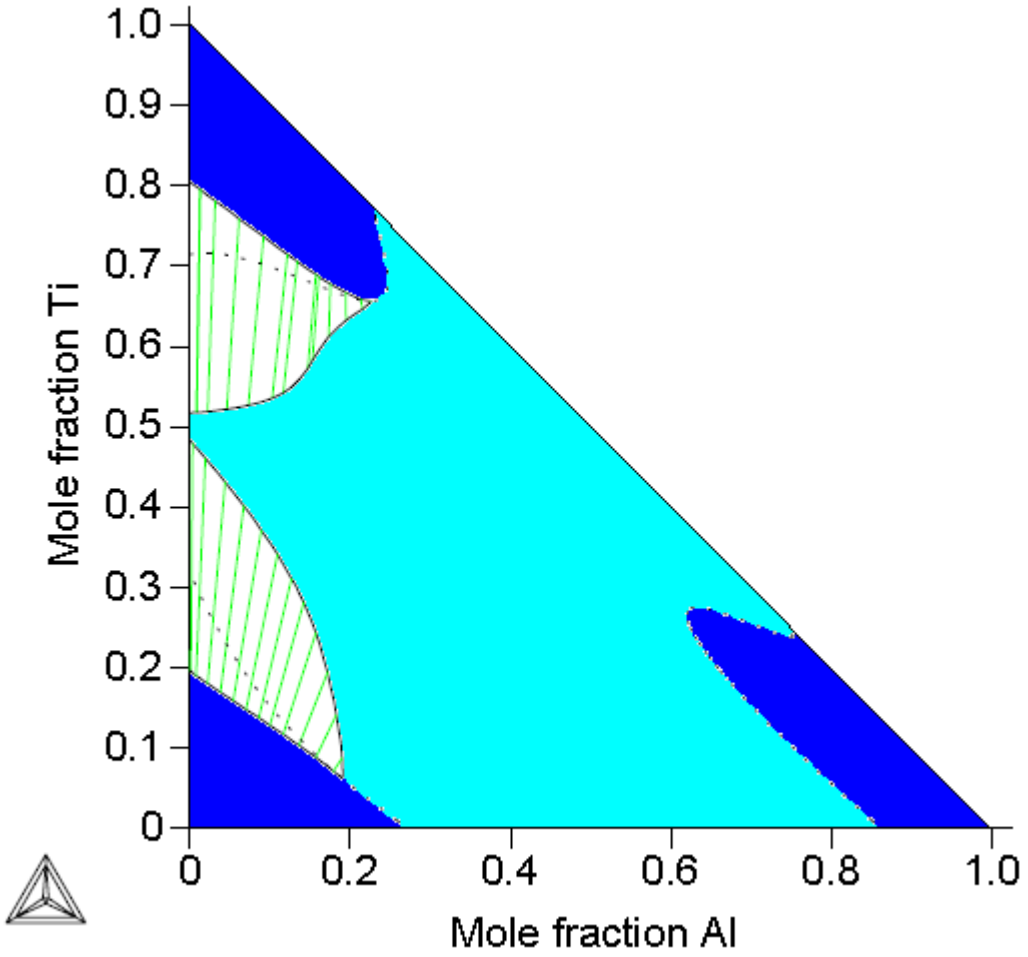
Al-Fe-Ti


Ti
900 °C
Fe
Al
at % Fe
at % Ti
at % Al
10
30
50
70
90

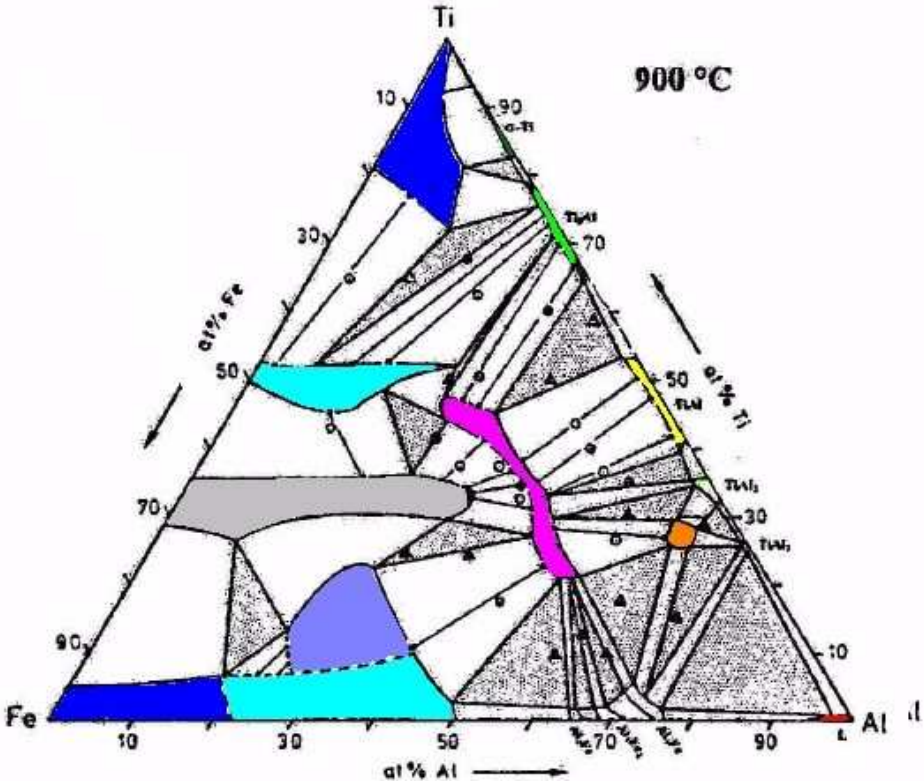

Mole fraction Ti
Mole fraction Al
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0

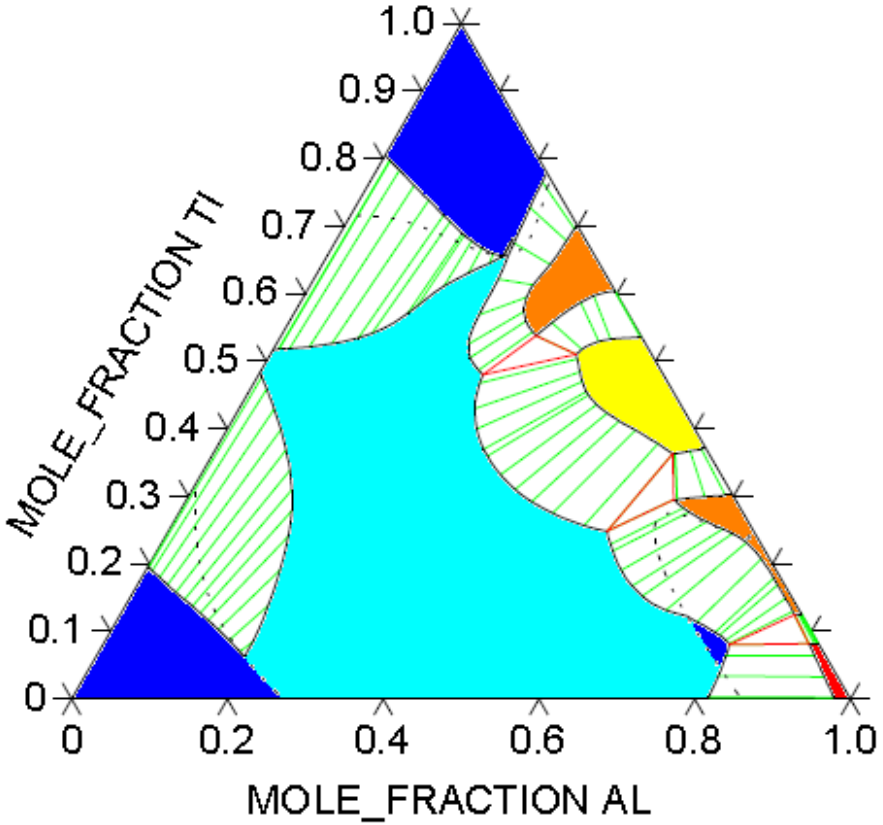
Al-Fe-Ti


FeTi
x_{Ti}
0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
first order
second order
experimental (L21/B2)
B2
$D0_3$ ($L2_1$)
A2
B2
0.00 0.05 0.10 0.15 0.20 0.25 0.30 0.35 0.40 0.45 0
Fe
x_{Al}


Mole fraction Ti
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0 0.2 0.4 0.6 0.8 1.0
Mole fraction Al

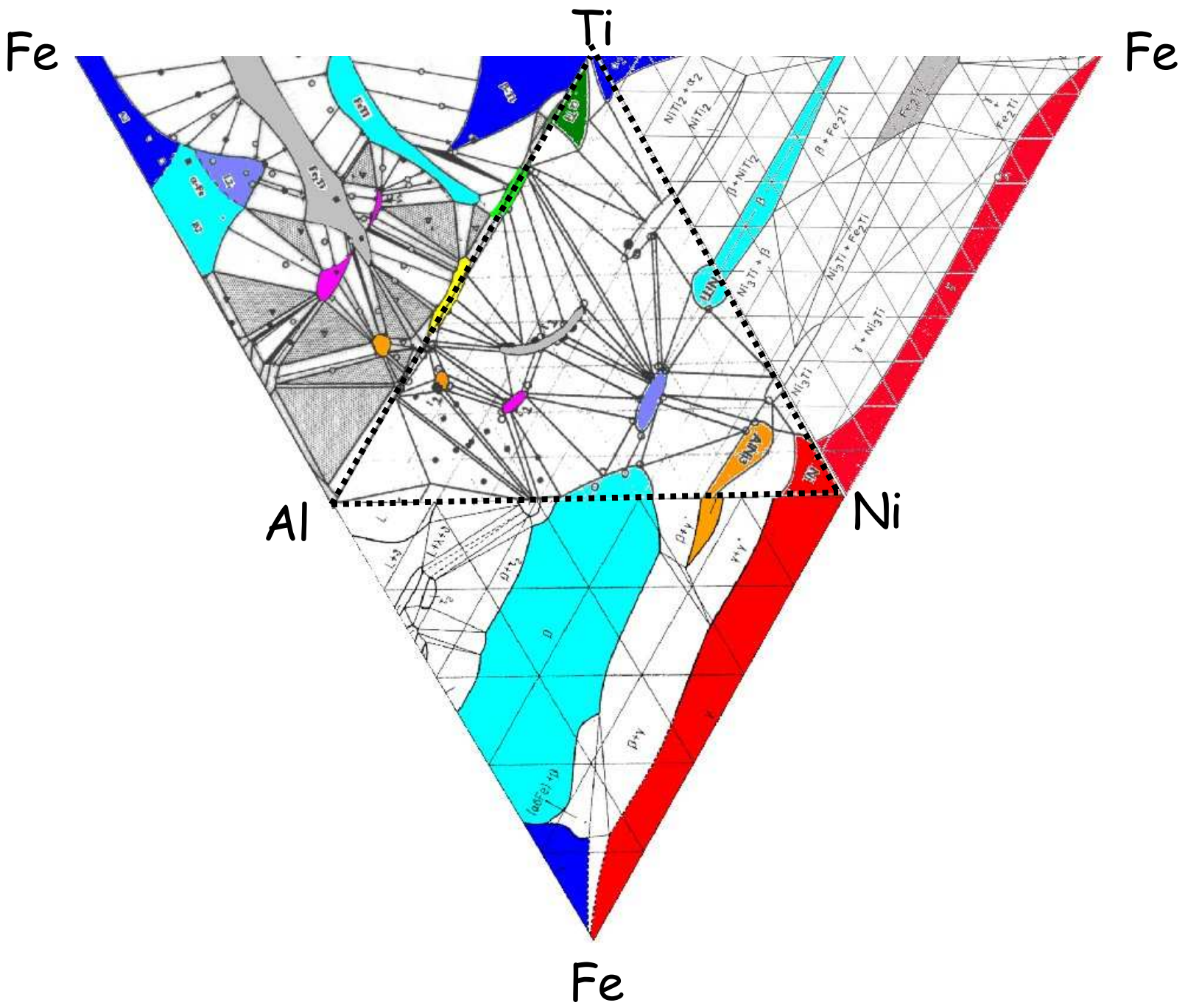
Al-Fe-Ti


Ti
900 °C
Fe
Al
at% Fe
at% Ti
at% Al
10
30
50
70
90


MOLE_FRACTION TI
MOLE_FRACTION AL
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0






Fe
Ti
Fe
Al
Ni
Fe