
Boat Bike Rentals

A case study of modelling order-disorder transformations: Al-Fe-Ni

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Calcul Thermodynamique

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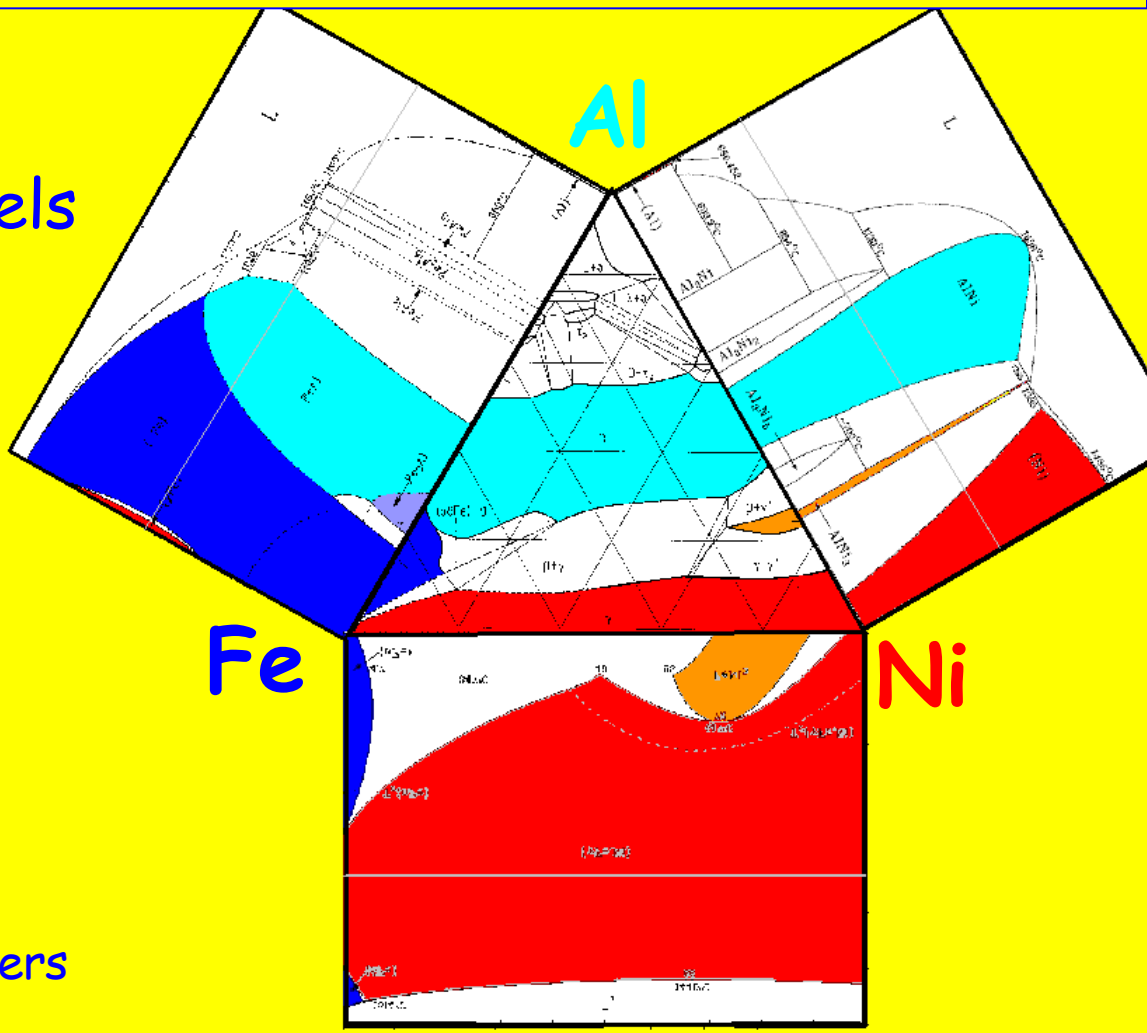
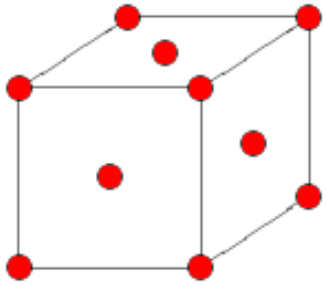
Outline

1. Crystallography
2. Thermodynamics models
3. Binary systems
   a. stable equilibria
   b. fcc detailed
   c. bcc quickly
7. Extrapolations in the ternary system
   a. ternary compounds
   b. ternary reciprocal parameters
10. Discussion

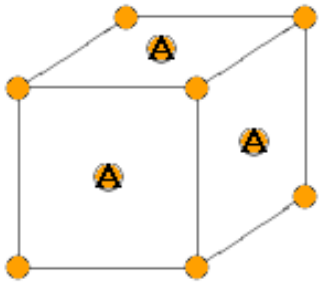


1. Crystallography

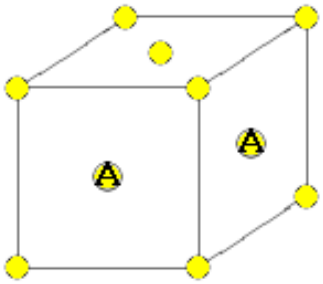
Ordering from the fcc lattice



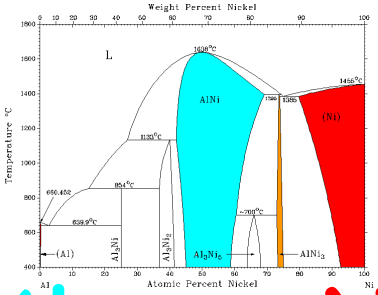
A1



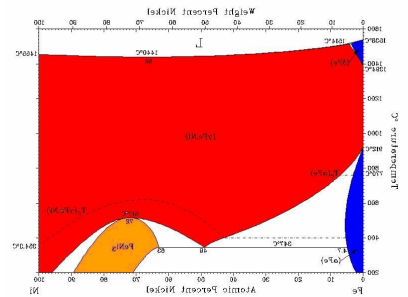
$L1_2$



$L1_0$

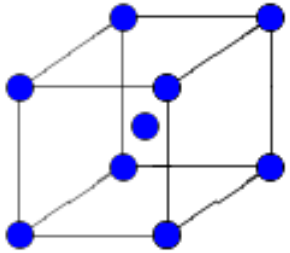


Al Ni

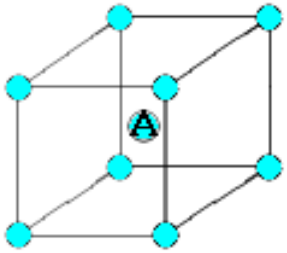


Ni Fe

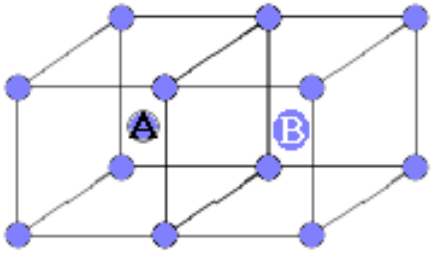
Ordering from the bcc lattice



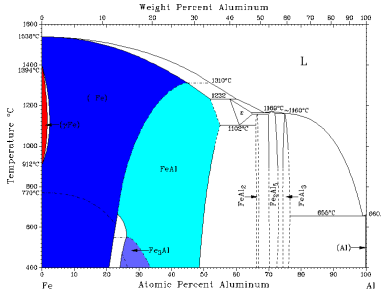
A2



B2



DO_3



Fe Al

2. Thermodynamic models

- The models for all ordered phases based on the Compound Energy Formalism (CEF).

$$G = G^{dis}(x_i) + G^{ord}(y_i^{(s)})$$

- For BCC ordered phases a 2 sublattice model with vacancies is used (Al,Fe,Ni,□)(Al,Fe,Ni,□).

- For FCC ordered phases a 4 sublattice model is used (Al,Fe,Ni)(Al,Fe,Ni)(Al,Fe,Ni)(Al,Fe,Ni).

- For FCC phases, the contribution from SRO is described as an excess Gibbs energy allowing correct topology for coherent binary phase diagram.

2. Thermodynamic models

$$G = G^{dis}(x_i) + G^{ord}(y_i^{(s)})$$

$$G^{dis}(x_i) = \sum_i x_i G_i^{dis} + RT \sum_i x_i \ln x_i + \sum_{i,j} x_i x_j L_{i,j}^{dis} + \sum_{i,j,k} x_i x_j x_k L_{i,j,k}^{dis} + G^{dis,mag}(x_i)$$

2. Thermodynamic models

$$G = G^{dis}(x_i) + G^{ord}(y_i^{(s)})$$

$$G^{ord}(y_i^{(s)}) = G^{SL}(y_i^{(s)}) - G^{SL}(y_i^{(s)} = x_i)$$

when $y_i^{(s)} = x_i$

$$G^{SL}(y_i^{(s)}) = G^{SL}(y_i^{(s)} = x_i)$$

$$G^{ord}(y_i^{(s)}) = 0 \qquad G = G^{dis}(x_i)$$

2. Thermodynamic models (fcc)

$$G^{ord}(y_i^{(s)}) = G^{SL}(y_i^{(s)}) - G^{SL}(y_i^{(s)} = x_i)$$

$$G^{SL}(y_i^{(s)}) = \sum_i \sum_j \sum_k \sum_l y_i^{(1)} y_j^{(2)} y_k^{(3)} y_l^{(4)} G^{SL}_{ijkl}$$

$$+ \tfrac{1}{4} RT \sum_s \sum_i y_i^{(s)} \ln y_i^{(s)}$$

$$+ \sum_s \sum_{i,j} y_i^{(s)} y_j^{(s)} L^{SL}_{i,j:*:*:*}$$

$$+ \sum_{s,r} \sum_{i,j} \sum_{k,l} y_i^{(s)} y_j^{(s)} y_k^{(r)} y_l^{(r)} L^{SL}_{i,j:k,l:*:*}$$

2. Thermodynamic models (fcc)

$$G^{ord}(y_i^{(s)}) = G^{SL}(y_i^{(s)}) - G^{SL}(y_i^{(s)} = x_i)$$

$$G^{SL}(y_i^{(s)} = x_i) = \sum_i \sum_j \sum_k \sum_l x_i x_j x_k x_l \, G^{SL}_{ijkl}$$

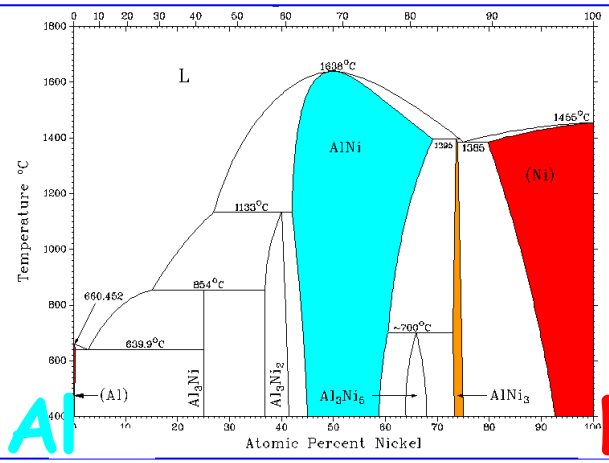
$$+ \tfrac{1}{4} RT \sum_s \sum_i x_i \ln x_i$$

$$+ \sum_s \sum_{i,j} x_i x_j \, L^{SL}_{i,j:*:*:*}$$

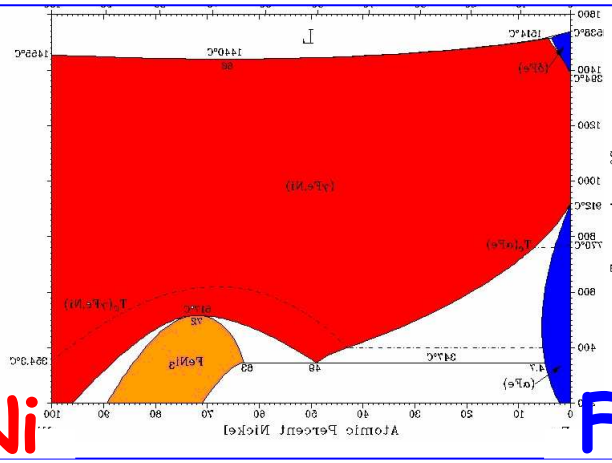
$$+ \sum_{s,r} \sum_{i,j} \sum_{k,l} x_i x_j x_k x_l \, L^{SL}_{i,j:k,l:*:*}$$

3.a. Stable binary phase diagrams

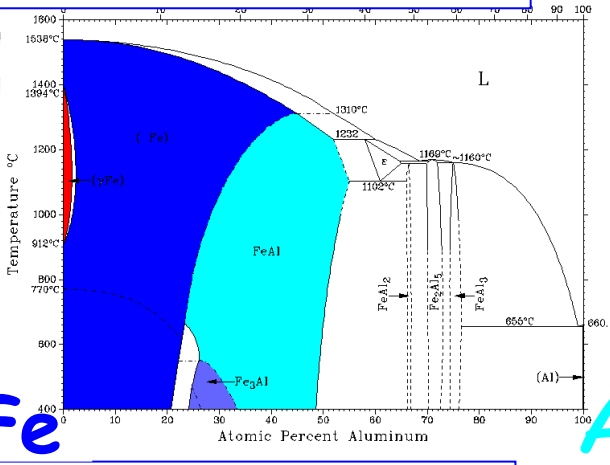
Critical assessments



Al

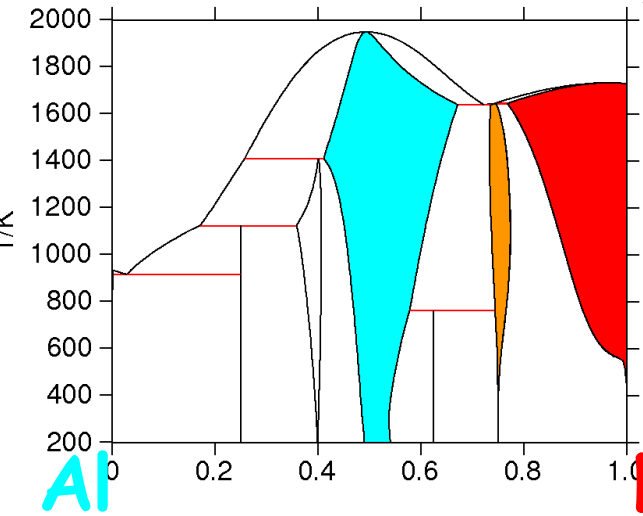


Ni



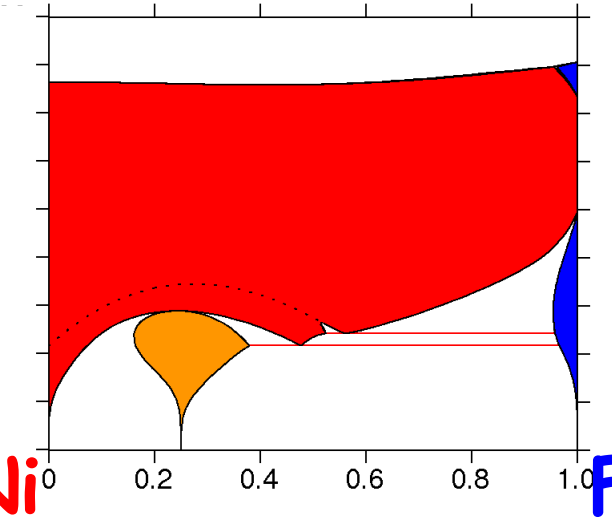
Fe Al

Thermodynamic descriptions



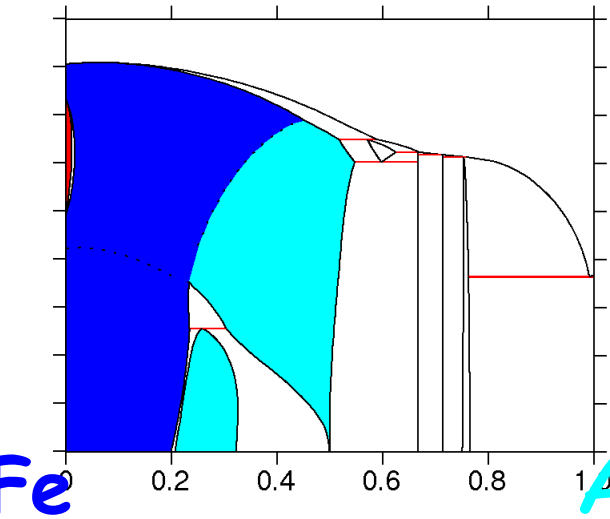
Al

1. Ansara, Dupin, Lukas, Sundman
2. Dupin, Sundman (4SL)



Ni

1. Chart, Dinsdale
2. Ansara ($L1_2$)

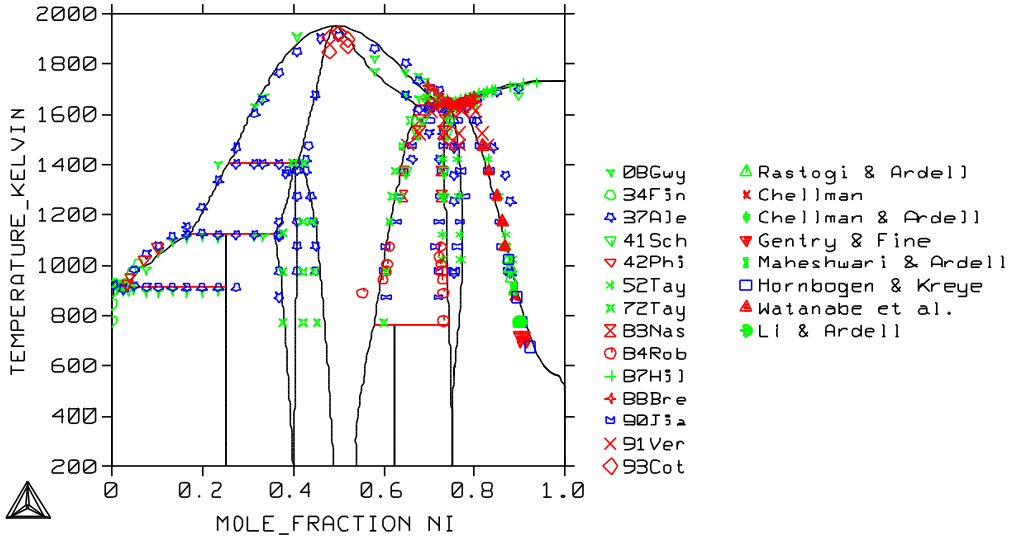


Fe Al

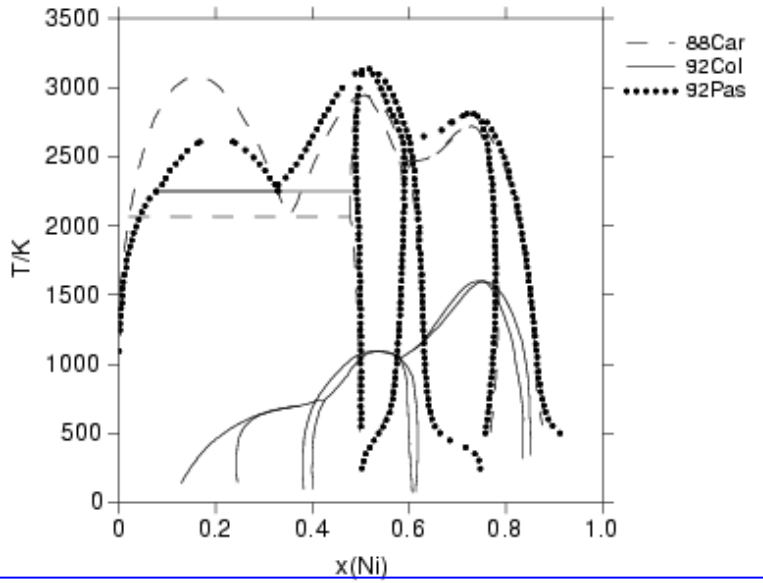
1. Seiersten (COST 507)
2. Ohnuma (A2/B2)

3.b. fcc ordering in Al-Ni

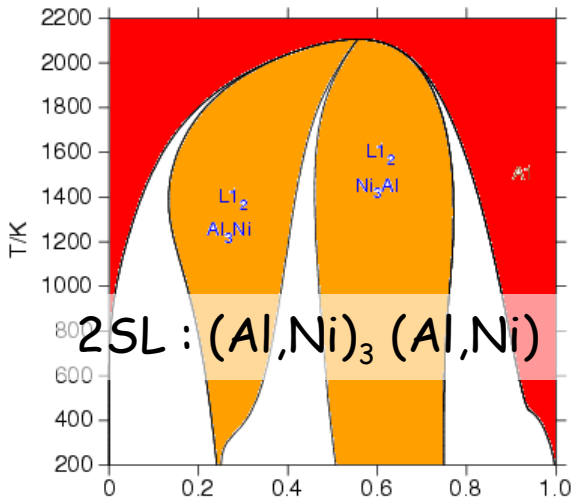
Calphad, stable phase diagram

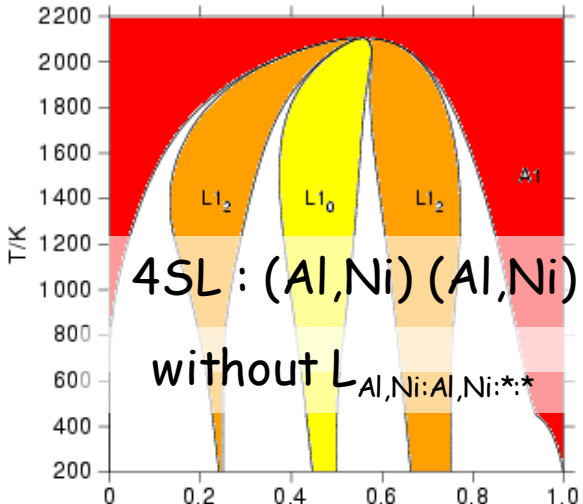


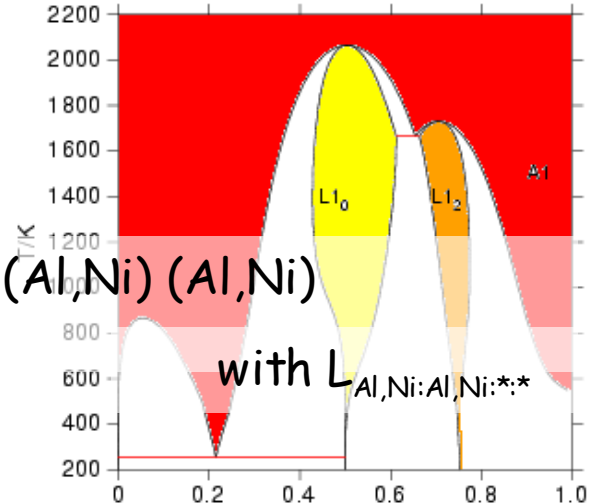
FP phase diagrams



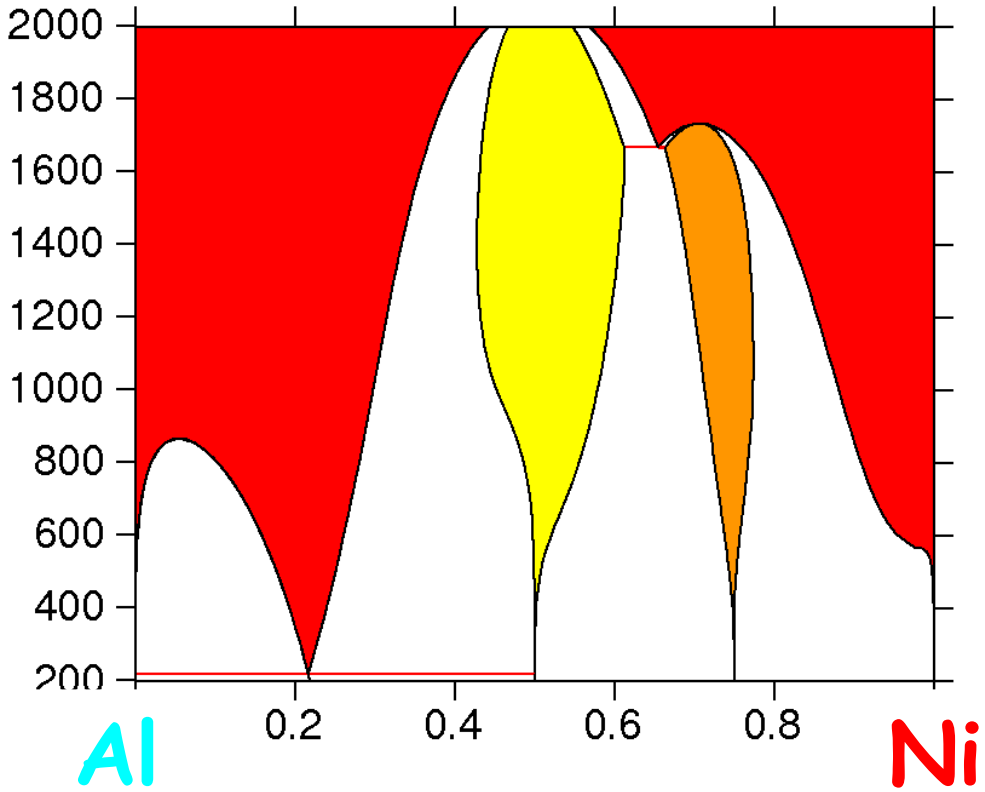
Calphad, metastable phase diagrams







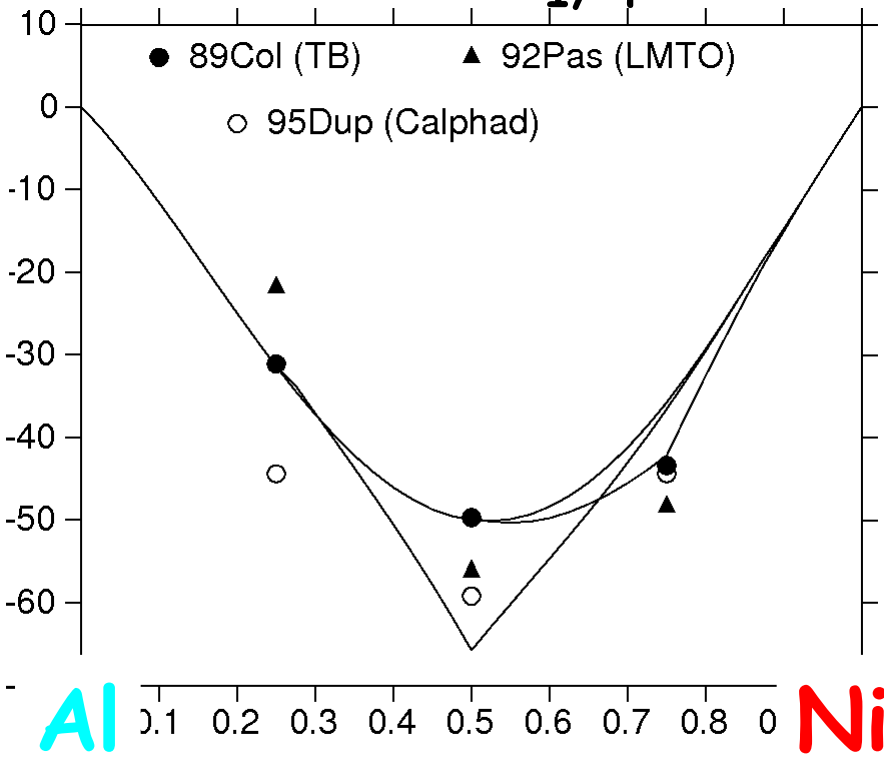
3.b. fcc ordering in Al-Ni



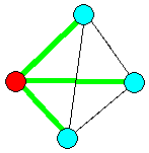
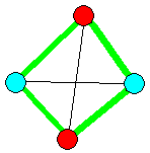
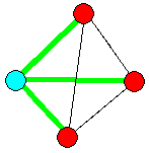
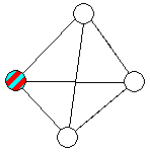
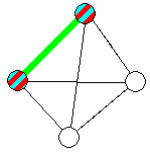
95Dup : u_{AlNi} = 1/3

= 1/3

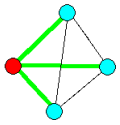
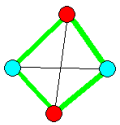
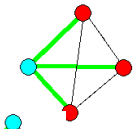
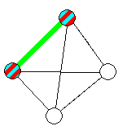
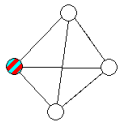
= 1/4

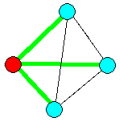
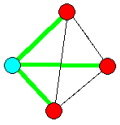


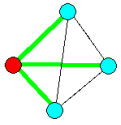
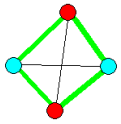
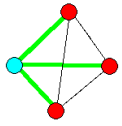
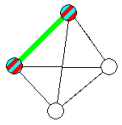
3.b. fcc ordering in Al-Ni

G_{Al_3Ni}	$G_{Al_2Ni_2}$	G_{AlNi_3}	$L_{Al,Ni:*:*:*}$	$L_{Al,Ni:Al,Ni:*:*}$
- 29600	- 66718	- 43590	+ 5310	- 34575
	+ 11.64 T	+ 6.22 T	- 1.46 T	+ 13.22 T

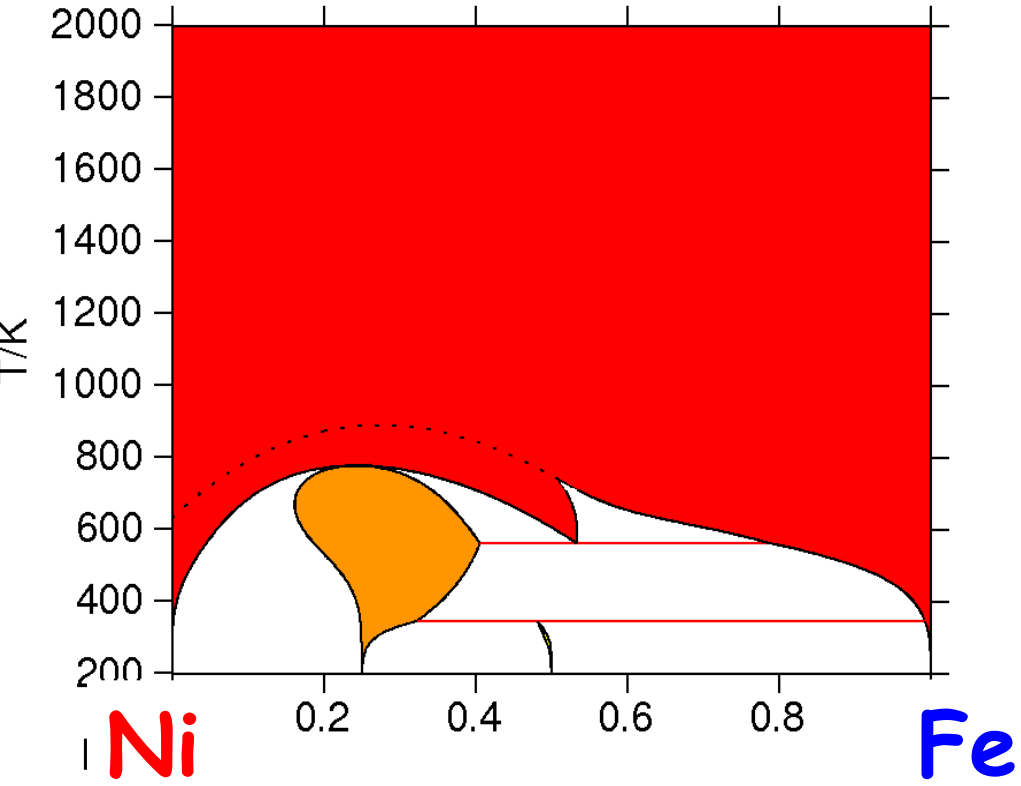
$$L^{fcc}_{Al,Ni} = \text{  } + 1.5 \text{  } + \text{  } + 1.5 \text{  } + 4 \text{  }$$

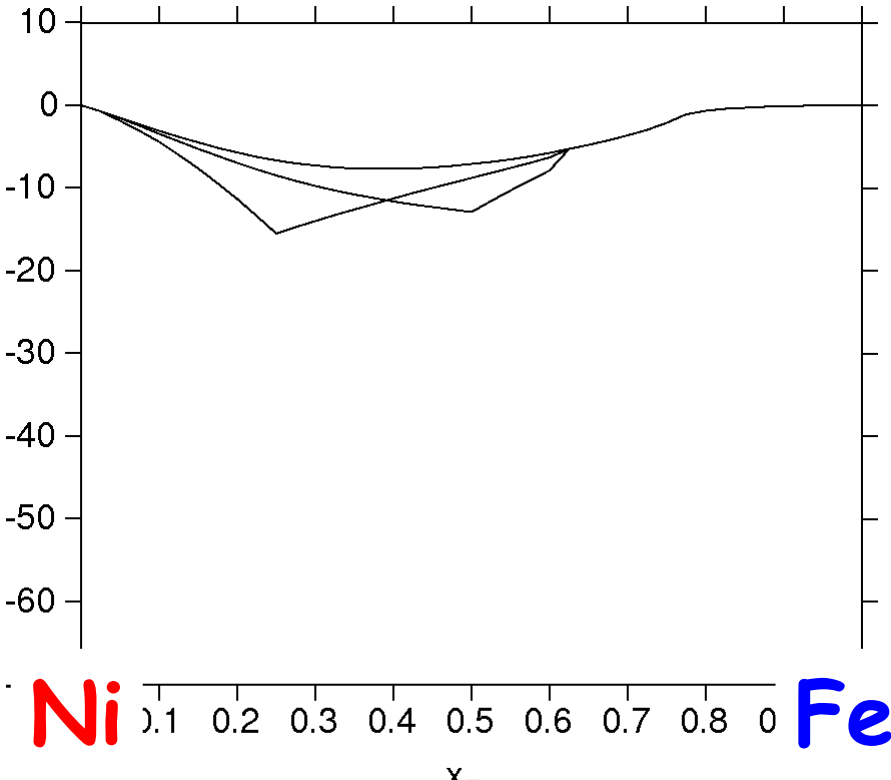
$$+ 2(x_{Al} - x_{Ni})(\text{  } - \text{  })$$

$$+ (x_{Al} - x_{Ni})^2(\text{  } - 1.5 \text{  } + \text{  } - 1.5 \text{  })$$

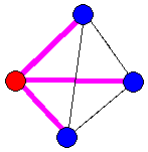
$$TC^{fcc}_{Al,Ni} = x_{Ni} TC^{fcc}_{Ni} + x_{Al} x_{Ni}[-1112 + (x_{Al} - x_{Ni})1745]$$

3.b. fcc ordering in Fe-Ni





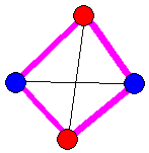
3.b. fcc ordering in Fe-Ni



G_{Fe_3Ni}

-16500

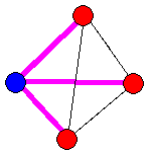
+ 41.1 T



$G_{Fe_2Ni_2}$

- 30000

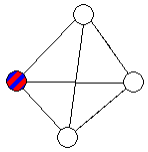
+ 54.8 T



G_{FeNi_3}

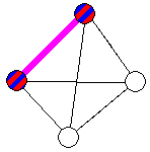
- 28815

+ 41.1 T



$L_{Fe,Ni:*:*:*}$

1200



$L_{Fe,Ni:Fe,Ni:*:*}$

- 7500

+ 13.7 T

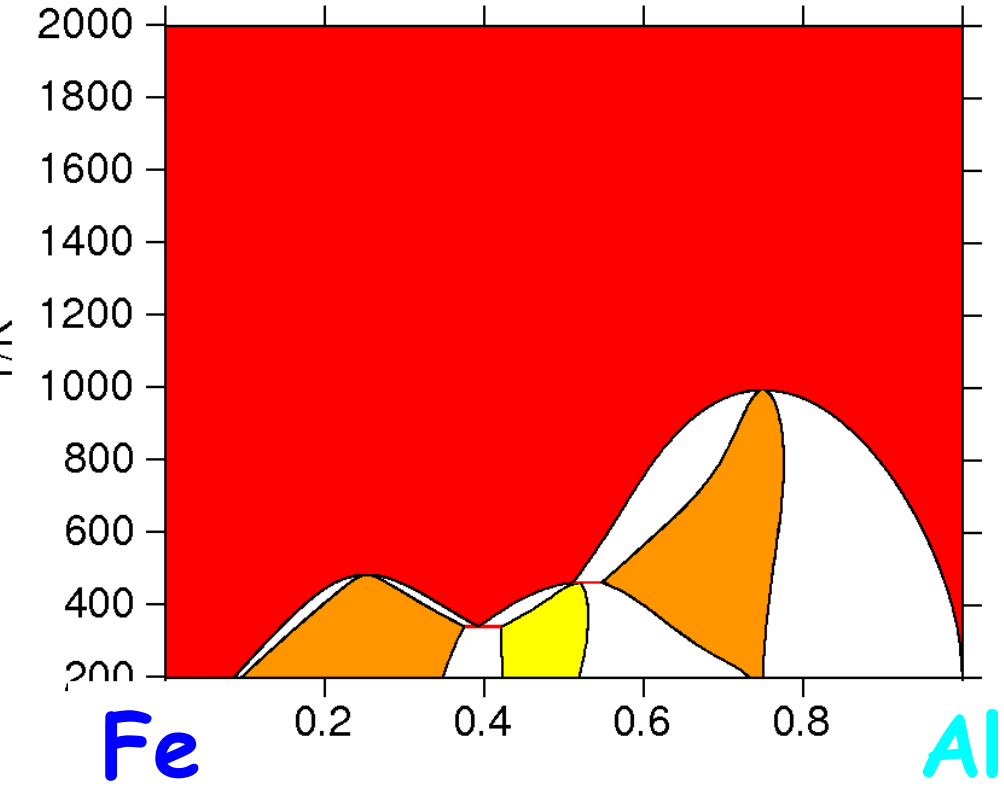
ie $G_{Fe_2Ni_2}/4$

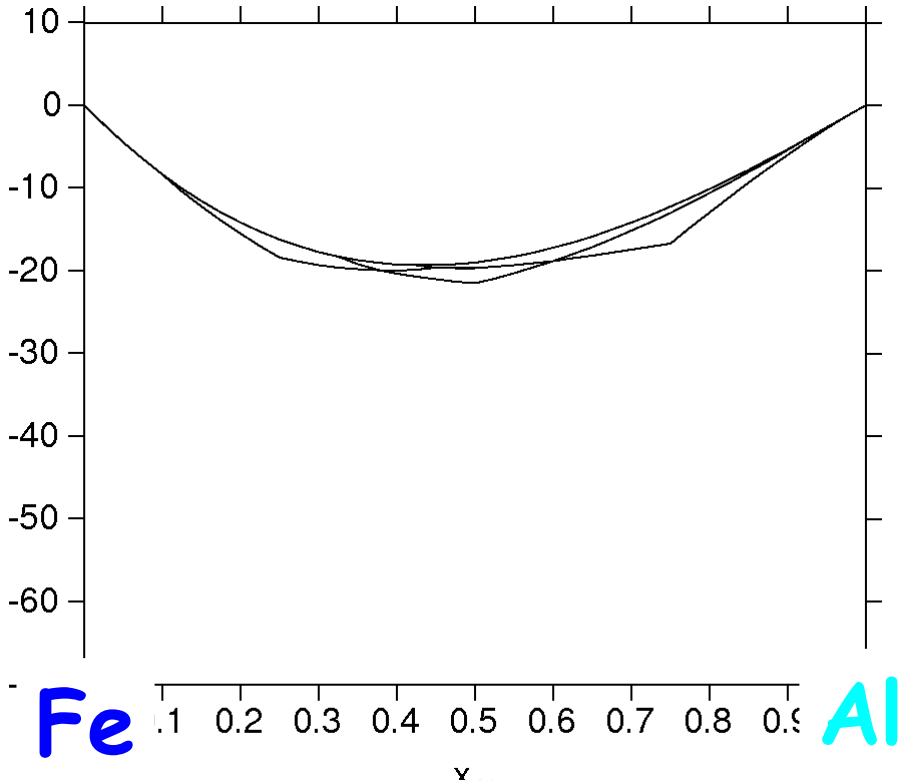
$$L^{fcc}_{Fe,Ni} = -12054 + 3.274T + (x_{Fe} - x_{Ni})(11082 - 4.45T) + (x_{Fe} - x_{Ni})^2(-725.8)$$

$$TC^{fcc}_{Fe,Ni} = x_{Fe}TC^{fcc}_{Fe} + x_{Ni}TC^{fcc}_{Ni} + x_{Fe}x_{Ni}[2133 - (x_{Fe} - x_{Ni})682]$$

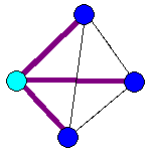
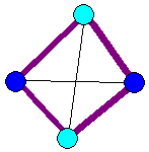
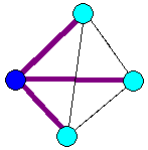
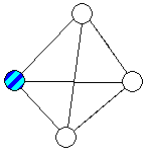
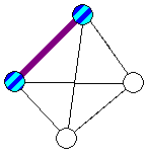
$$BMAG^{fcc}_{Fe,Ni} = x_{Fe}BMAG^{fcc}_{Fe} + x_{Ni}BMAG^{fcc}_{Ni} + x_{Fe}x_{Ni}[\,9.55 + (x_{Fe} - x_{Ni})7.23 + (x_{Fe} - x_{Ni})^2 5.93 + (x_{Fe} - x_{Ni})^3 6.18\,]$$

3.b. fcc ordering in Al-Fe





3.b. fcc ordering in Al-Fe

G_{Al_3Fe} $G_{Al_2Fe_2}$ G_{AlFe_3} $L_{Al,Fe:*:*:*}$ $L_{Al,Fe:Al,Fe:*:*}$

-18000 - 20000 - 14400 0 - 5000

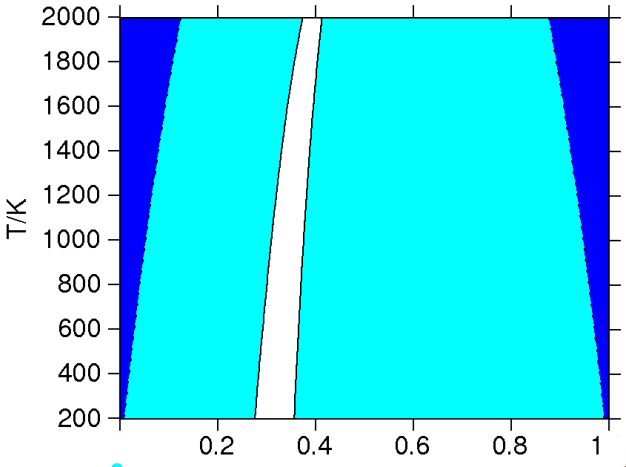
From Ab initio by Watson and Weinert

ie $G_{Al_2Fe_2}/4$

$$L^{fcc}_{Al,Fe} = -76066.1 + 18.6758T + (x_{Al} - x_{Fe})(21167.4 + 1.3398T)$$

$$TC^{fcc}_{Al,Fe} = x_{Fe} TC^{fcc}_{Fe}$$

3.c. bcc ordering

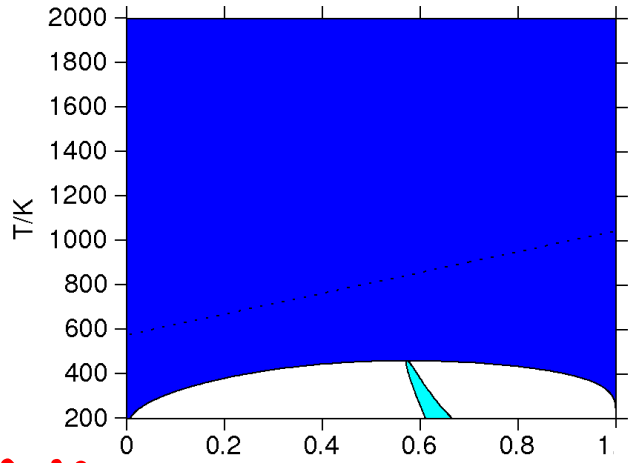


Al

Only B2 stable.

Constitutional defects largely studied and well described in the range of stability.

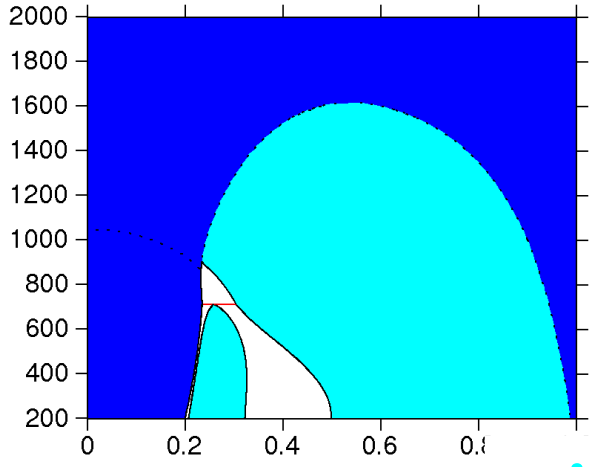
Ab initio on the metastable transition could be worthy.



Ni

Only A2 stable.

Ab initio on the metastable transition would be worthy.



Fe

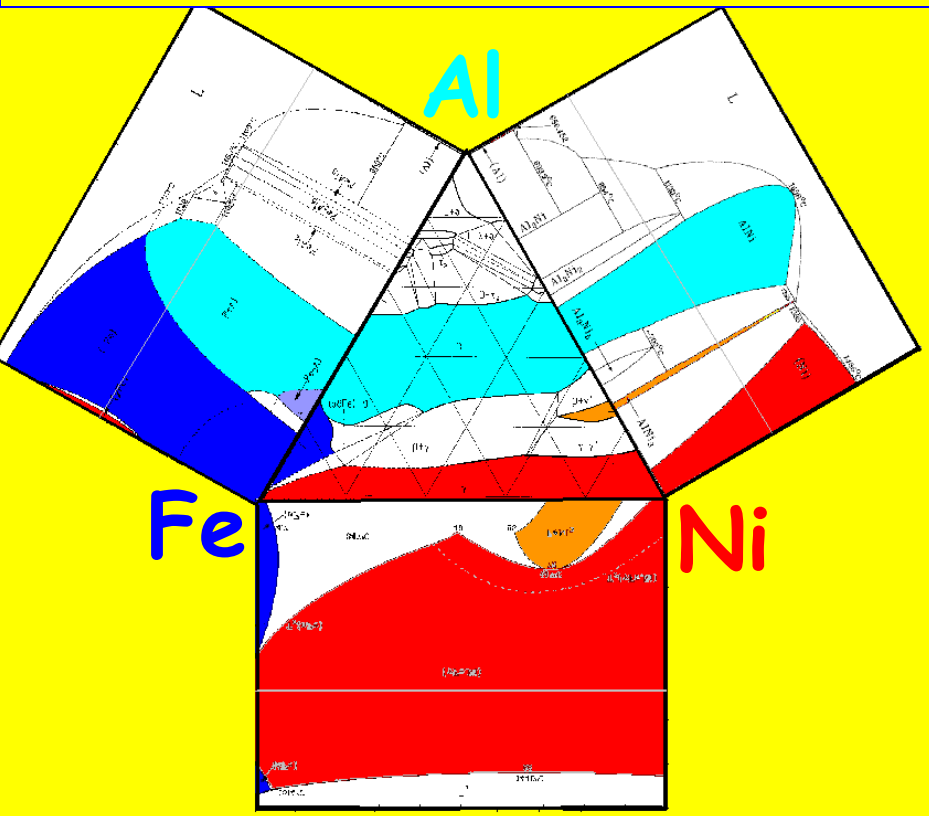
Al

Both A2 and B2 stable.

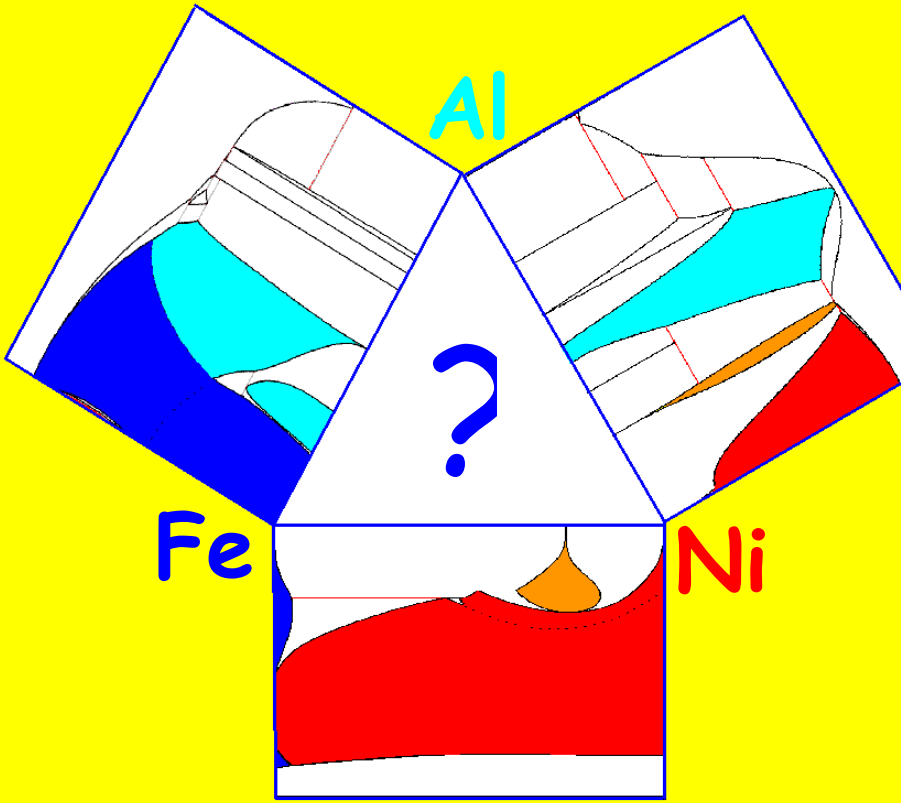
Vacancies not taken into account as a tool for the modelling of the B2 phase.

The stability of the DO3 needs 4SL modelling.

4. Extrapolation to the ternary

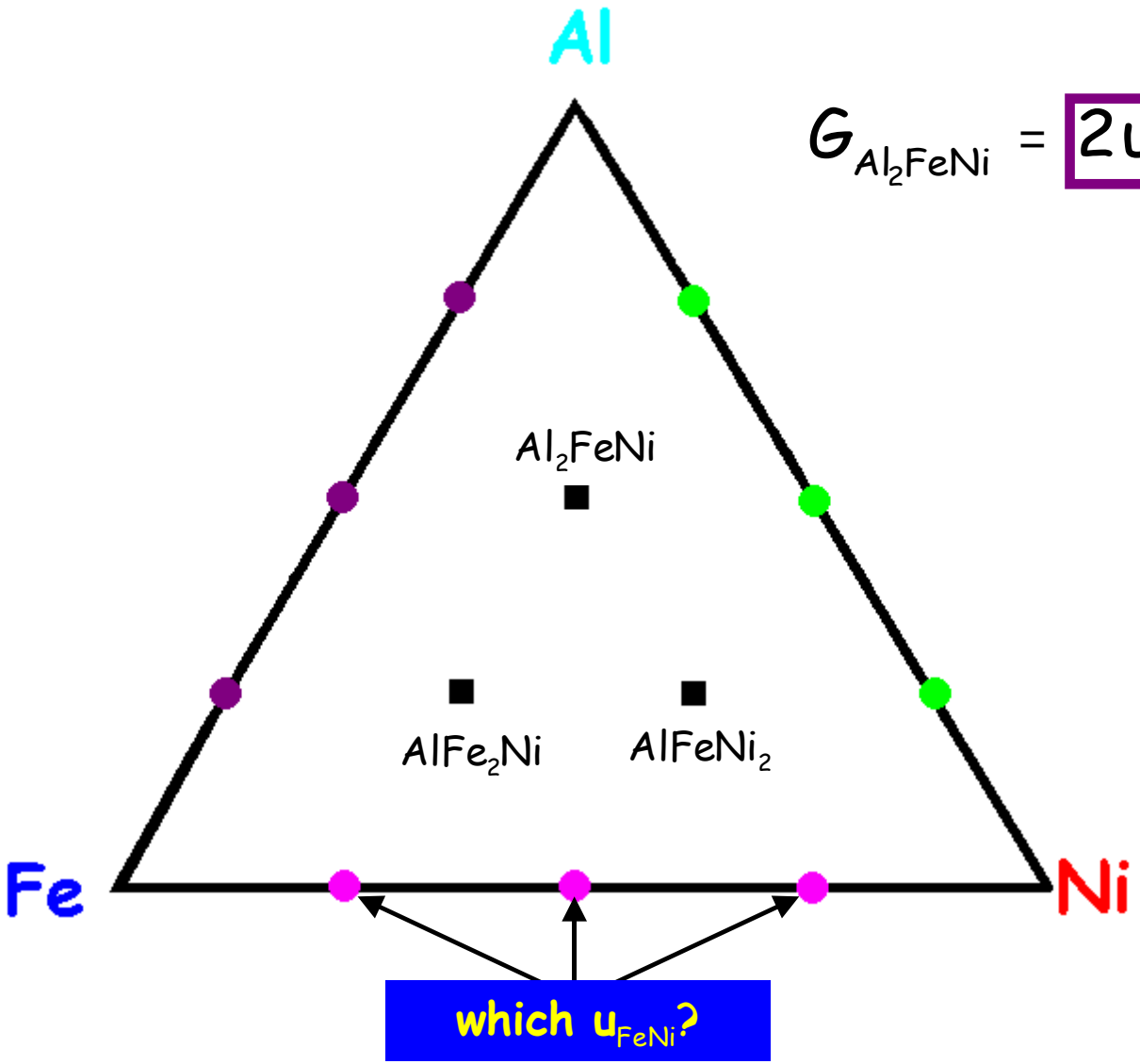


Critical assessment

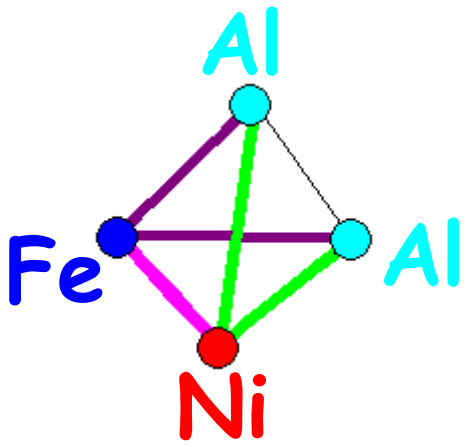


Thermodynamic description

4.a. Ternary fcc "compounds"

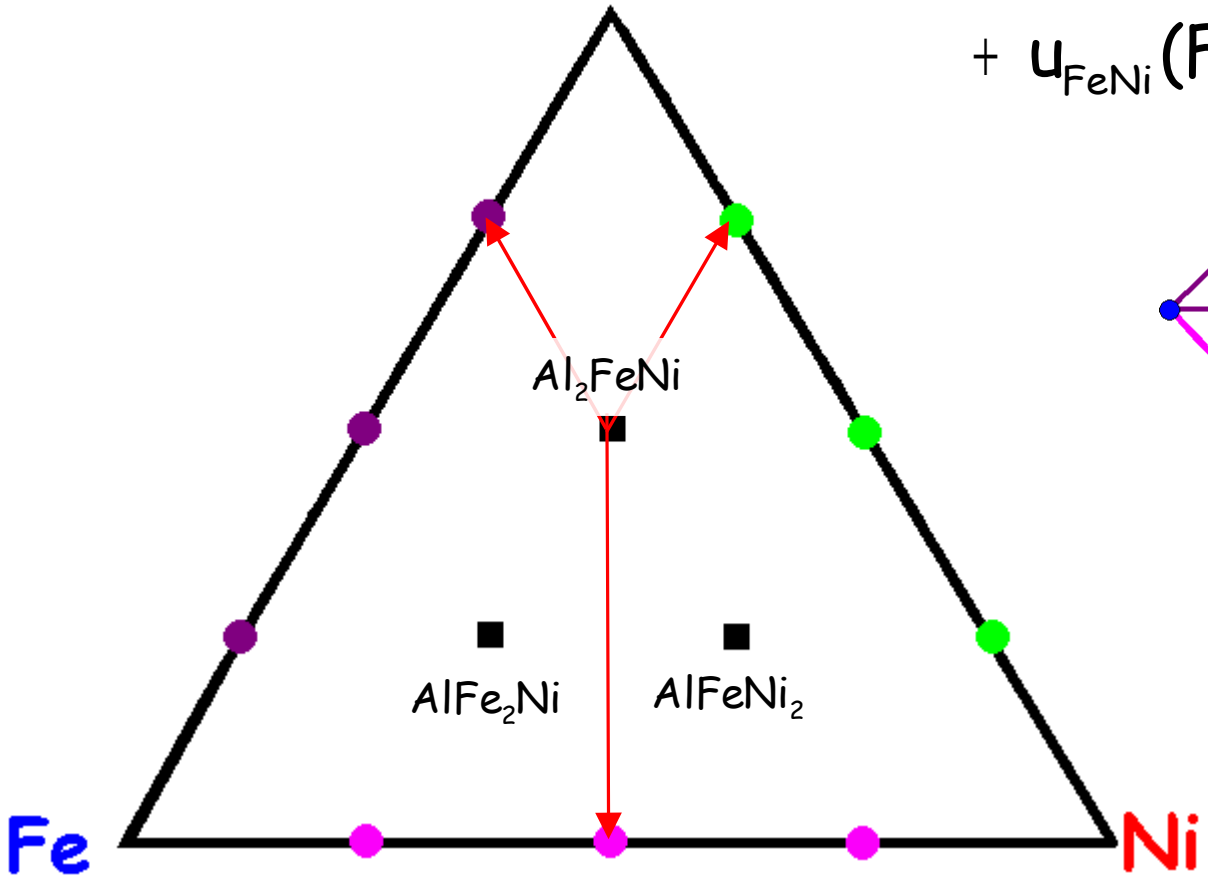


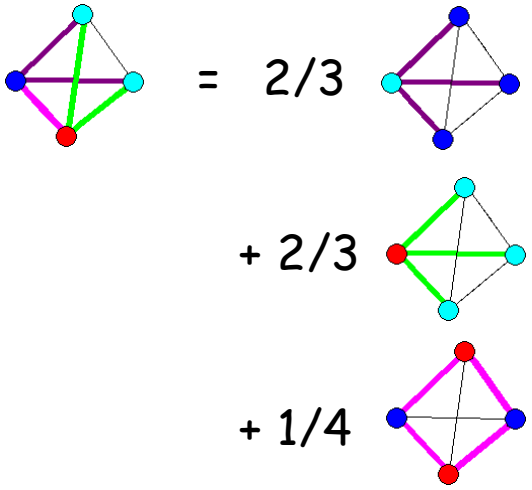
$$G_{Al_2FeNi} = \boxed{2u_{AlFe}} + \boxed{2u_{AlNi}} + \boxed{u_{FeNi}}$$



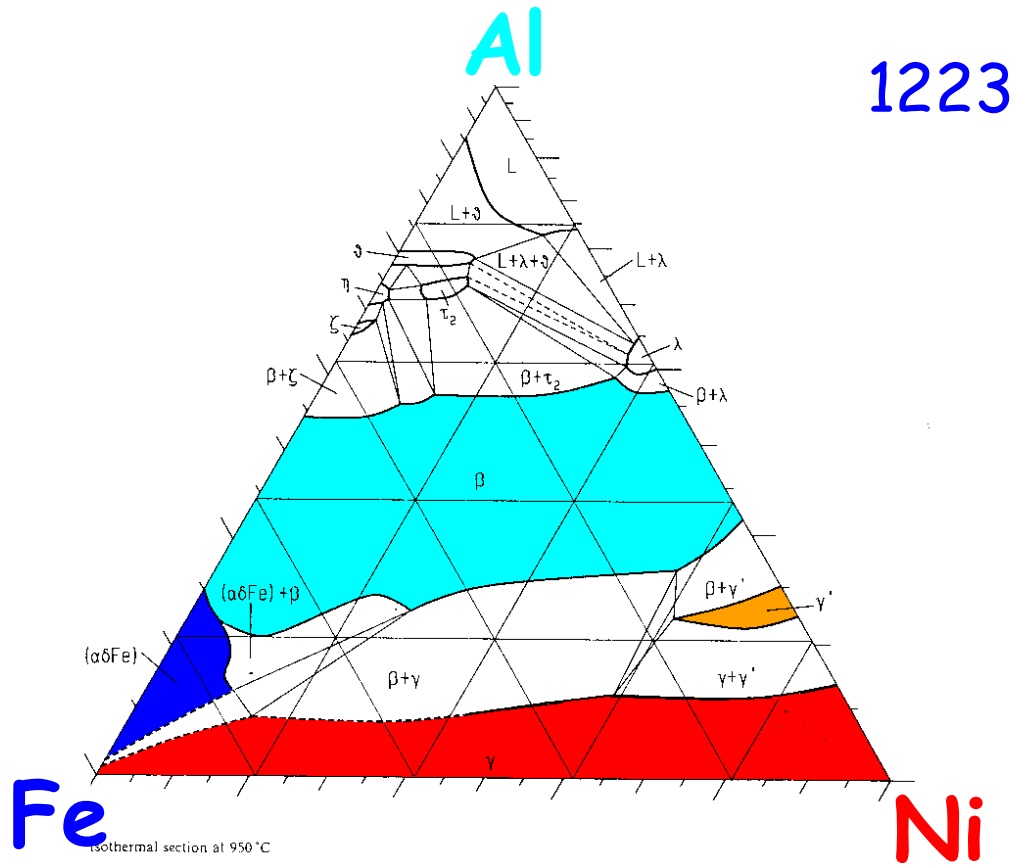
4.a. Ternary fcc "compounds"

$$G_{Al_2FeNi} = 2u_{AlFe}(Al_3Fe) + 2u_{AlNi}(Al_3Ni) + u_{FeNi}(Fe_2Ni_2)$$





4.a.Ternary fcc "compounds"



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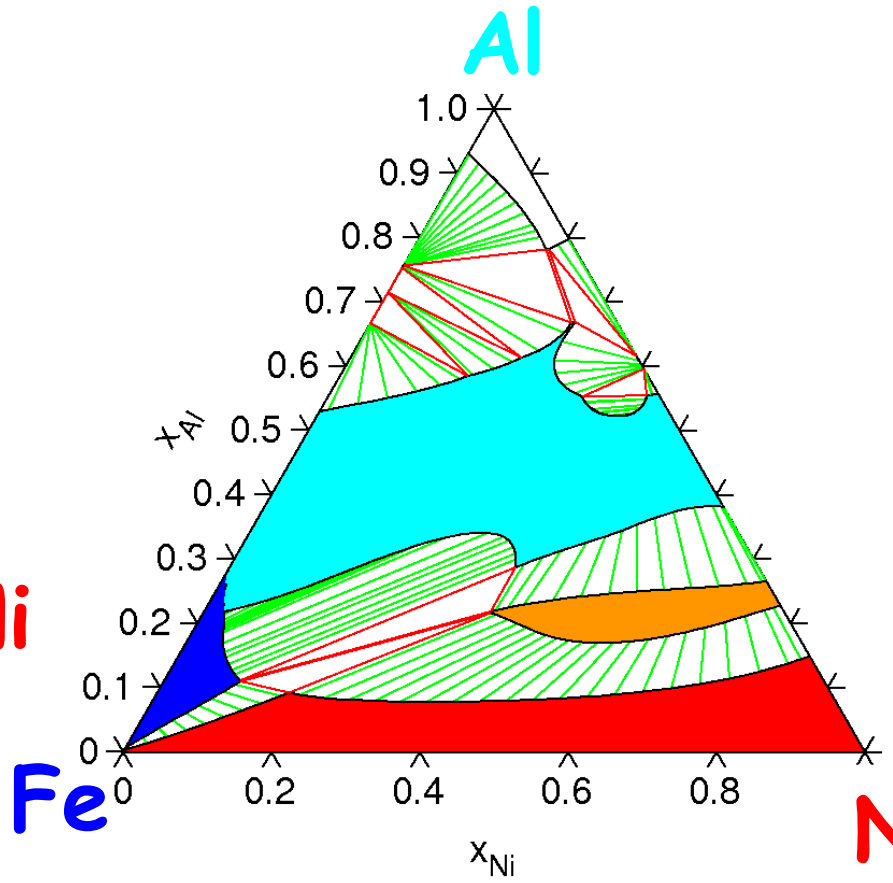


Critical assessment

Thermodynamic description

4.b.Ternary fcc reciprocal parameters

In the binary systems, the reciprocal parameters have been shown to be able to simulate the effect of SRO.

In a paper dedicated to Himo Ansara dealing with fcc prototypes, it has been proposed to expressed these parameters in ternary systems

$$L_{A,B:A,C:*:*} = \frac{1}{2}u_{AB} + \frac{1}{2}u_{AC} - \frac{1}{2}u_{BC}$$

used in the following

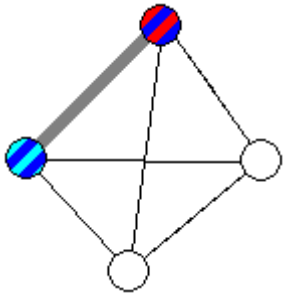
4.b.Ternary fcc reciprocal parameters

$$L_{A,B:A,C:*:*} = \frac{1}{2}u_{AB} + \frac{1}{2}u_{AC} - \frac{1}{2}u_{BC}$$

actually applied as

$$L_{A,B:A,C:*:*} = \frac{1}{2}L_{A,B:A,B:*:*} + \frac{1}{2}L_{A,C:A,C:*:*} - \frac{1}{2}L_{B,C:B,C:*:*}$$

4.b.Ternary fcc reciprocal parameters



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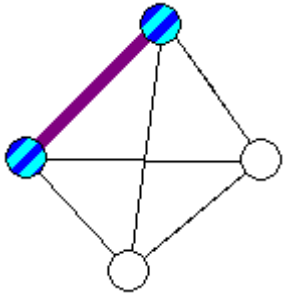

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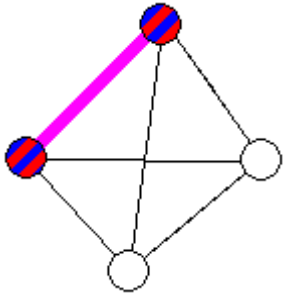

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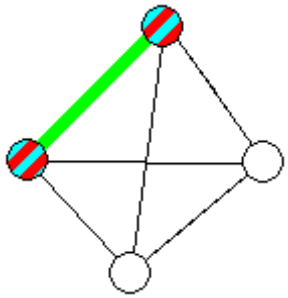

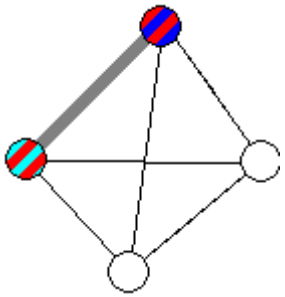

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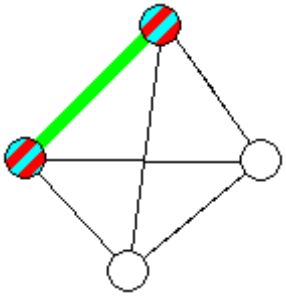

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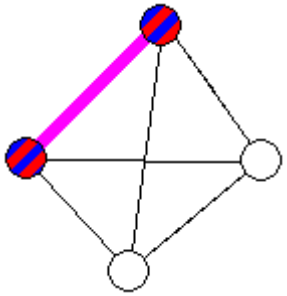

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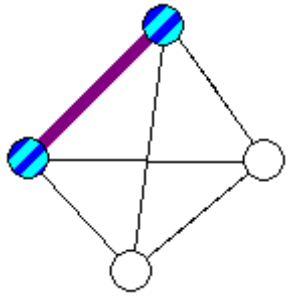

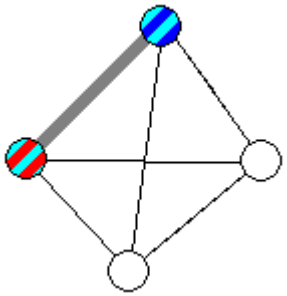

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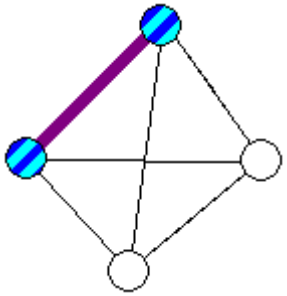

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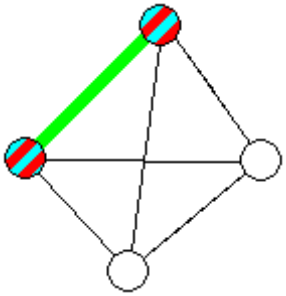

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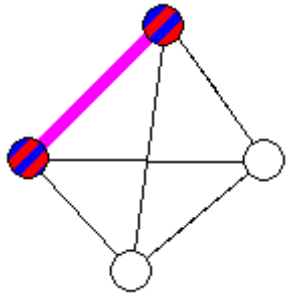
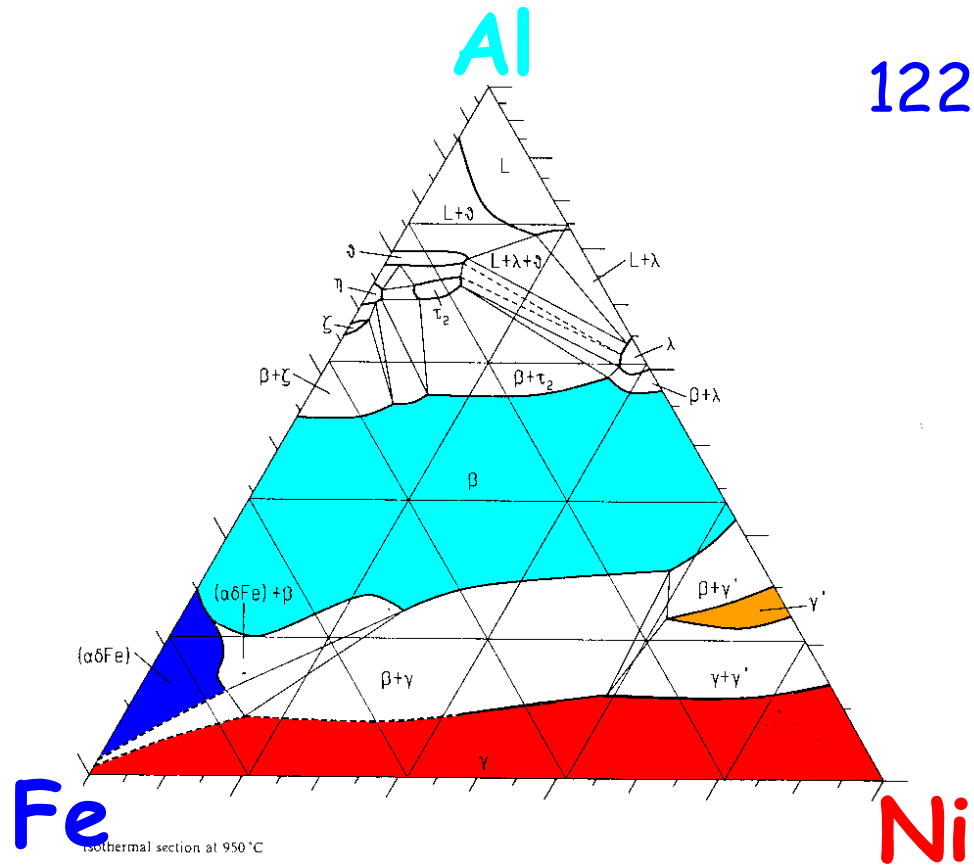


4.b.Ternary fcc reciprocal parameters



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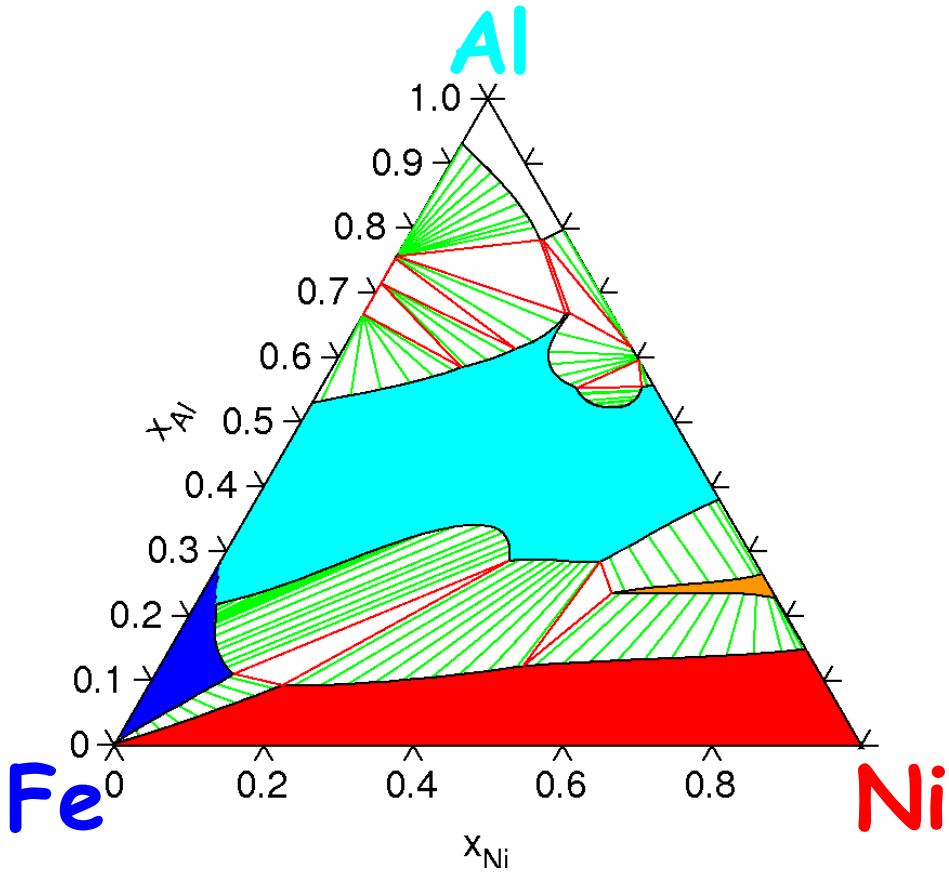

Critical assessment

Thermodynamic description

5. Discussion

Very good starting values are obtained to describe the equilibria envolving the A1, L12, A2 and B2 phase just **extrapolating the binary descriptions**

Before the optimisation procedure, it is planned to

- change the model used for the bcc ordering : 2SL → 4SL,

- test recent ab initio results, in particular for Fe-Ni bcc and Al-Fe fcc,

- acquire more experiments, in particular liquidus/ solidus in the Fe-rich corner.