The GTT Aluminium database

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Introduction:

Why an additional Al-database?

- starting from existing database (former project, exp. results)
- several metastable phases in Al-Mg-Si system considered by Povoden-Karadeniz et al.[1]
  (great importance for production of light-weight alloys)
- more emphasis on experimental results (c_p-functions)

[1] E. Povoden-Karadeniz, P. Lang, P. Warczok, A. Falahati, W. Jun, E. Kozeschnik, Calphad 43 (2013) 94

Database:

Contents:

elements 8: Al, Cu, Fe, Mg, Mn, Ni, Pb, Si

binary systems (28/28): Al-Cu, Al-Fe, Al-Mg, Al-Mn, Al-Ni, Al-Pb, Al-Si, Cu-Fe, Cu-Mg, Cu-Mn, Cu-Ni, Cu-Pb, Cu-Si, Fe-Mg, Fe-Mn, Fe-Ni, Fe-Pb, Fe-Si, Mg-Mn, Mg-Ni, Mg-Pb, Mg-Si, Mn-Ni, Mn-Pb, Mn-Si, Ni-Pb, Ni-Si, Pb-Si, (Al-Zr) optimised

Database:

ternary systems (10/56): Al-Cu-Mg, Al-Cu-Si, Al-Fe-Mg, Al-Fe-Ni, Al-Mg-Si, Cu-Fe-Ni, Al-Fe-Mn, Al-Fe-Si, Al-Mg-Mn, Al-Mn-Si

ternary systems containing Al (9/21) ⇒ still not complete

solution phases: 65
stoichiometr. condensed phases: 52
reference states for elements (s, l)

Database:

metastable Al,Mg,Si phases contained in the database[1]:

CL_MGSI	MgSi-co-clusters	$(Mg,Si)_1$
GP_MAT	Guinier-Preston-zones	$(Al,Mg,Si)_1(Al,Mg,Si)_1$
	(GP) "Matsuda-phase"	$(Al,Mg,Si)_1(Al,Mg,Si)_1$
	ordered FCC phase	
Al2Mg5Si4	Al-ß"	$(Al)_2(Mg)_5(Si)_4$
Al4Mg8Si7	B'_H	$(Al)_4(Mg)_8(Si)_7$
Al3Mg9Si7	B'_L	$(Al)_3(Mg)_9(Si)_7$
Mg9Si5	ß'	$(Mg)_9(Si)_5$
Mg5Si6	ß"	$(Mg)_5(Si)_6$
u1_phase	u1	$(Al)_2(Mg)_1(Si)_2$
u2_phase	u2	$(Al)_1(Mg)_1(Si)_1$

[1]E. Povoden-Karadeniz, P. Lang, P. Warczok, A. Falahati, W. Jun, E. Kozeschnik, Calphad 43 (2013) 94

The ternary Al-Mg-Si system:

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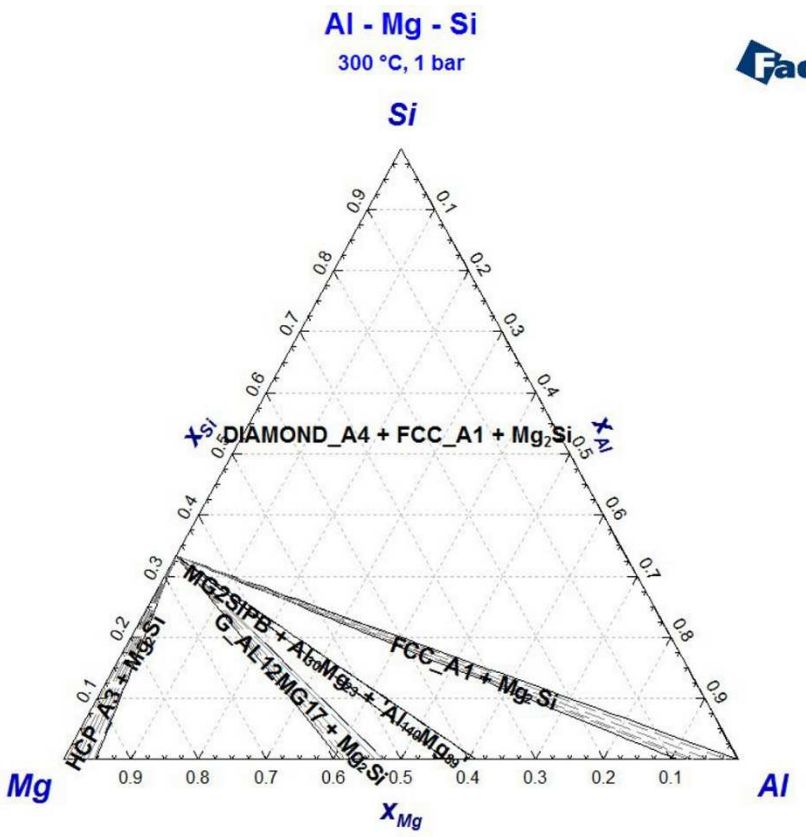
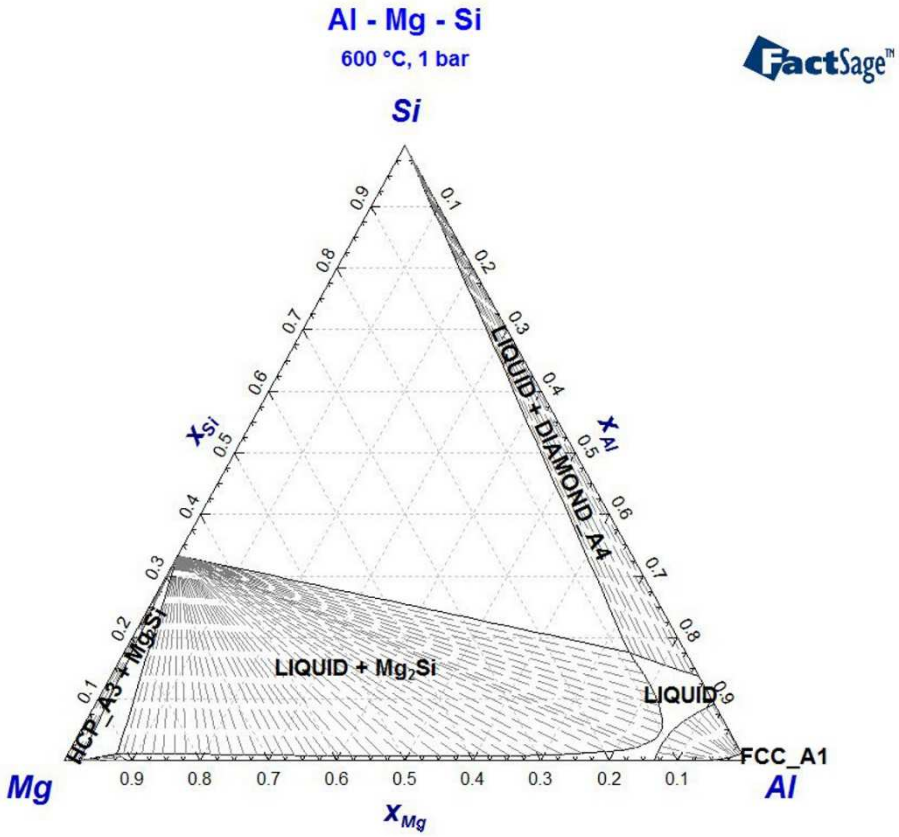
isothermal cross sections (300°C, 600°C)





dominating phase: Mg_2Si

The ternary system Al-Fe-Ni

ternary system Al-Fe-Ni neither in SGTE nor FSstel

Thermodynamic assessment from literature:

ELSEVIER

Available online at www.sciencedirect.com
ScienceDirect
Acta Materialia 57 (2009) 5324–5341

Acta MATERIALIA
www.elsevier.com/locate/actamat

Thermodynamic properties of the Al–Fe–Ni system acquired via a hybrid approach combining calorimetry, first-principles and CALPHAD

Lijun Zhang [a], Jiong Wang [a], Yong Du [a,*], Rongxiang Hu [b], Philip Nash [b], Xiao-Gang Lu [c], Chao Jiang [a]

[a] *State Key Laboratory of Powder Metallurgy, Central South University, Changsha, Hunan 410083, China*
[b] *Thermal Processing Technology Centre, Illinois Institute of Technology, 10 West, 32nd Street, Chicago, IL 60616, USA*
[c] *Thermo-Calc Software AB, Björnnäsvägen 21, 113 47 Stockholm, Sweden*

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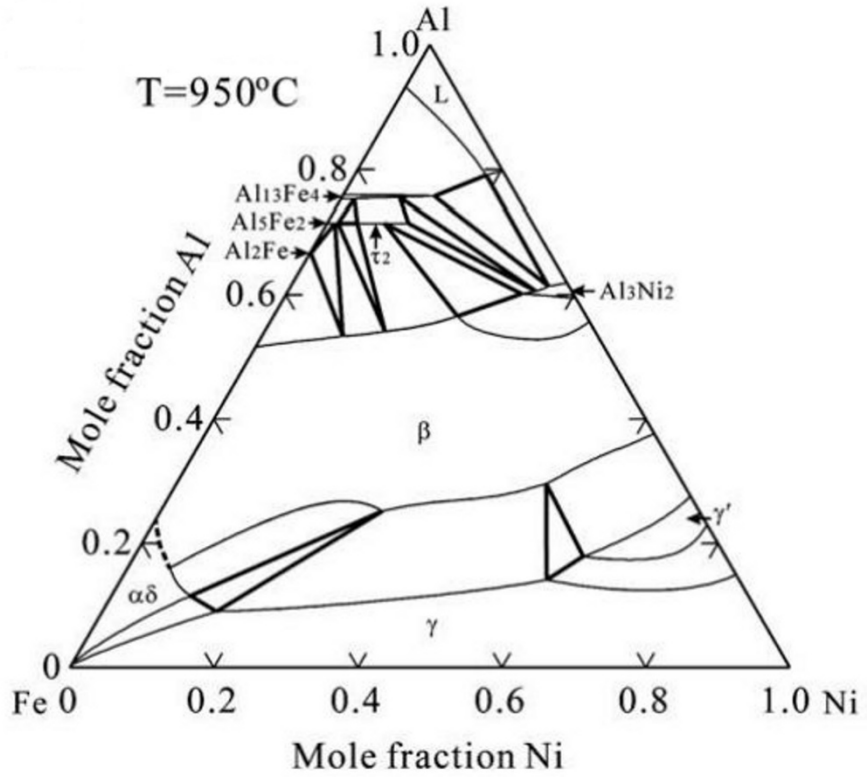
Available online 21 August 2009

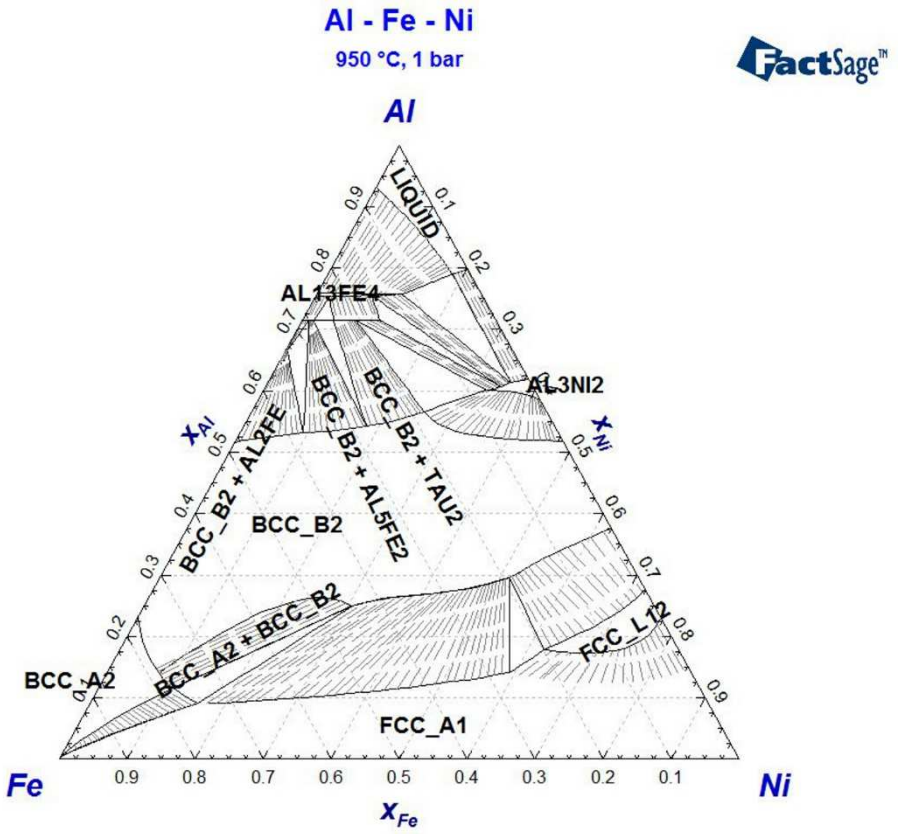
incorporation into database after critical inspection!

The ternary system Al-Fe-Ni

comparison of isothermal sections:



Zhang et al. (2009)

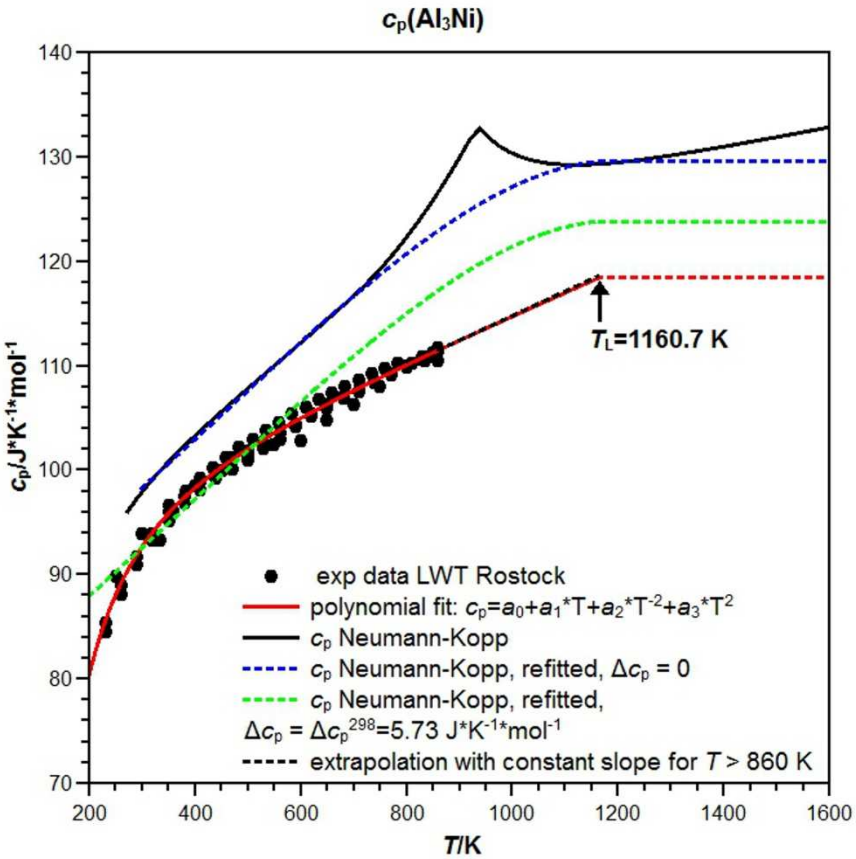


calculated from database

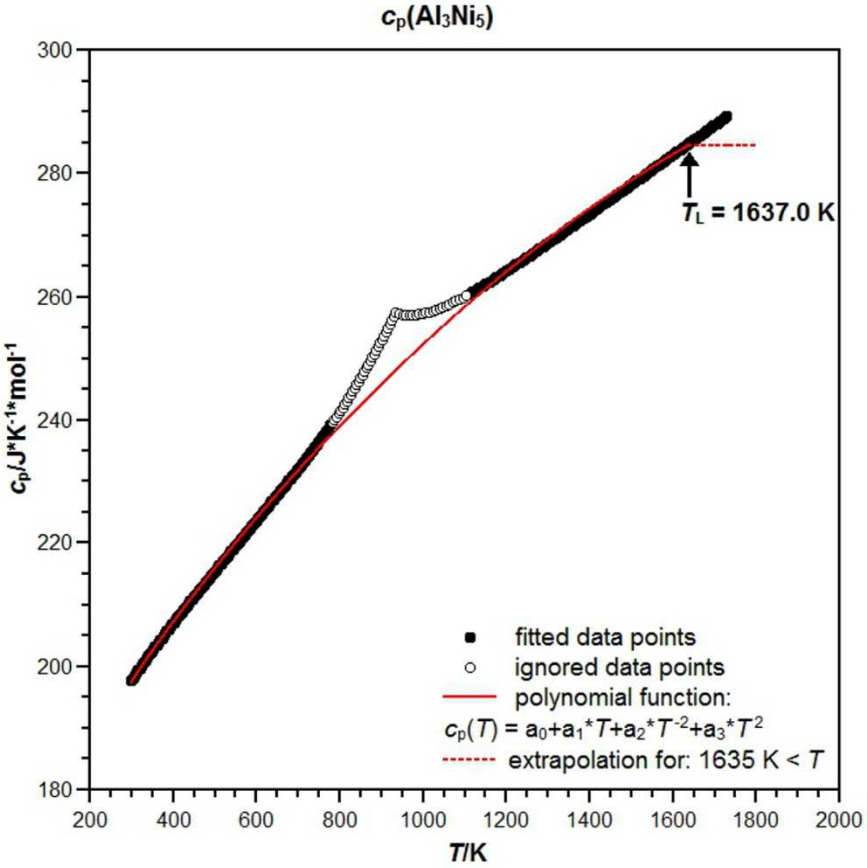
Experimental data for c_p:

Al-Ni binary system:

$c_p(Al_3Ni)$: (LWT Rostock)

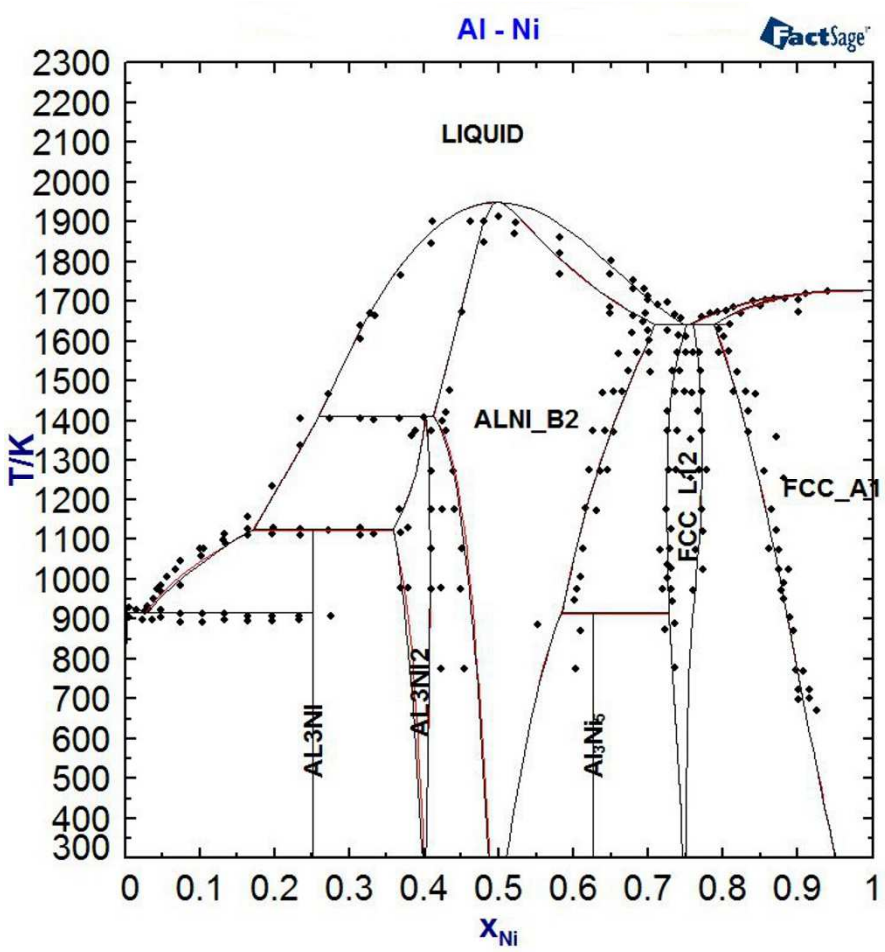


$c_p(Al_3Ni_5)$: refitted Neumann-Kopp



Experimental data for c_p:

reoptimization of binary Al-Ni:

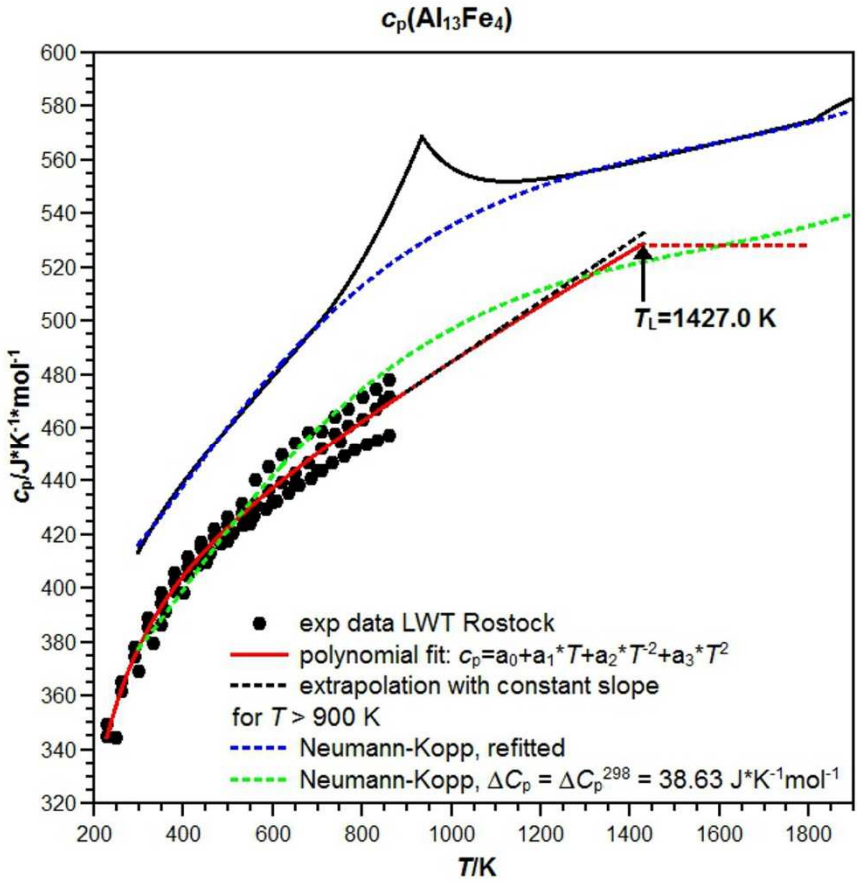


comparison between:

initial phase diagram (black),
optimised phase diagram (red)
experimental data

Experimental data for c_p:

Al-Fe binary system:



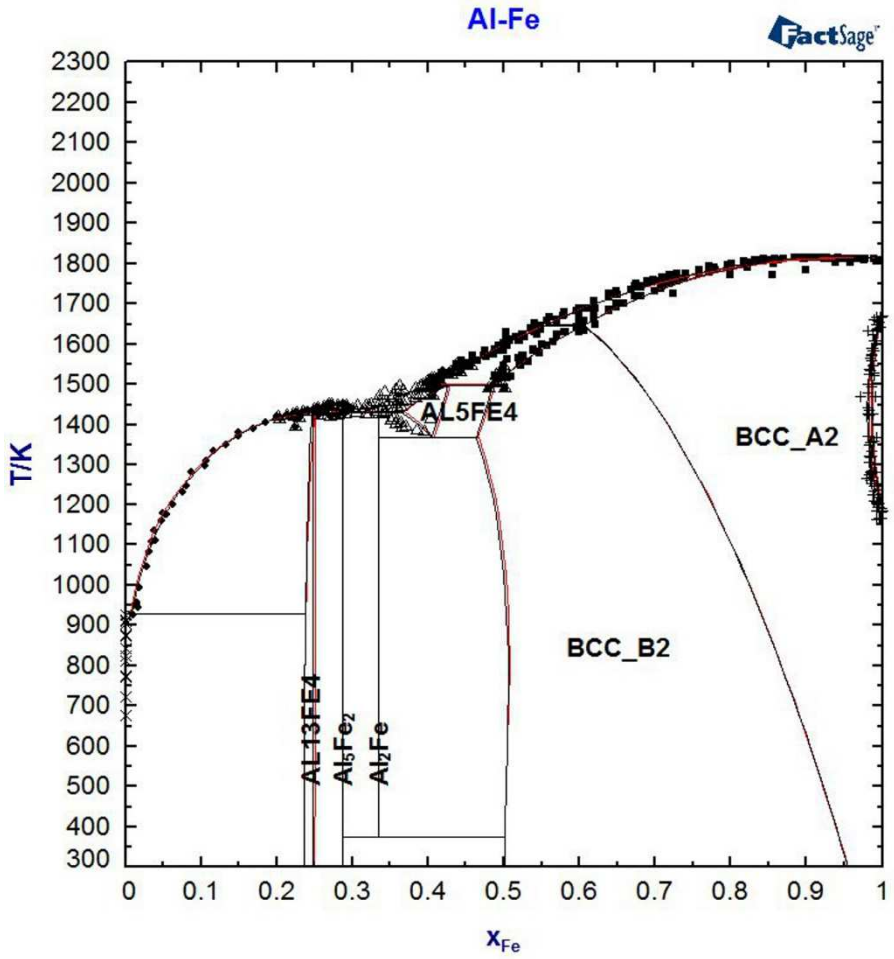
AL13FE4 is non-stoichiometric (solution phase), modelled $(Al)_{32}(Fe)_{12}(Al,Va)_7$,

end-members:
$(Al)_{32}(Fe)_{12}(Al)_7 = (Al)_{13}(Fe)_4$
$(Al)_{32}(Fe)_{12}(Va)_7 = (Al)_8(Fe)_3$

Assumption (within experimental precision):
$c_p(Al_8Fe_3)/11 = c_p(Al_{13}Fe_4)/17$
per moles of atoms

Experimental data for c_p:

reoptimization of binary Al-Fe:

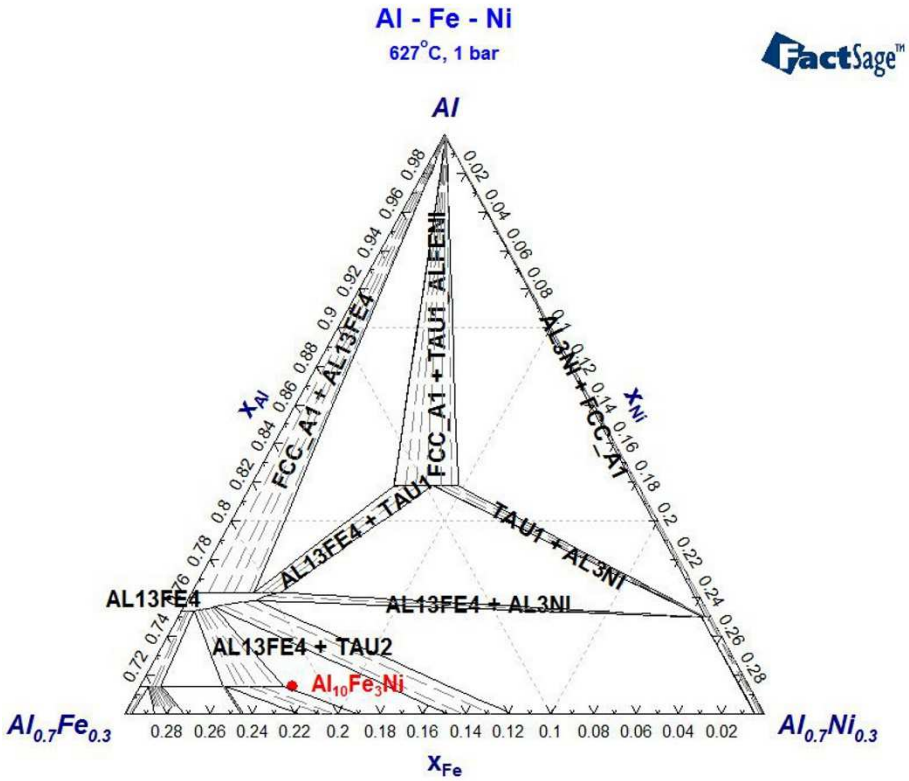


comparison between:

initial phase diagram (black),
optimised phase diagram (red)
experimental data

Experimental data for c_p:

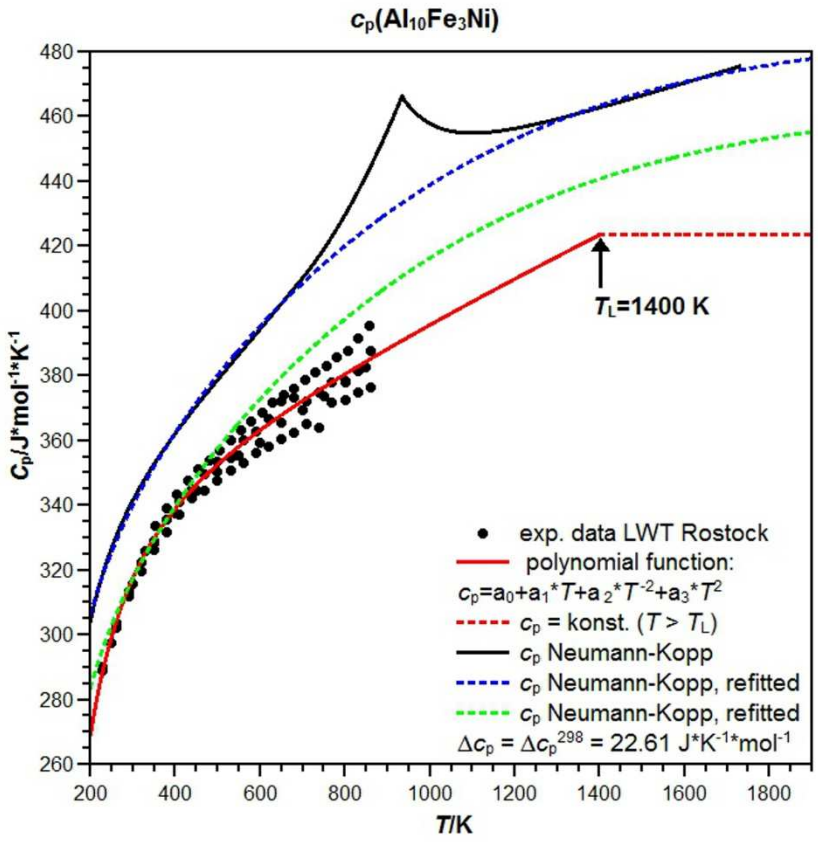
c_p-measurement for $Al_{10}Fe_3Ni$ (TAU2) (LWT Rostock)



TAU2:
model $(Al)_5(Fe,Ni)_2$
end members:
Al_5Fe_2 – Al_5Ni_2

Experimental data for c_p:

TAU2: $(Al)_5(Fe,Ni)_2$
end members: Al_5Fe_2 – Al_5Ni_2



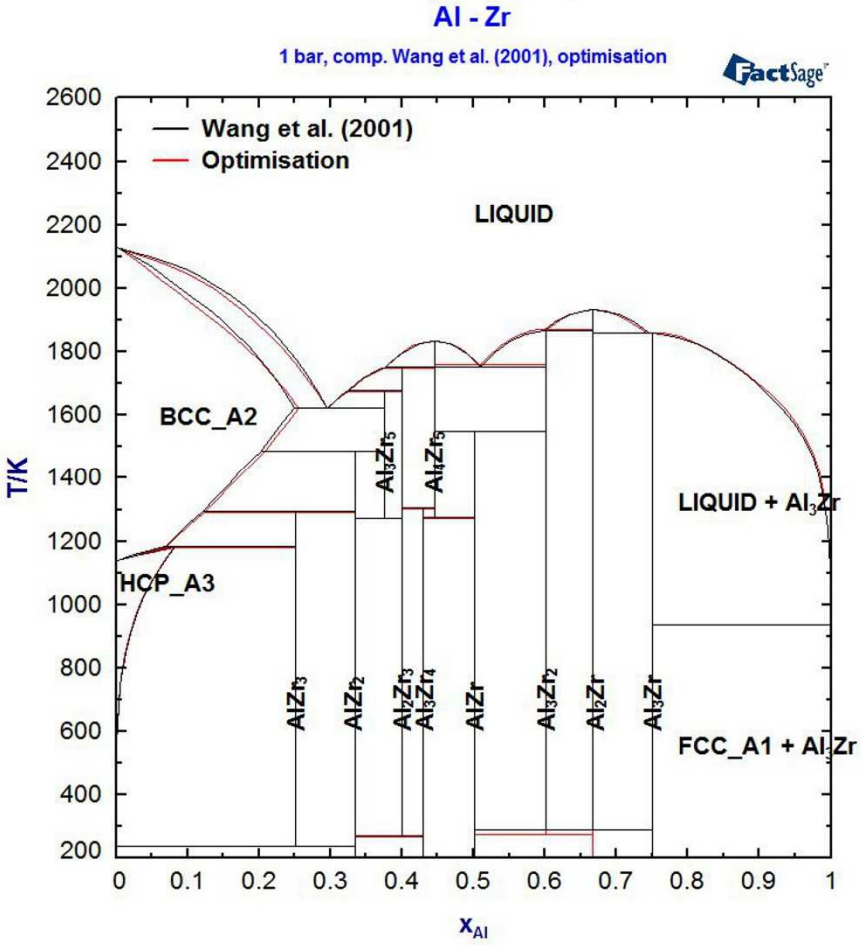
same assumption as for AL13FE4:

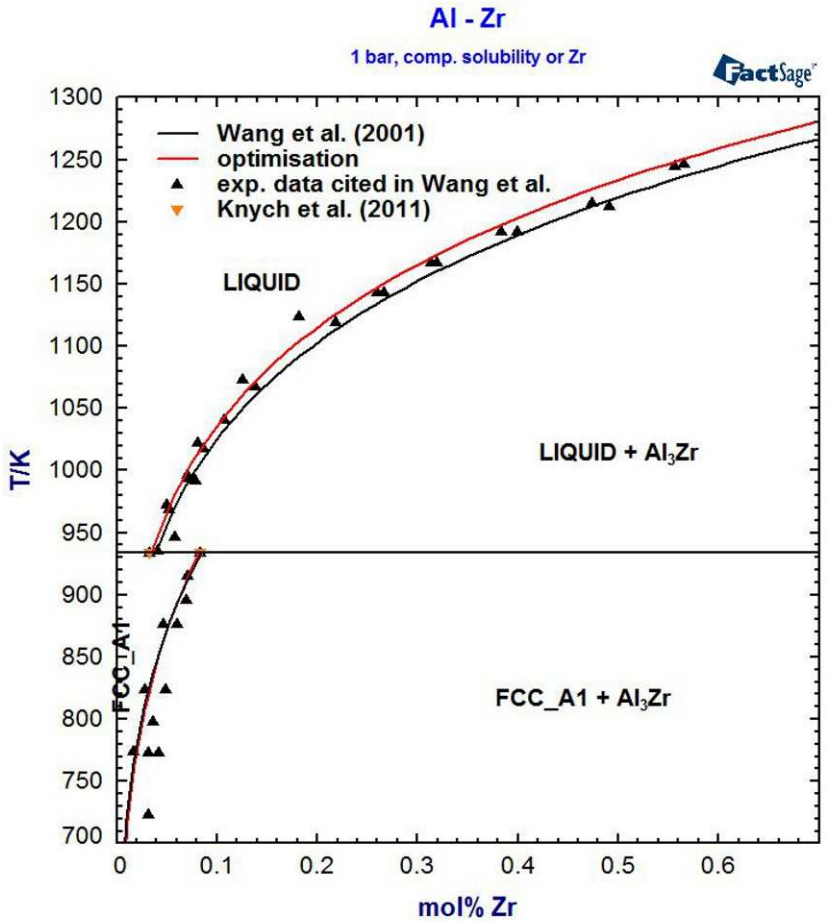
$c_p(Al_5Fe_2)/7 = c_p(Al_5Ni_2)/7 = c_p(Al_{10}Fe_3Ni)/14$ per mole of atoms

Reoptimization of ternary Al-Fe-Ni system with experimentally based c_p-functions in progress

Experimental data for c_p:

binary system Al-Zr optimized with exp. $c_p(Al_3Zr)$[2] and solubility of Zr in Al(fcc) and LIQUID[3]





[2]T. Knych et al., Archives Met. Mater. 56(3) (2011) 685

[3]LWT Rostock

Metastable phases in Al-Mg-Si :

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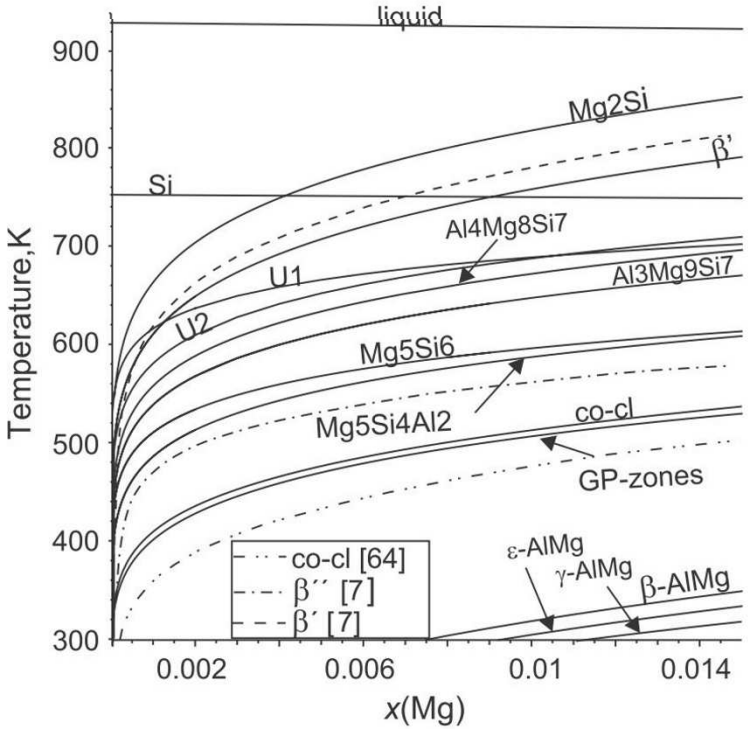
metastable equilibria in Al-Mg-Si system of great importance for precipitation hardening[1]:

supersatured solid solution (rt) → clusters → co-clusters → GP-zones → ß" → ß', $ß'_H$, $ß'_L$, u_1, u_2



solvi of metastable phases compared to Mg_2Si for an AA6016 alloy (0.76at% Si)[2]

[1] E. Povoden-Karadeniz, P. Lang, P. Warczok, A. Falahati, W. Jun, E. Kozeschnik, Calphad 43 (2013) 94

Metastable phases in Al-Mg-Si :

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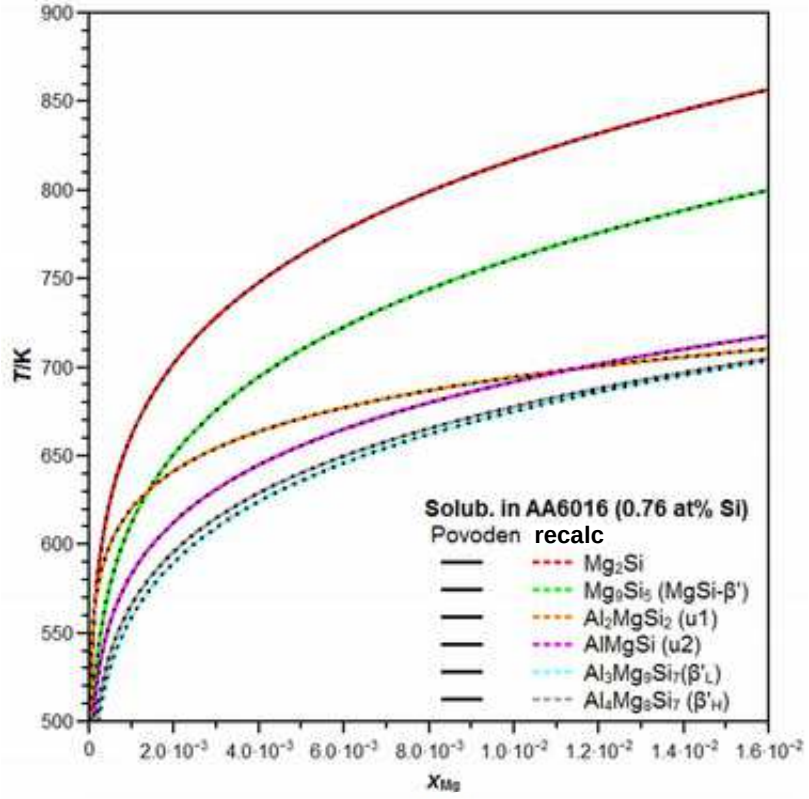
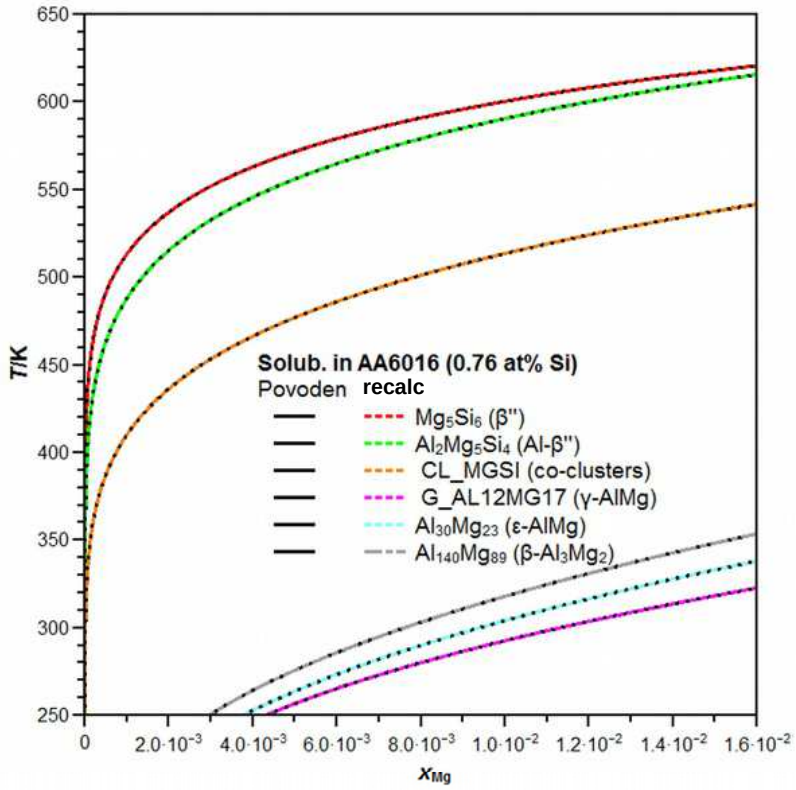
recalculation of solvi in Al(fcc), comp. to Povoden-Karadeniz et al.



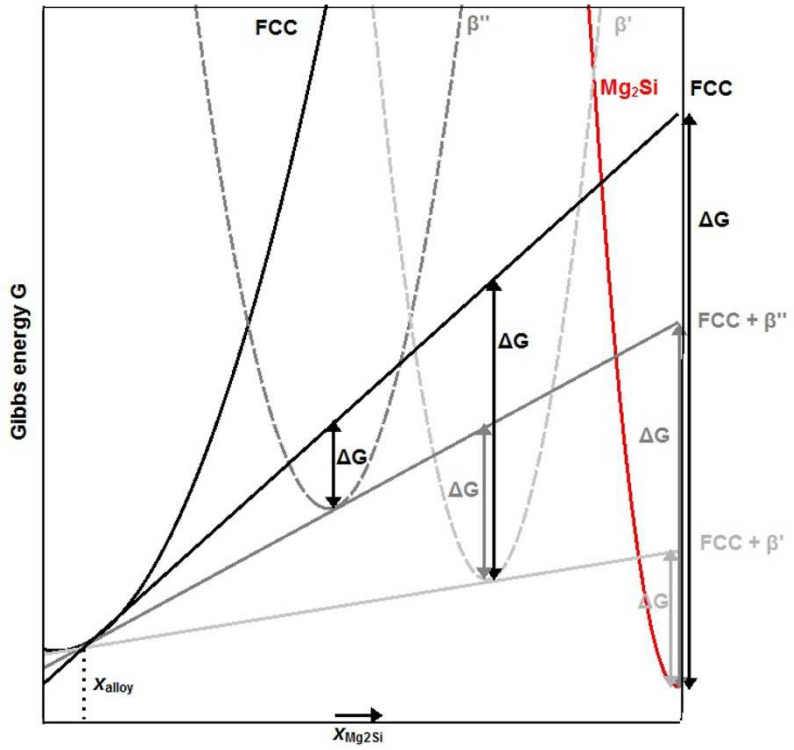
stable phase: Mg_2Si



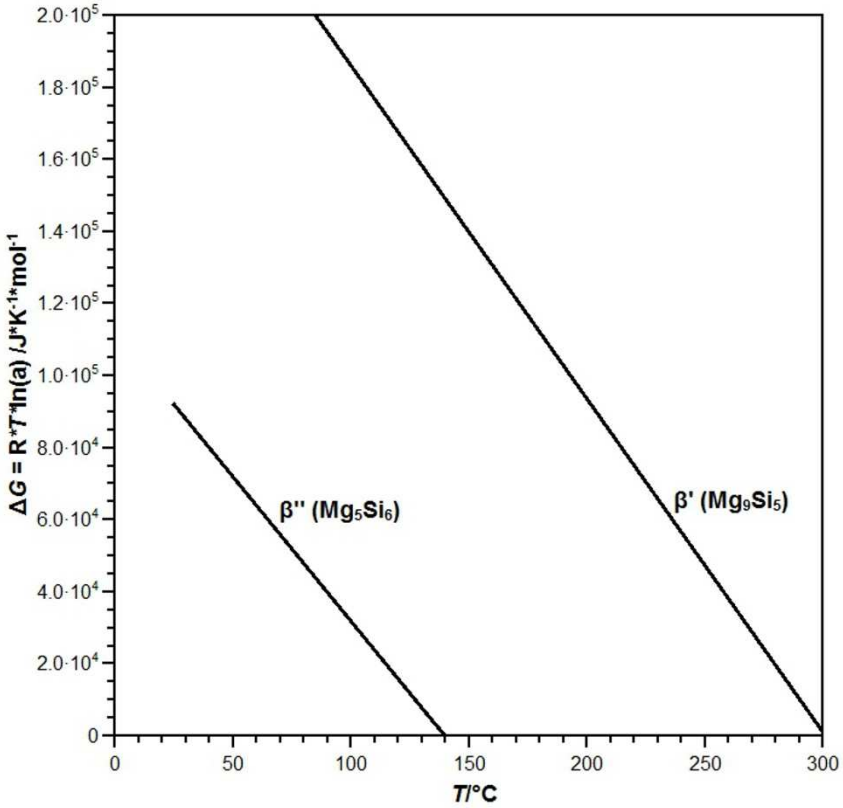
stable phases: β-, γ-, ε-AlMg

Metastable phases in Al-Mg-Si :

Gibbs energy diagram of selected metastable phases (sketch)

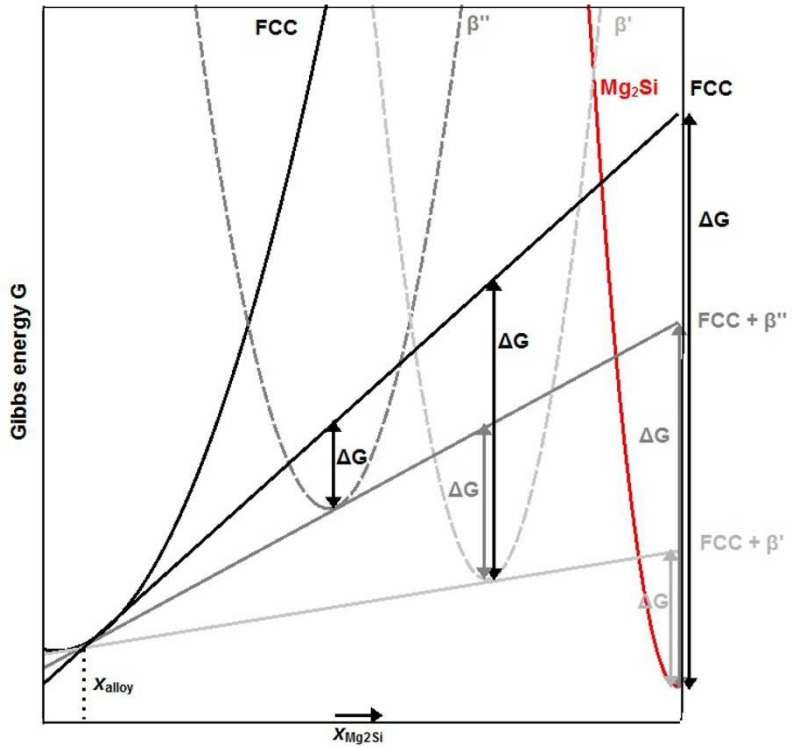


driving forces only FCC present

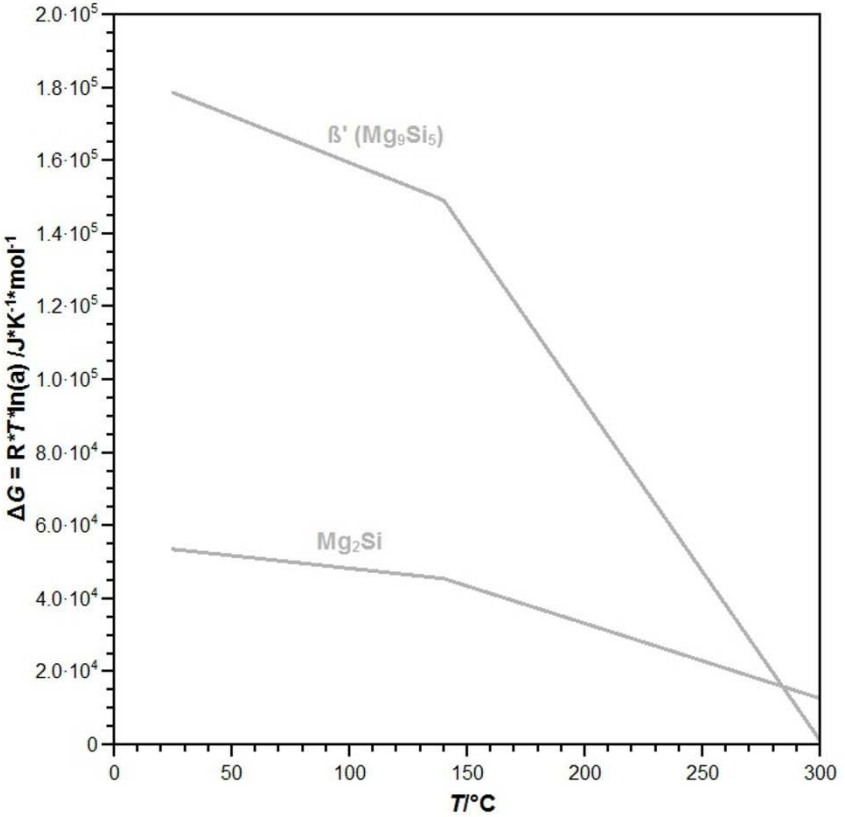


Metastable phases in Al-Mg-Si :

Gibbs energy diagram of selected metastable phases (sketch)



driving forces, FCC + ß" present



Summary:

- **Actual contents of database:**
  8 elements, 28 binary-, 10 ternary systems, 65 solution phases, 52 stoichiometr. compounds, metastable phases (Al-Mg-Si: 9)

- **New thermodynamic assessment for Al-Fe-Ni (Zhang et al. 2009)**

- **Use of exp. $c_p(T)$ for Al_3Ni, "$Al_{13}Fe_4$", Al_3Zr, "$Al_{10}Fe_3Ni$" (TAU2) $\Rightarrow$ reoptimization of Al-Ni, Al-Fe, Al-Zr binary systems, Al-Fe-Ni ternary system ongoing**

- **Calculations using the database (examples), metastable phases in the Al-Mg-Si ternary system**

Thanks for your attention !