Modelling chemical ordering with Thermo-Calc

Nathalie Dupin

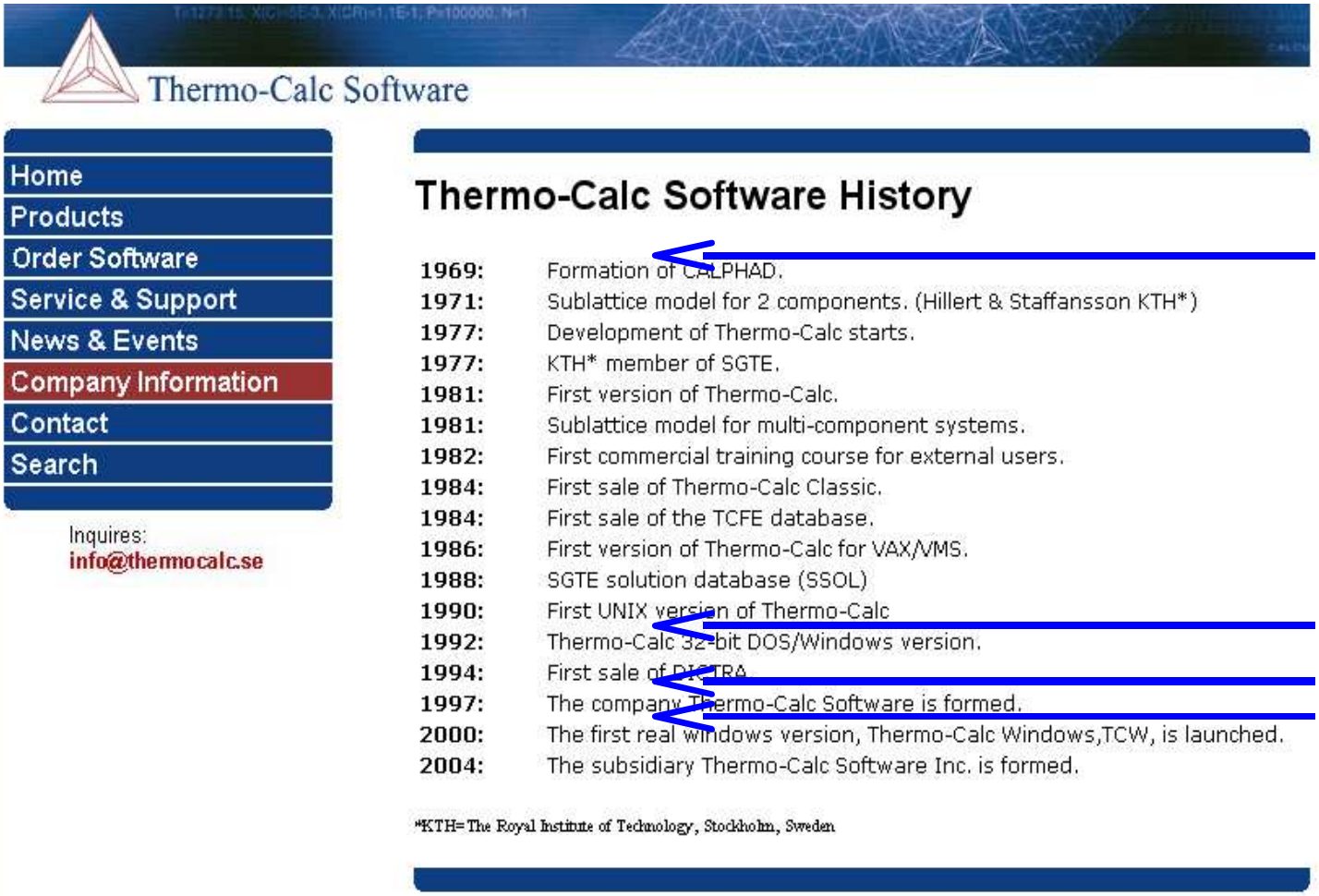
Stockholm - 2007 October 18th

My personnal experience Modelling chemical ordering with Thermo-Calc

Nathalie Dupin

Stockholm - 2007 October 18th

My short history



Thermo-Calc Software

- Home
- Products
- Order Software
- Service & Support
- News & Events
- Company Information
- Contact
- Search

Inquires:
info@thermocalc.se

Thermo-Calc Software History

1969:	Formation of CALPHAD.
1971:	Sublattice model for 2 components. (Hillert & Staffansson KTH*)
1977:	Development of Thermo-Calc starts.
1977:	KTH* member of SGTE.
1981:	First version of Thermo-Calc.
1981:	Sublattice model for multi-component systems.
1982:	First commercial training course for external users.
1984:	First sale of Thermo-Calc Classic.
1984:	First sale of the TCFE database.
1986:	First version of Thermo-Calc for VAX/VMS.
1988:	SGTE solution database (SSOL)
1990:	First UNIX version of Thermo-Calc
1992:	Thermo-Calc 32-bit DOS/Windows version.
1994:	First sale of DICTRA
1997:	The company Thermo-Calc Software is formed.
2000:	The first real windows version, Thermo-Calc Windows,TCW, is launched.
2004:	The subsidiary Thermo-Calc Software Inc. is formed.

*KTH= The Royal Institute of Technology, Stockholm, Sweden

Birth

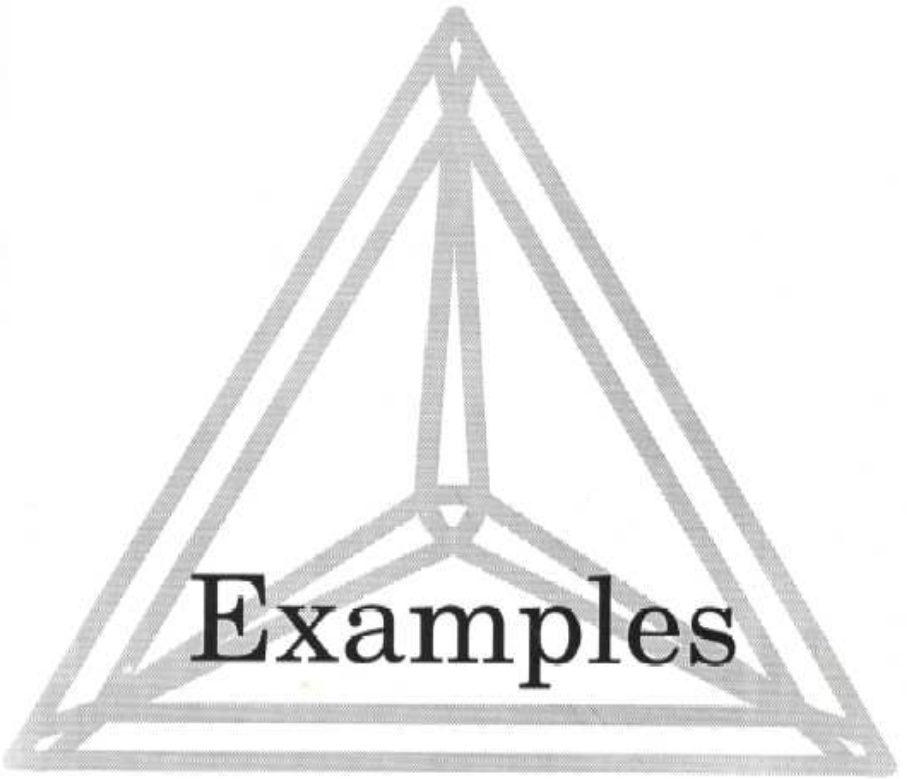
TCG on VAX in Grenoble

Doctor !

Self employed

Grenoble, October 1991

Thermo-Calc



Bo Sundman
Div of Computational Thermodynamics
Dept of Material Science and Engineering
Royal Institute of Technology
S-100 44 Stockholm, Sweden

easy!

Grenoble, October 1991

Acta metall. Vol. 36, No. 4, pp. 977–982, 1988
Printed in Great Britain. All rights reserved

0001-6160/88 $3.00 + 0.00
Copyright © 1988 Pergamon

88Ans

THERMODYNAMIC MODELING OF ORDERED PHASES IN THE Ni–Al SYSTEM

I. ANSARA[1], B. SUNDMAN[2] and P. WILLEMIN[1]

[1]Laboratoire de Thermodynamique et de Physico-Chimie Métallurgiques, UA 29 CNRS, ENSEEG, BP 75, 38400 Saint Martin d'Héres Cédex, France and [2]Division of Physical Metallurgy, Royal Institute of Technology, S-10044, Stockholm, Sweden

(*Received* 1 *October* 1986; *in revised form* 23 *June* 1987)

Abstract—The thermodynamic properties of the ordering in the $L1_2$, $D5_{13}$ and B_2 phases existing in the Al–Ni system were described using the sub-lattice model. For the B2 phase, aluminium and nickel are considered to occupy one of the sub-lattices whereas vacancies and nickel occupy the second. For the $L1_2$, $D5_{13}$ phases, aluminium and nickel mix on both sub-lattices. When, the phases are disordered the site fractions of the two elements are equal on both sub-lattices. The interaction parameters are evaluated using an assessment procedure taking into account available experimental information on thermochemical properties and phase diagram data. The calculated phase diagram is compared to previously calculated ones using different models.

$(Al,Ni)_{0.75}(Al,Ni)_{0.25}$

Relations between parameters from dG min for disorder

mit zwei Teilgittern wird angenommen, dass Alum Leerstellen das andere. In den $L1_2$ und $D5_{13}$ Pha besetzen. Im regellosen Zustand sind alle Teilgitter g werden unter Berücksichtigung der verfügbaren t Wechselwirkungsenergien bestimmt. Das mit die früheren Rechnungen verglichen.

INTRODUCTION

The Ni–Al phase diagram is characterised by a liquid phase, an f.c.c. (Al) phase at both the Al and Ni rich ends, a non congruently melting compound Al_3Ni and three intermediate phases with variable range of

shown in Fig. 1. Sigli *et al.* [3] also calculated the phase diagram by describing the thermodynamic behaviour of the NiAl and Ni_3Al phases by the cluster variation method, the other ordered phases

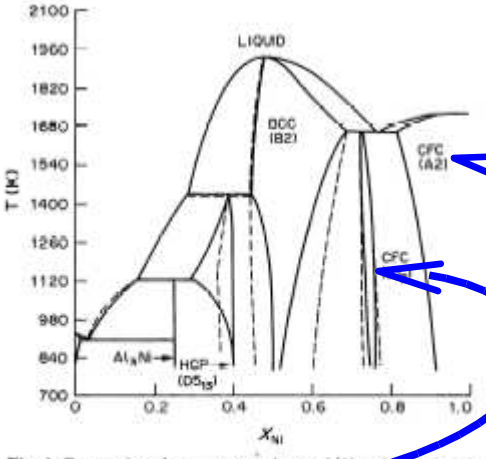


Fig. 4. Comparison between experimental [1] and calculated phase diagram [present work]. The equilibrium lines between Al_3Ni and the liquid, f.c.c. and b.c.c. phases correspond to metastable equilibria.

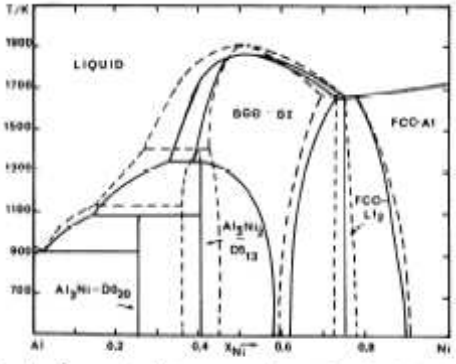


Fig. 1. Comparison between experimental and calculated phase diagram [2].

2. L. Kaufman and H. Nesor, *Calphad* **2,** 325 (1978).

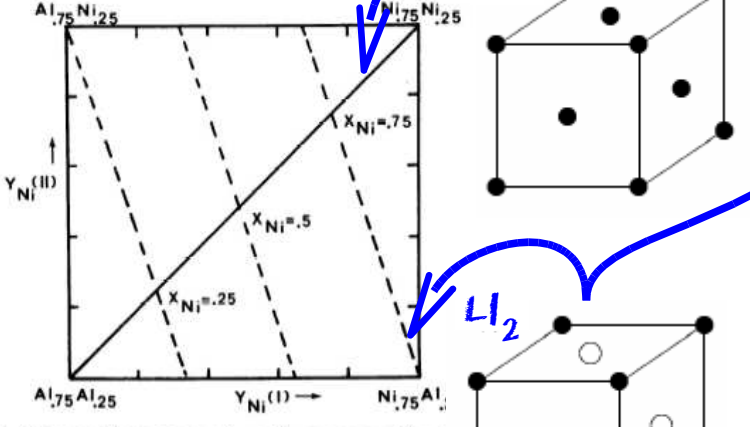


Fig. 3. Composition plane $y'_{Ni} = y''_{Ni}$ corresponding t ous molar fraction of Ni in the ordered state. The di represent the locus of composition in the disordere

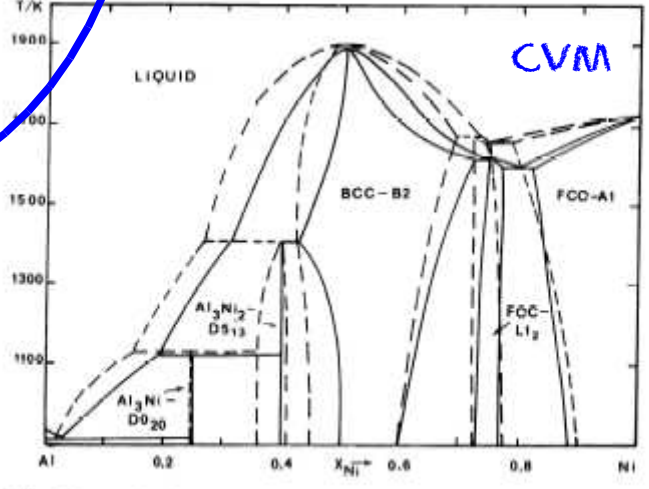
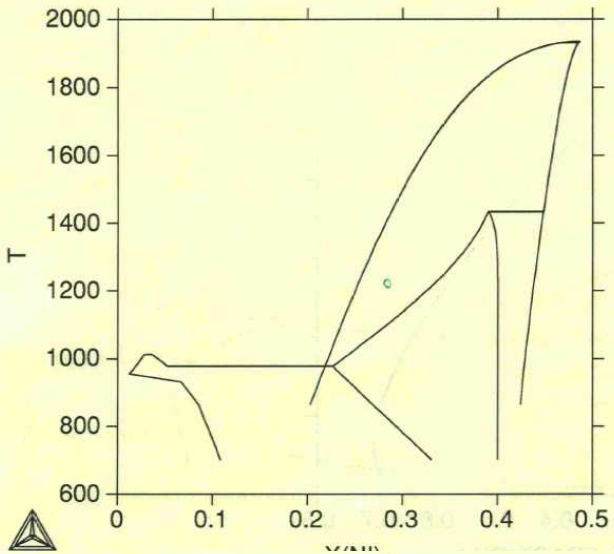


Fig. 2. Comparison between experimental [1] and calculated phase diagram [3].

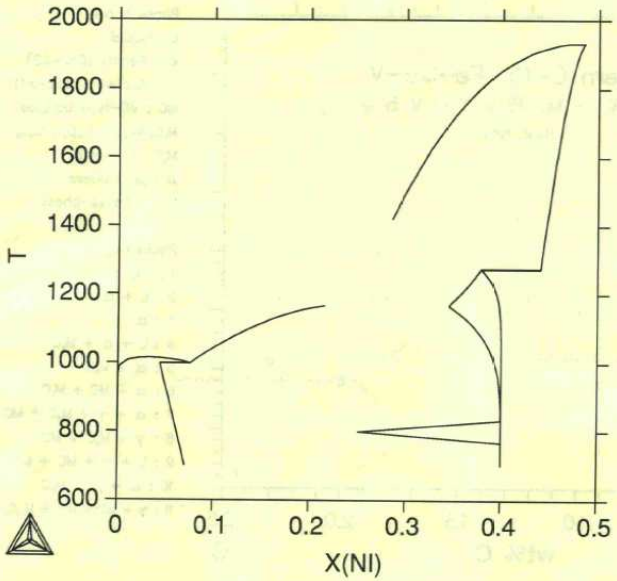
3. C. Sigli and J. M. Sanchez, *Acta metall.* **33,** 1097 (1985).

Grenoble, ...

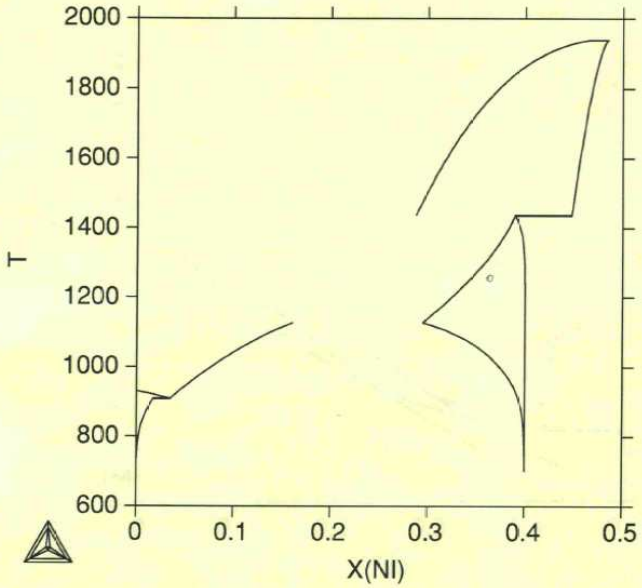
THERMO-CALC (91.11.15:13.39) :



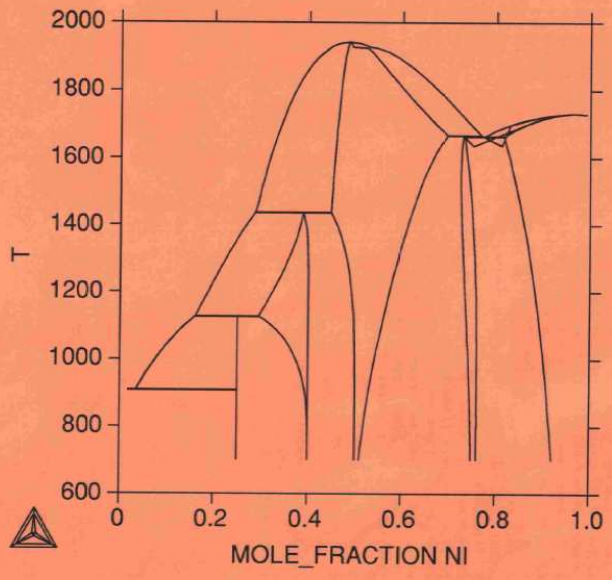
THERMO-CALC (91.11.15:14.40) :



THERMO-CALC (91.11.13:15.18) :



THERMO-CALC (92. 1.10: 8.44) :



ERROR: timeout
OFFENDING COMMAND: timeout
STACK:

on 13-NOV-1991 15:18:28.75

Help !

```
Date: 1991-11-14 06:24:15
                              Msg-ID: RFC-822
                              0095199F.62D35800.4268@ortho.matsc.kth.se  OU=
                              CICG-GW

To:   bosse@ortho.matsc.kth.se   OU=CICG-GW
From: "BO SUNDMAN, KTH. BOSSE@MATSC.KTH.SE"
bosse@ortho.matsc.kth.se      OU=CICG-GW

Subj: AL-NI

------------ Letter Body Part 1 - Text  ------------

RFC-822-HEADERS:
Received: by ortho.matsc.kth.se (MX V2.3-1) id 4268; Thu, 14 Nov 1991 00:13:06
          CET
Date: Thu, 14 Nov 1991 00:13:06 CET


------------ Letter Body Part 2 - Text  ------------

Hello Himo,

I have checked the data and there is one error. The parameters
for G(AL3NI2,AL:NI) and G(AL3NI2,NI:AL) are referred to GHSERNI
and GHSERAL, it should be GHCPAL and GHCPNI. However, this is
a quite small error and cannot explain why AL3Ni2 does not appear
where it should. The reason for that is that one has to give explicit
start composition for this phase, otherwise it becomes disordered.
Below is your command file slightly edited.

I have still not managed to calculate the whole diagram

$ set verify
$ TC
GO DATA
DEF-SYS AL NI
REJ P BCC-A2
GET
GO P-3
S-C P=1E5 N=1 X(NI)=0.35 T=1200
L-C
S-A-S
Y
C-E
S-S-C AL3NI2
NONE
.0001
.9999
C-E
```

one has to give explicit start composition

The recipe for many cases

I have still not managed to calculate the whole diagram

Not that easy...!

Help !

Date: 1992-01-21 03:40:38
Msg-ID: RFC-822
00954F14.89492460.5787@ortho.matsc.kth.se OU=
CICG-GW

To: bosse@ortho.matsc.kth.se OU=CICG-GW
From: "BO SUNDMAN, KTH. BOSSE@MATSC.KTH.SE"
bosse@ortho.matsc.kth.se OU=CICG-GW

Subj: FAX about activity stepping

---------- Letter Body Part 1 - Text ----------

RFC-822-HEADERS:
Received: by ortho.matsc.kth.se (MX V2.3-1) id 5787; Tue, 21 Jan 1992 00:55:14
CET
Date: Tue, 21 Jan 1992 00:55:14 CET

---------- Letter Body Part 2 - Text ----------

Hello Himo,

When you give the STEP command you use STEP SEPARATE and then
the activity is calculated in each phase separately. Thus you will
not have constant activity in the two-phase region. In order to
get that use STEP NORMAL

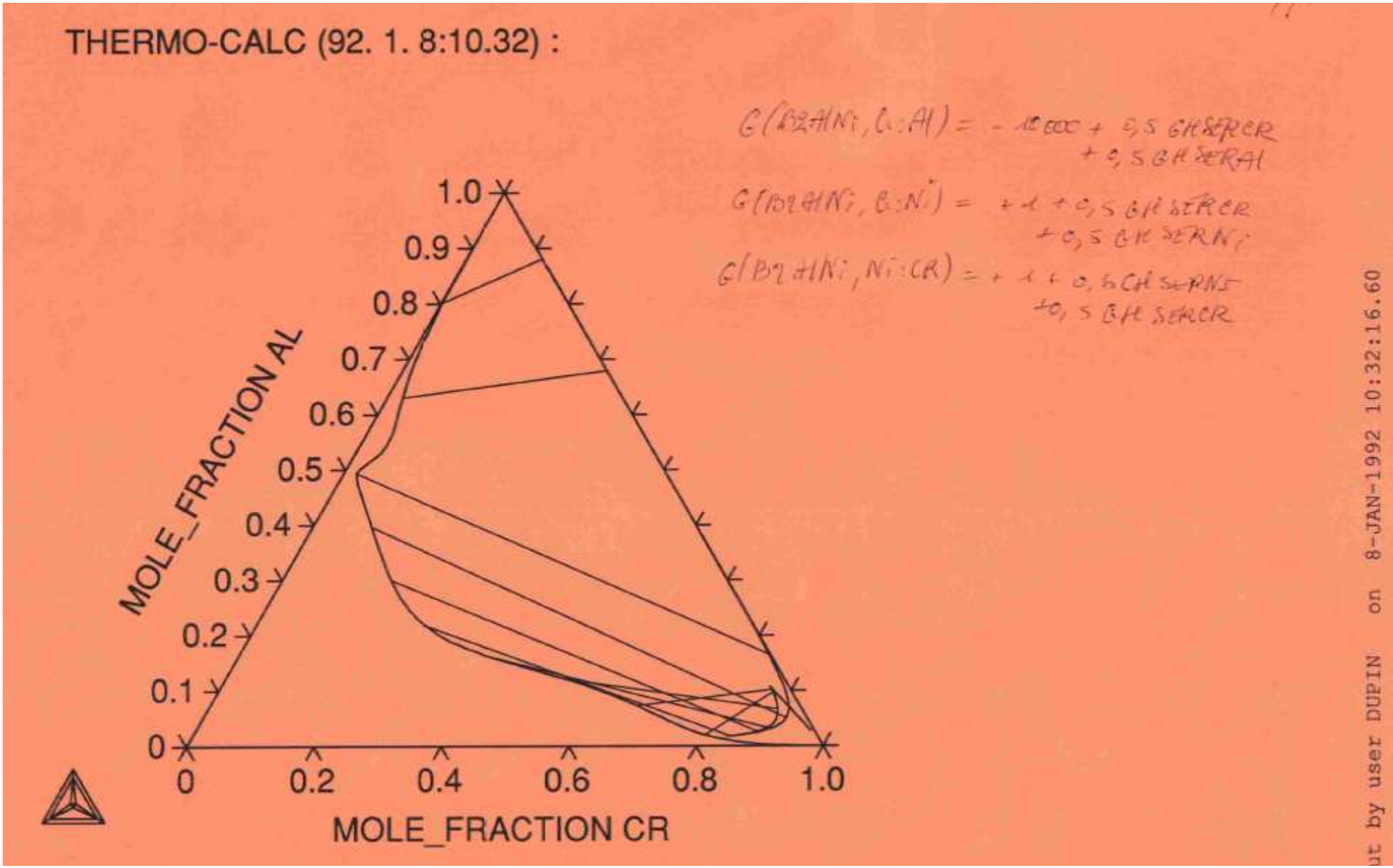
Even with step separately you get the one and two-phase regions
outputted during the STEP command. That is a bug. With step SEP
you calculate each phase separately.

Bosse

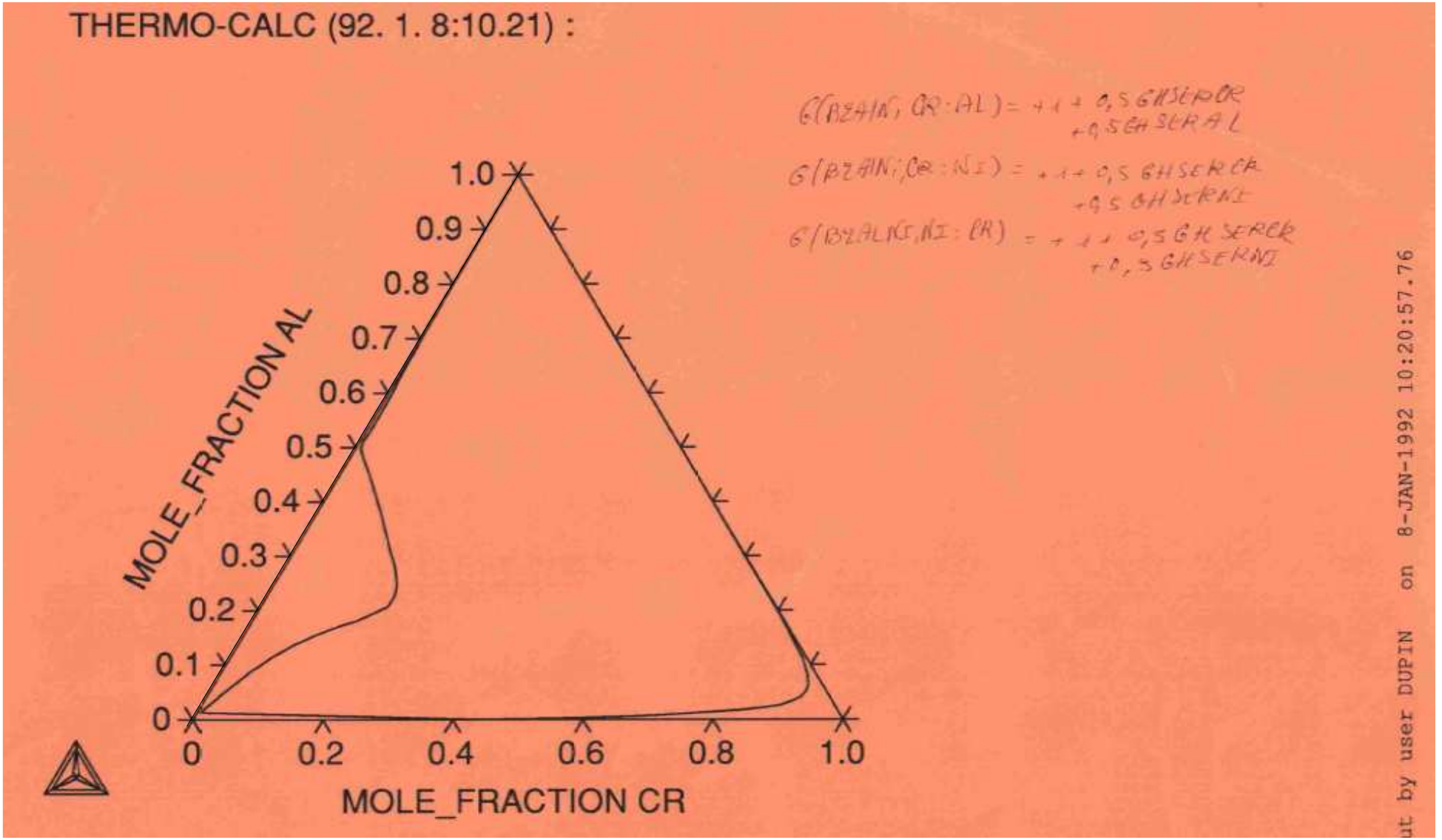
** END OF MESSAGE **

That is a bug.

Grenoble,...


THERMO-CALC (92. 1. 8:10.32) :
MOLE_FRACTION AL
MOLE_FRACTION CR
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
0
0.2
0.4
0.6
0.8
1.0
8-JAN-1992 10:32:16.60

Grenoble,...


THERMO-CALC (92. 1. 8:10.21) :
G(BZHAN;CR:AL) = +1 + 0,5 GHSERCR + 0,5 GHSERAL
G(BZHAN;CR:NI) = +1 + 0,5 GHSERCR + 0,5 GHSERNI
G(BZALNI,NI:CR) = +1 + 0,5 GHSERCR + 0,5 GHSERNI
MOLE_FRACTION AL
MOLE_FRACTION CR
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
0.2
0.4
0.6
0.8
1.0
Plot by user DUPIN on 8-JAN-1992 10:20:57.76

THÈSE

présentée par

Nathalie DUPIN

pour obtenir le titre de **DOCTEUR**
de l'**INSTITUT NATIONAL POLYTECHNIQUE de GRENOBLE**
(Arrêté ministériel du 30 Mars 1992)
Spécialité : Science et Génie des Matériaux

CONTRIBUTION À L'ÉVALUATION THERMODYNAMIQUE DES ALLIAGES POLYCONSTITUÉS À BASE DE NICKEL

Soutenue le 29 Mars 1995

Composition du jury :

W. KURZ	Président
Y. BIENVENU	Rapporteur
J.C. MATHIEU	Rapporteur
C. BERNARD	
B. SUNDMAN	
I. ANSARA	

Thèse préparée au
Laboratoire de Thermodynamique et de Physico-Chimie Métallurgiques de Grenoble

... March 1995

Contribution to the thermodynamic assessment of the multicomponent Ni based alloys

ELSEVIER

Journal of Alloys and Compounds 247 (1997) 20–30

Journal of ALLOYS AND COMPOUNDS

97Ans

Thermodynamic assessment of the Al–Ni system

Ibrahim Ansara[a], Nathalie Dupin[a], Hans Leo Lukas[b], Bo Sundman[c]

[a]Laboratoire de Thermodynamique et de Physico-Chimie Métallurgiques, CNRS/INPG/UJF, ENSEEG, B.P. 75, 38402 Saint-Martin d'Hères, France
[b]MPI für Metallforschung, Institut für Werkstoffwissenschaft, Heisenbergstr. 5, D-70569 Stuttgart, Germany
[c]Department of Materials Science and Engineering, Royal Institute of Technology, Stockholm, Sweden

Abstract

The sub-lattice model is used to describe the thermodynamic behaviour of the ordered phases existing in the Al–Ni system. The model parameters are derived from an optimisation procedure using all available experimental data. The order–disorder transformation f.c.c.-A1:$L1_2$ phase is modelled using either two or four sub-lattices which are mathematically equivalent.

Keywords: Al–Ni; Thermodynamic modelling; Sub-lattice model; Order–disorder transition; γ–γ' equilibria

1. Introduction

The use of the sub-lattice model, developed by Hillert and Staffanson [1] based on Temkin's model for ionic solutions [2] and extended by Sundman and Ågren [3], allows a variety of solution phases to be treated. This model is thus very adequate to describe the thermodynamic properties of the ordered phases in the Al–Ni system which is characterised by five intermetallic compounds with different structures: the $AlNi_3$-$L1_2$ phase disorders to an f.c.c.-A1 structure; AlNi b.c.c.-B2 is of the CsCl type; Al_3Ni_2 presents a range of non-stoichiometry; Al_3Ni_5 is formed by five sub-lattices and decomposes above 1173 K; Al_3Ni is stoichiometric.

2. Experimental information

2.1. Phase diagram data

The phase diagram of the Al–Ni system is rather well established. The solid phases and their crystal structures are presented in Table 1.

The experimental results relative to the phase diagram obtained by several investigators are represented in Fig. 1 together with the assessed diagram by Okamoto [19]. There is a general agreement between these different investigations. The main important differences appear in the solubility of aluminium in the nickel-rich solid solution γ. Alexander and Vaughan [6], who were the first to analyse in detail the phase diagram, determined lower solubilities compared with more recent investigations.

There are several studies of the region where equilibria between the liquid, γ and γ' phases exist because of the uncertainty of the nature of the invariant equilibria involving the formation of the γ' phase. Alexander and Vaughan [6] suggested the following reactions:

liquid$\rightleftharpoons\gamma+\gamma'$ at 1385 °C (1658 K)
liquid + $\beta\rightleftharpoons\gamma'$ at 1395 °C (1668 K)

which differ notably from Schramm's [7]

liquid + $\gamma\rightleftharpoons\gamma'$ at 1362 °C (1635 K)
liquid$\rightleftharpoons\gamma'+\beta$ at 1360 °C (1633 K)

In recent publications, Bremer and coworkers [13,14] confirm that the eutectic reaction takes place with the B2 phase as suggested by Schramm. The invariant temperatures measured by Hilpert et al. [13] are respectively 1642 K and 1645 K for the eutectic and peritectic reactions, approximately 10 K higher than Schramm's. By directional solidification measurements, Verhoeven et al. [17] confirmed Schramm's observation on the nature of the eutectic reaction, as well as Lee and Verhoeven [20] who used the same technique but lower cooling rates.

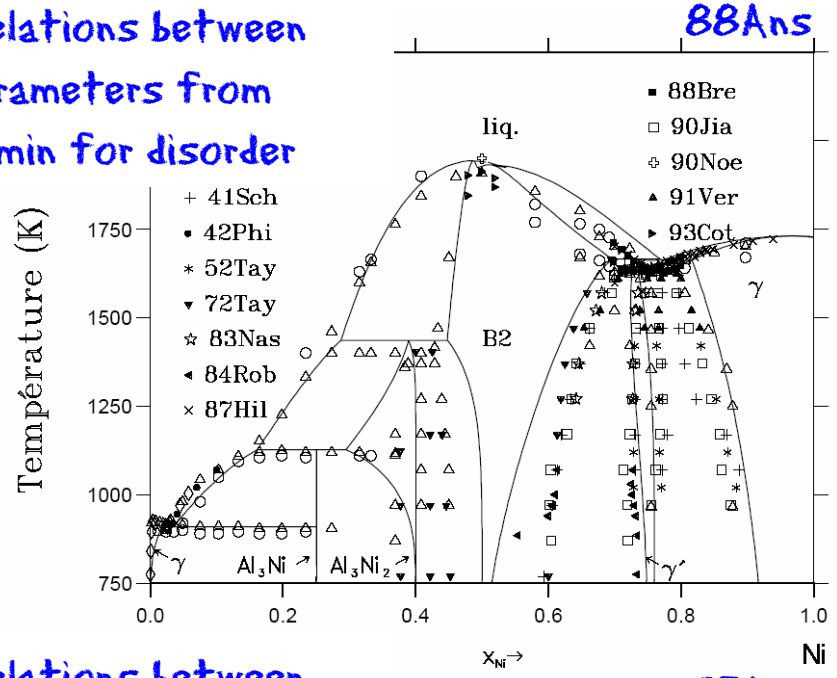
2.2. Thermodynamic data

The thermodynamic properties of the liquid, B2 and f.c.c. phases have been determined by various techniques

0925-8388/97/$17.00 © 1997 Elsevier Science S.A. All rights reserved
PII S0925-8388(96)02652-7

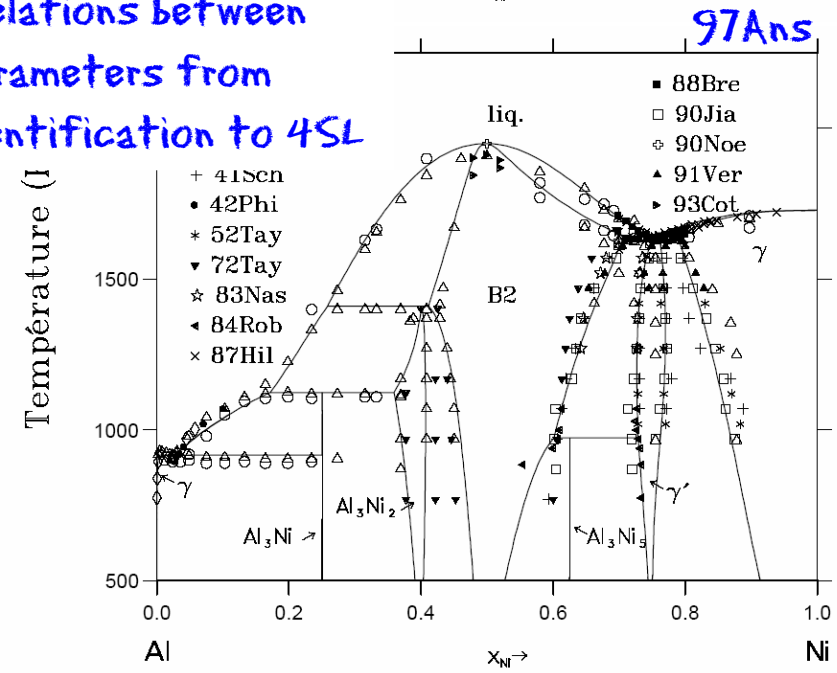
Relations between parameters from G min for disorder

88Ans



Relations between parameters from identification to 4SL

97Ans



$$G_m = G_m^{dis}(x_i) + G_m^{ord}(y_i', y_i'') - G_m^{ord}(x_i)$$

Scandinavian Journal of Metallurgy 2001; 30: 184–192
Printed in Denmark. All rights reserved

Copyright © Munksgaard 2001

SCANDINAVIAN
JOURNAL OF METALLURGY
ISSN 0371-0459

OlDup

A thermodynamic database for Ni-base superalloys

N. Dupin[1] and B. Sundman[2]

[1]Calcul Thermodynamique, 63670 Orcet, France; [2]Department of Materials Science and Engineering, Royal Institute of Technology, Stockholm, Sweden

A thermodynamic database has been developed for Ni-base superalloys. Following the CALPHAD procedure, it is based on the assessment of thermodynamic behaviour of the relevant constituting sub-systems of the complex system of interest. The current database contains 7 elements: Al, Co, Cr, Ni, Ti, W, Re. The thermodynamics of the γ and γ' phases are modelled with a single Gibbs energy function taking into account the crystallographic relation between these two phases. The formalism of the thermodynamic models used is briefly introduced. A few phase diagrams calculated with the current database in assessed binary and ternary systems are presented. Some experiments available in higher order systems are compared with the results of calculations wi… ation of the database is verified for solid state equilibria as well as for solidification behaviour (liquidus temperature and partition ratios). The introduction of Mo and Ta to the current database is in progress. Other elements (Nb, Fe, Zr, Hf, C, B, ···) are planed to be introduced.

Key words: CALPHAD, superalloys, thermodynamic database, γ/γ' equilibria, order-disorder modelling, solid-liquid partition ratio, liquidus.

© Munksgaard, 2001

…0

G = GRK(x) + GSL(y) - GSL(y=x)
applied to A1/L12
and also to A2/B2

Complex com… hanical properties
of elaboration … sible because both
superalloys to … A1 is a disordered
der to develo… appears between
the engineering … ally illustrated by
ria and thermodynamic behaviour of the complex systems under consideration need to be known. The CALPHAD procedure allows an estimation of them from the combination of the thermodynamic description of lower order sub-systems. In the current work, it has been applied in order to obtain a thermodynamic database for Ni superalloys.

The coherency of the γ (A1) and γ' ($L1_2$) phases is … Fig. 1. A single thermodynamic description depending on the site fractions of the elements in the different crystallographic sites has been used for these two phases as introduced by Ansara et al. [1].

The use of a single Gibbs energy curve for the γ and γ' phases and thus making the thermodynamics more closely related to the crystallography of these phases is the main difference between the present work and previous studies of the thermodynamic behaviours of the superalloys or of their relevant sub-system carried out following the CALPHAD method [2–7]. The γ' was modelled stoichiometric in the work of Kaufman and Nesor and with the sublattice formalism but totally independent of the γ phase in Saunders' work.

The current database contitutes a revision and an extension of a previous work [9, 14]. It is constituted by seven elements: Al, Co, Cr, Ni, Re, Ti, W. The thermodynamic description of the 21 binary systems have been either extracted from the available litterature or assessed in the present work. Ternary systems involving Ni have also been studied. The relations necessary to allow the stability of the disordered

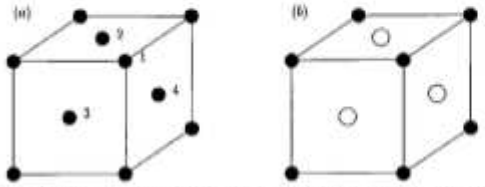
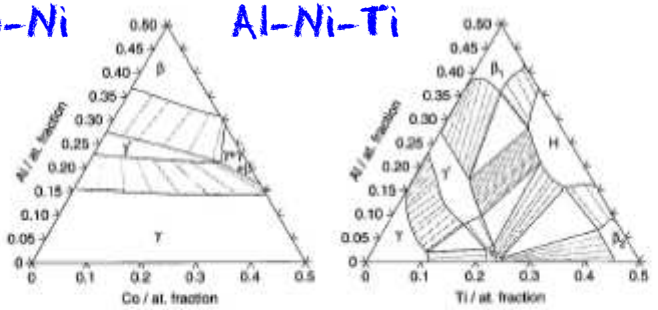
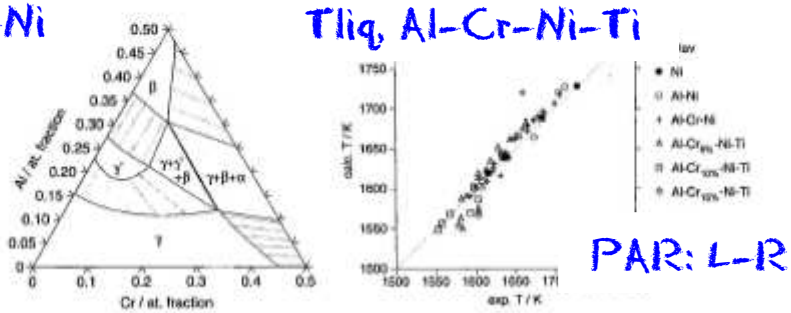


Fig. 1. Schematic representation of the crystallographic structures of the γ (A1) and γ' ($L1_2$) phases. (a) All the sites are equivalent. (b) The sites at the corners (4) are mainly occupied by the Al, Ti atoms, those in the center of each face (1, 2 and 3) by Ni, Co.

Al-Co-Ni Al-Ni-Ti



Al-Cr-Ni Tliq, Al-Cr-Ni-Ti



PAR: L-R G

Fig. 3. Isothermal section calculated at 1273 K for three important assessed ternary systems constituting the current database: Al–Co–Ni, Al–Ti, Al–Cr–Ni and comparison of calculated and experimental liquidus temperatures in the ternary Al–Cr–Ni and quaternary Al–Cr–Ni–Ti sys…

Re-Ti Re-W

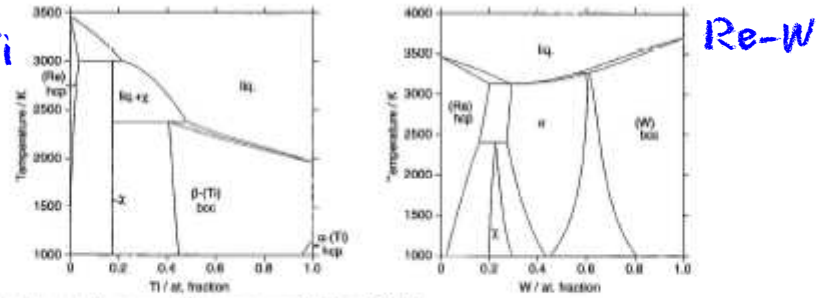


Fig. 4. Calculated phase diagram of two assessed binary systems: Re–Ti and Re–W.

Ni-Re-Ti Ni-Re-W

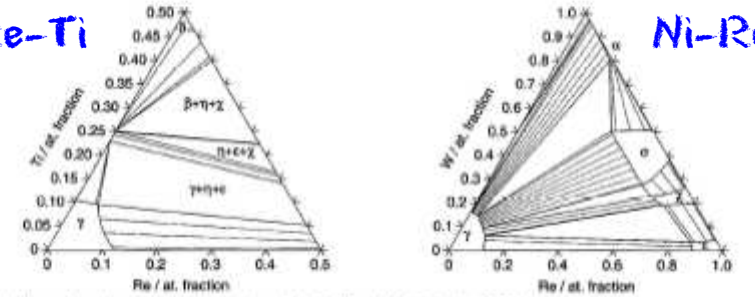
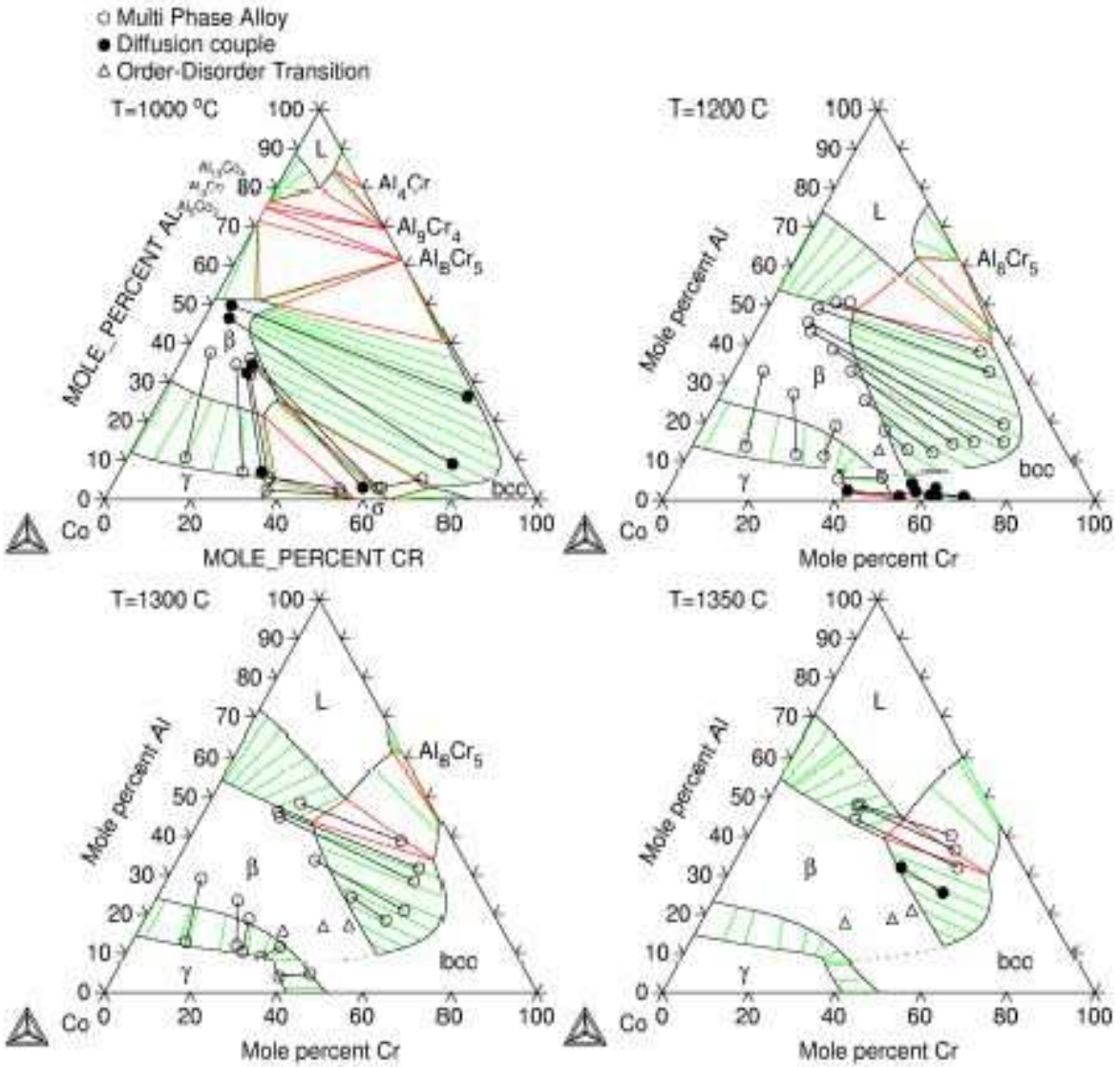
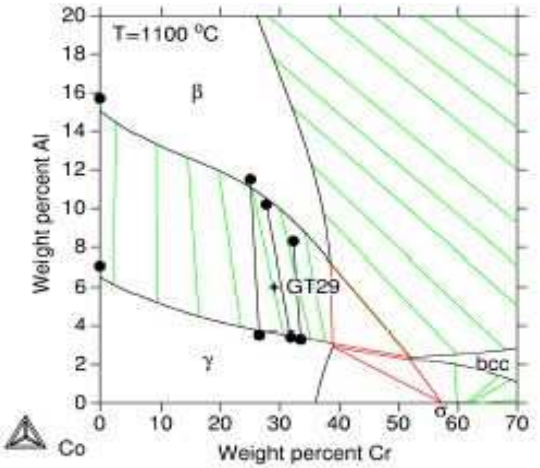


Fig. 5. Calculated isothermal section of the ternary systems Ni–Re–Ti and Ni–Re–W at 1273K.

T. Gomez-Acebo et al., 2004



Exp. : K. Ishikawa et al., 1998



Exp. : T. Gomez-Acebo et al.

Using TCNI where Al-Co-Cr is just extrapolated from binary systems

Pergamon

Calphad, Vol. 25, No. 4, pp. 549–565
© 2002 Published by Elsevier Scien
0364-5916/01/$ - see front

PII: S0364-5916(02)00007-X

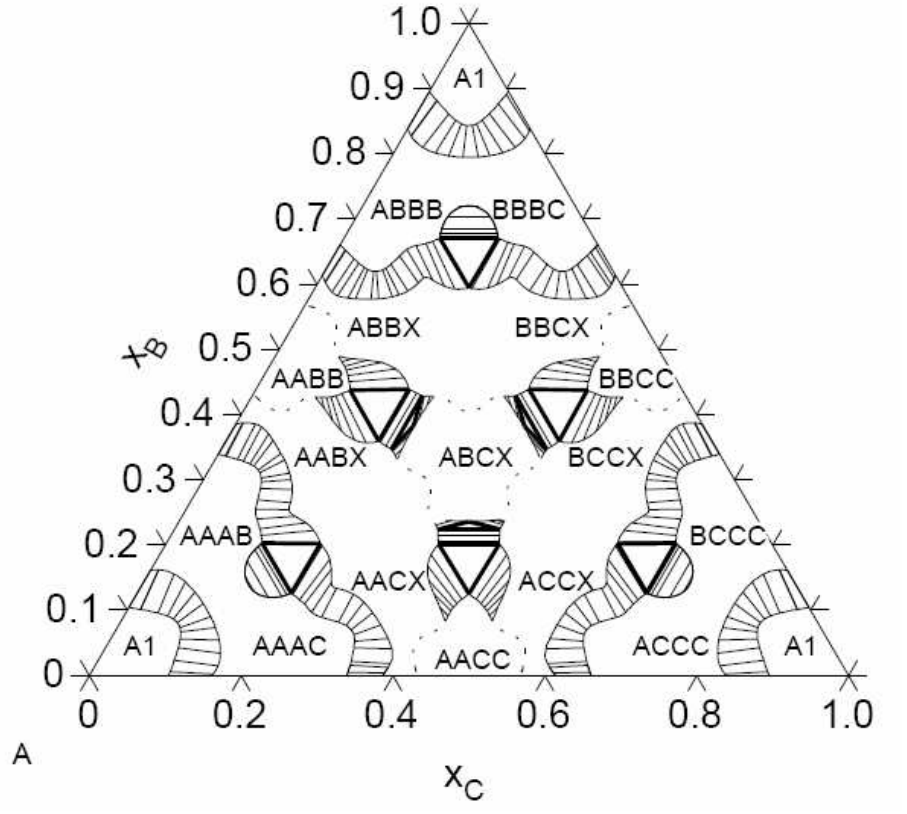
OIKus

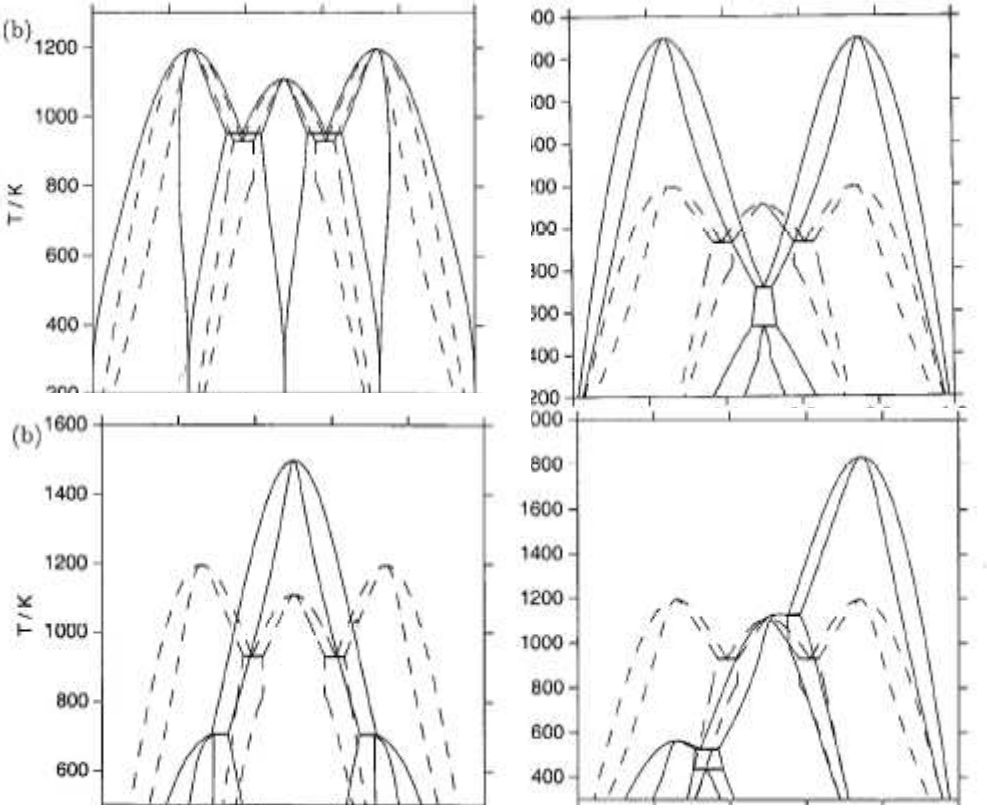
On the Compound Energy Formalism Applied to fcc Ordering.

A. Kusoffsky*, N. Dupin** and B. Sundman*
* Computational Thermodynamics, Department of Materials Science and Engineering,
Royal Institute of Technology, Stockholm, Sweden
** Calcul Thermodynamique, 3, rue de l'avenir, 63670 Orcet, France.
corresponding author's email:sandra@met.kth.se

(Received September 21, 2001)

Abstract The influence on the phase diagram and thermodynamic properties of some parameters i
Compound Energy Formalism (CEF) is studied for different simple binary and ternary cases sh
fcc ordering. It is shown that the flexibility of this formalism should enable to model most real
Recommendations for the ternary parameters that should be set from the binary systems are made.
© 2002 Published by Elsevier Science Ltd.





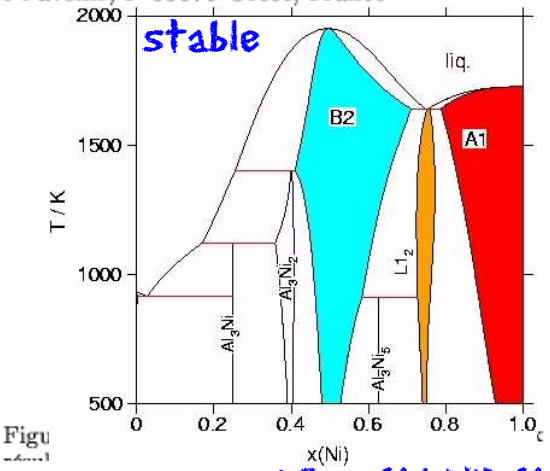
Une nouvelle évaluation thermodynamique du système Al-Ni

JEEP 2003 Lyon

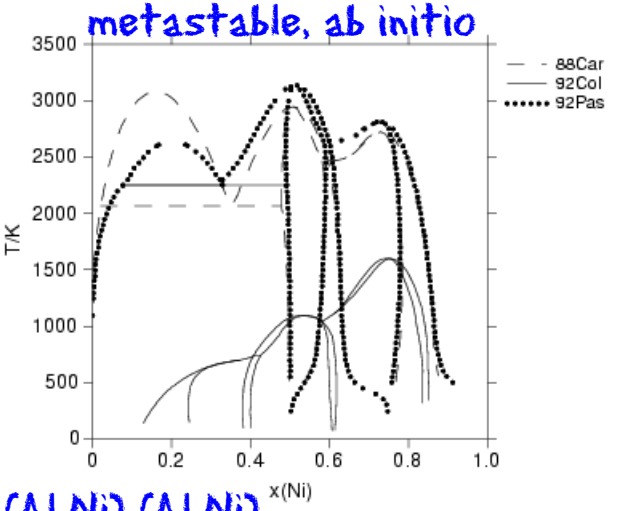
Bo Sundman
Material Science and Engineering Royal Institute of Technology S 100 44 Stockholm, Sweden
Nathalie Dupin
Calcul Thermodynamique 3, rue de l'avenir, F-63670 Orcet, France

1 Introduction

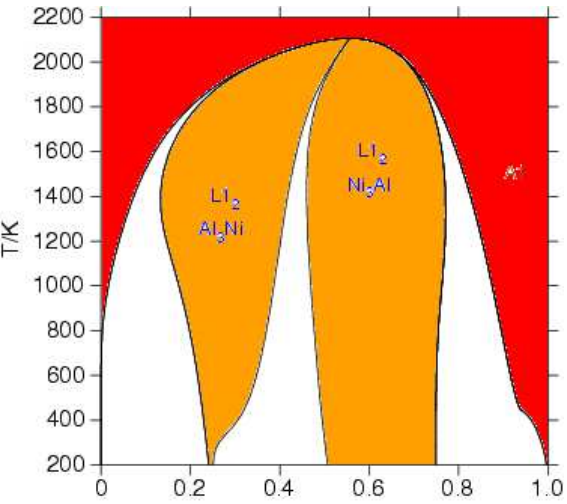
Le système Al-Ni, abondamment étudié, est en particulier intéressant parce qu'il constitue la base des superalliages base nickel. Différents types de calcul thermodynamique ont été effectués sur ce système suivant soit une approche *ab initio* [2,6,7,8] soit une approche *CALPHAD* [2,9,11]. L'extension des descriptions *CALPHAD* à des systèmes polycontitués a permis le développement de différentes bases de données commerciales [10,12] décrivant de manière globalement satisfaisante les équilibres de phases dans les alliages



Figu



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



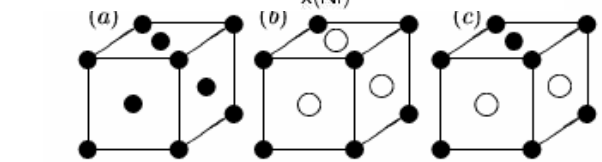
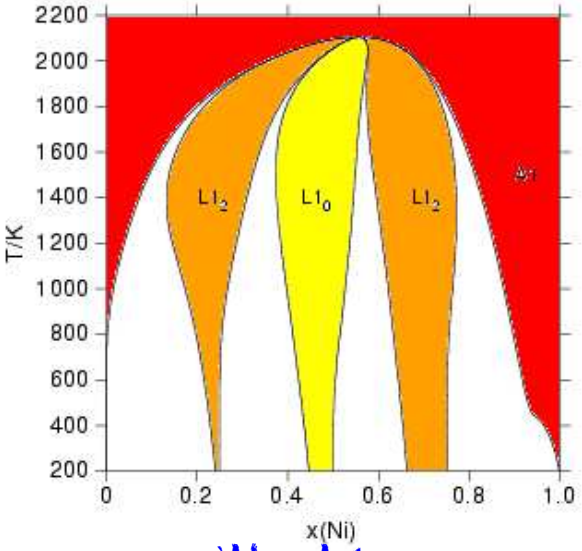
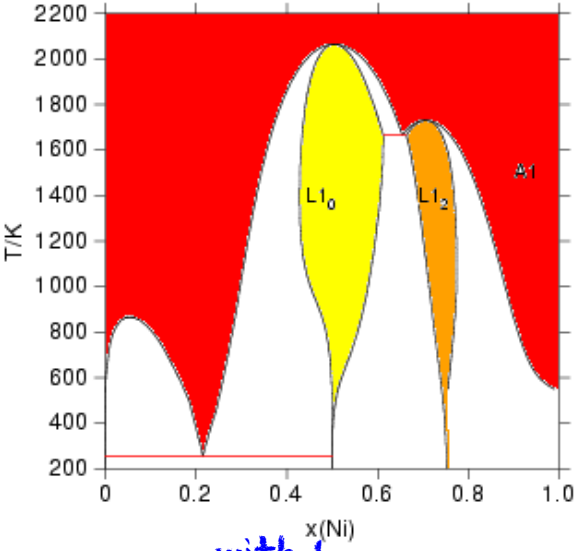


Figure 1: Schéma de la structure crystallographique des phases $A1$ (a), $L1_2$ (b) et $L1_0$ (c).

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



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

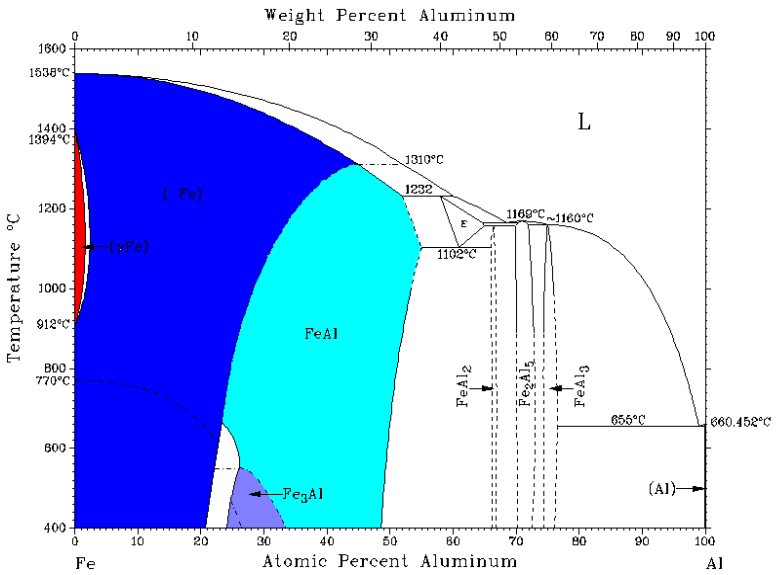


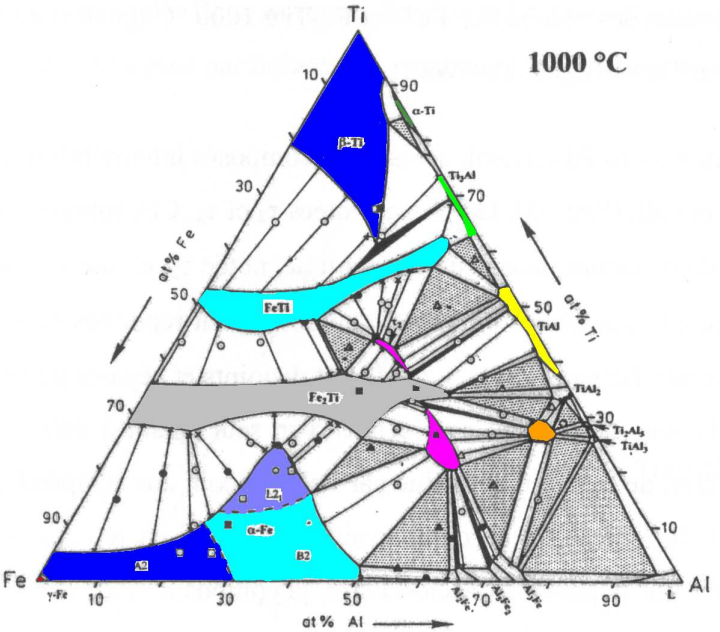
with $L_{Al,Ni:Al,Ni}$

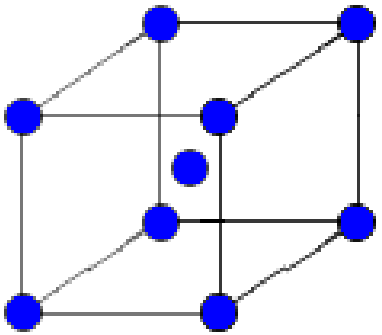
$$G^{des.}(x) = \sum_i x_i\, G_i^{des.} + G_{mag}^{des} + RT \sum_i x_i \ln x_i + x_{Al}\, x_{Ni} \sum_\nu (x_{Al} - x_{Ni})\, L_{Al,Ni}^{des.,\nu} \quad (2)$$

La contribution de mise en ordre est nulle

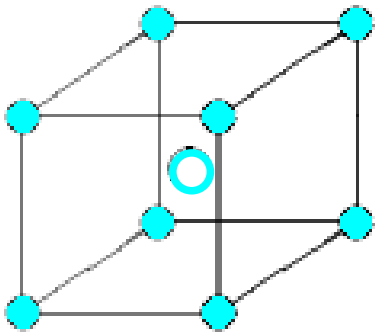
TofA 2004 Vienna



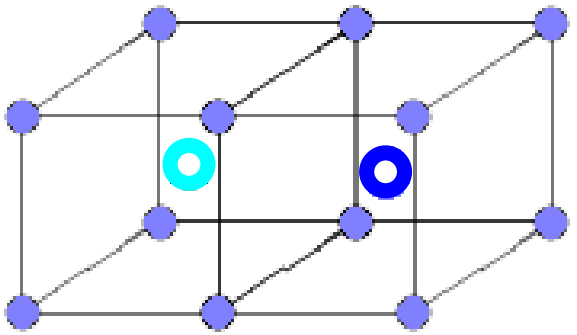




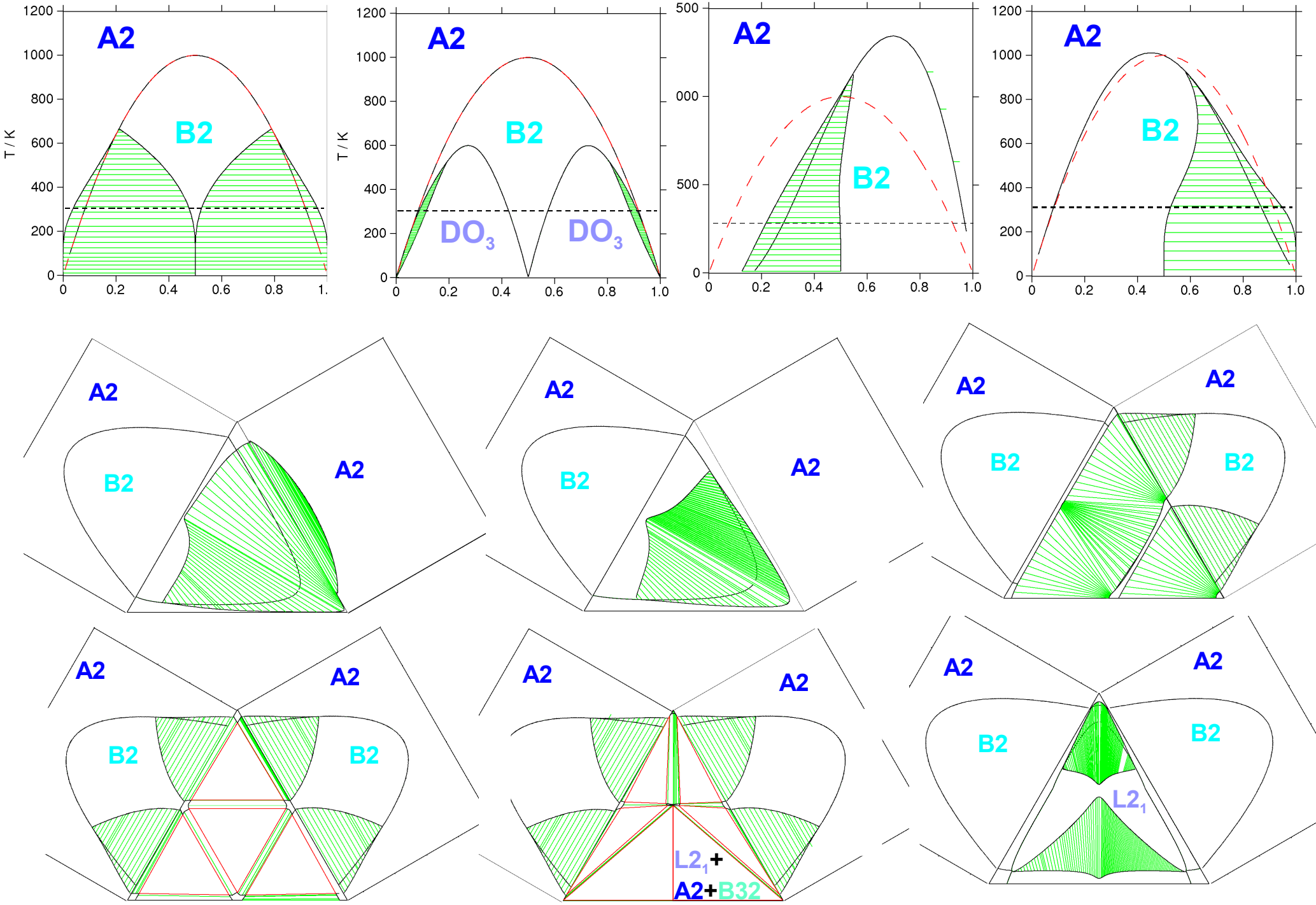
A2



B2



$DO_3, L2_1$


A2
B2
T / K
1200
1000
800
600
400
200
0
0.2
0.4
0.6
0.8
1.0
A2
B2
DO3
DO3
T / K
500
000
500
0
A2
B2
A2
B2
A2
A2
B2
A2
A2
A2
B2
B2
A2
A2
B2
B2
L21+
A2+B32
A2
A2
B2
B2
L21

Available online at www.sciencedirect.com
SCIENCE DIRECT
ELSEVIER
Computer Coupling of Phase Diagrams and Thermochemistry xx (xxxx) xxx–xxx
www.elsevier.com/locate

06Hal

Thermodynamic models for crystalline phases. Composition depende models for volume, bulk modulus and thermal expansion

Bengt Hallstedt[a,*], Nathalie Dupin[b], Mats Hillert[c], Lars Höglund[c], Hans Leo Lukas[d], Julius C. Schuster[e], Nuri Solak[d]

[a] RWTH Aachen, Aachen, Germany
[b] Calcul Thermodynamique, Orcet, France
[c] Royal Institute of Technology, Stockholm, Sweden
[d] Max-Planck-Institut für Metallforschung, Stuttgart, Germany
[e] Universität Wien, Vienna, Austria

Received 14 February 2006; accepted 17 February 2006

Abstract

The thermodynamic modelling of solid (crystalline) phases forms a central topic within the *Calphad* approach and a variety of a been discussed at previous Ringberg workshops. At the present Ringberg workshop, modelling of volume and its temperature, p composition dependence formed a major part of the discussions. In addition, modelling of the heat capacity above the (equilibriu temperature, sublattice modelling of complex phases, modelling of ordering and interstitial solutions in the bcc lattice and the effect of were addressed.
© 2006 Elsevier Ltd. All rights reserved.

1. In

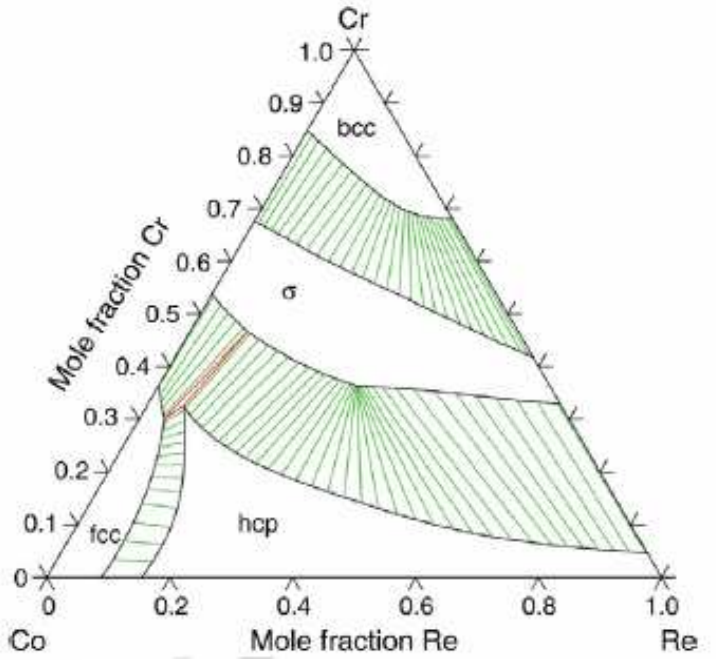
$$G_m^{\sigma} = G_m^{\mathrm{dis}}(x_i) + \Delta G_m^{\mathrm{conf}}\left(y_i^s\right),$$

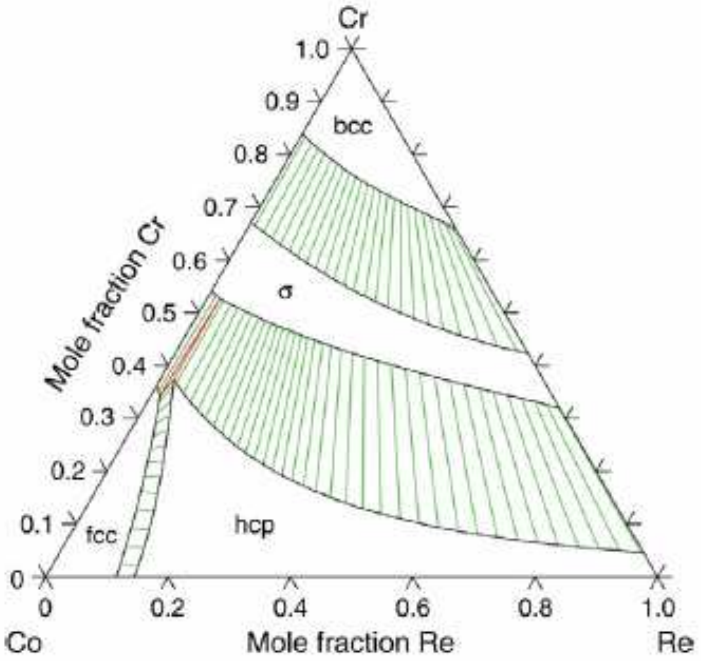
$$G_m^{\mathrm{dis}}(x_i) = \sum x_i\, {}^{\mathrm{o}}G_i^{\sigma} + \sum\sum\sum x_i x_j \left(x_i - x_j\right)^{\nu} L_{i,j}^{\nu,\sigma}$$

$$\Delta G_m^{\mathrm{conf}}\left(y_i^s\right) = \sum_i \sum_j \sum_k y_i^{(1)} y_j^{(2)} y_k^{(3)} \Delta G_{i:j:k}^{\sigma} + a^{(s)} RT \sum_s \sum_i y_i^{(s)} \ln y_i^{(s)},$$

Th
phase
recon
discu
of the
orderi
state i
enviro
interm
while
solutions in the hcp host lattice [8] were discussed in 1999. Order–disorder modelling has been frequently discussed [4,8,9]. Ionic solutions were discussed in 1996 [10] and 1999 [5,11] and semiconductors in 1996 [12] and 1997 [4].

the calculation of volume changes on for example hea melting, volume fractions, lattice mismatch in cubic str and phase diagrams at increased pressure. Pressure indep volumes can be used up to about 1 GPa. At pressures





Ordered phases that do not disorder

UNCORRECTED PROOF

Some improvements...

An early macro

```
GO D
sw
u
alni.tdb
def-sy al ni
get
go g
a-p-d fcc
COMPOSITION_SETS
2



a-p-d l12
COMPOSITION_SETS
2



a-p-d l12
maj
1
ni
ni
va
a-p-d l12
maj
2
ni
al
va

go p-3
s-c p=1e5 n=1 t=1200 x(ni)=.8
ch-st p l12 l12#2
e
1
s-s-c l12 *
s-s-c l12#2 *
c-e
l-e

nx
s-a-v 1 x(ni) 0 1

s-a-v 2 t 500 2000

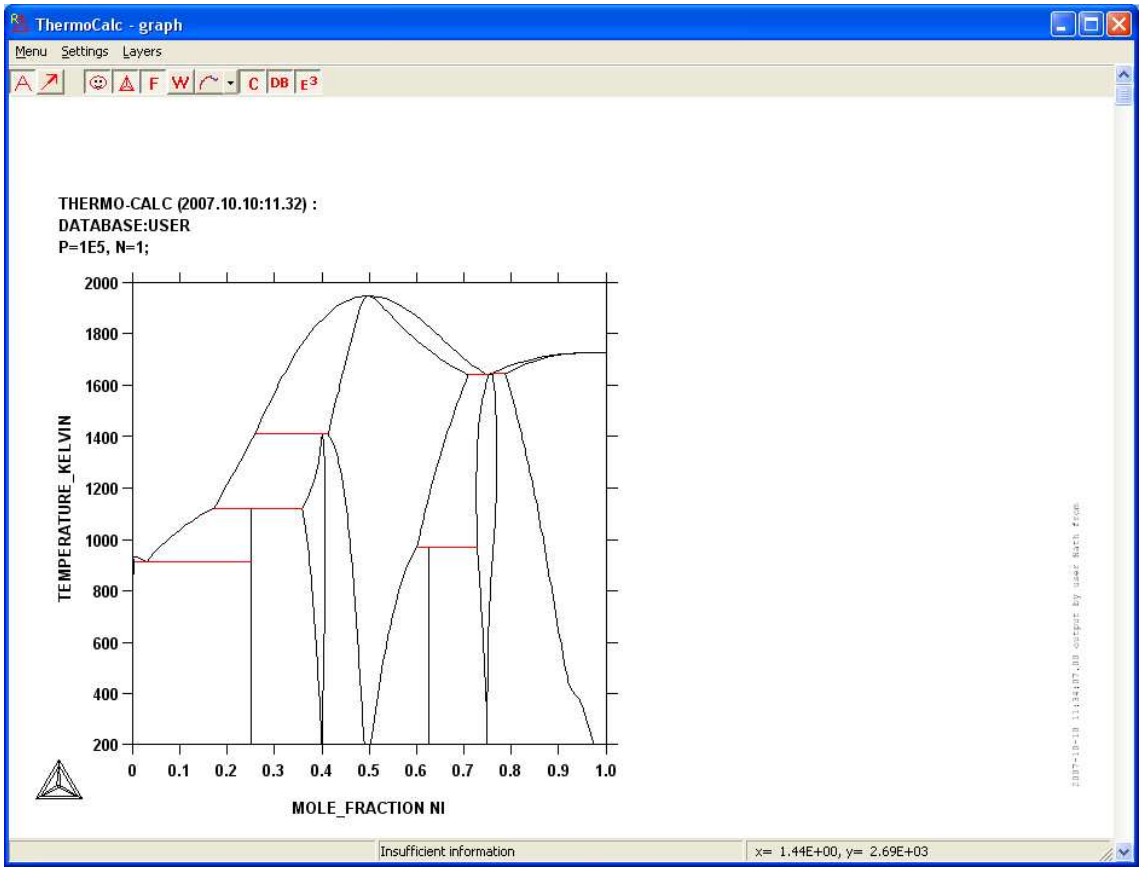
sa
alni
y
add

map
$EXIT -> CPU time          55  seconds
```

alni.TCM last modified 17/05/94

run 10/10/2007

CPU time 4 seconds



```
GO D
sw
u
alni.tdb
def-sy al ni
get
go g
a-p-d fcc
COMPOSITION_SETS
2



a-p-d l12
COMPOSITION_SETS
2



a-p-d l12
maj
1
ni
ni
va
a-p-d l12
maj
2
ni
al
va

go p-3
s-c p=1e5 n=1 t=1200 x(ni)=.8
ch-st p l12 l12#2
e
1
s-s-c l12 *
s-s-c l12#2 *
c-e
l-e

nx
s-a-v 1 x(ni) 0 1

s-a-v 2 t 500 2000

sa
alni
y
add

map
$EXIT -> CPU time          55  seconds
```

Improving tdb

TYPE_DEFINITION O GES A_P_D L12 C_S 2 NI:AL:VA !
TYPE_DEFINITION O GES A_P_D L12 MAJ 1 NI:NI:VA !

```
go d
sw u
NAT
def_sy al ni
get
go pol
s_c p=1E5 n=1 t=1200 x(ni)=.75
c_e
c_e
s_a_v 1 x(ni) 0 1,,
s_a_v 2 T 200 2000,,
sa alni y
add 1
map
po
set_tit Al-Ni
pl,,
set_int
```

Note

no more starting constitution

automatic axis

```
GO D
sw
u
alni.tdb
def-sy al ni
get
go g
a-p-d fcc
COMPOSITION_SETS
2



a-p-d l12
COMPOSITION_SETS
2



a-p-d l12
maj
1
ni
ni
va
a-p-d l12
maj
2
ni
al
va

go p-3
s-c p=1e5 n=1 t=1200 x(ni)=.8
ch-st p l12 l12#2
e
1
s-s-c l12 *
s-s-c l12#2 *
c-e
l-e

nx
s-a-v 1 x(ni) 0 1

s-a-v 2 t 500 2000

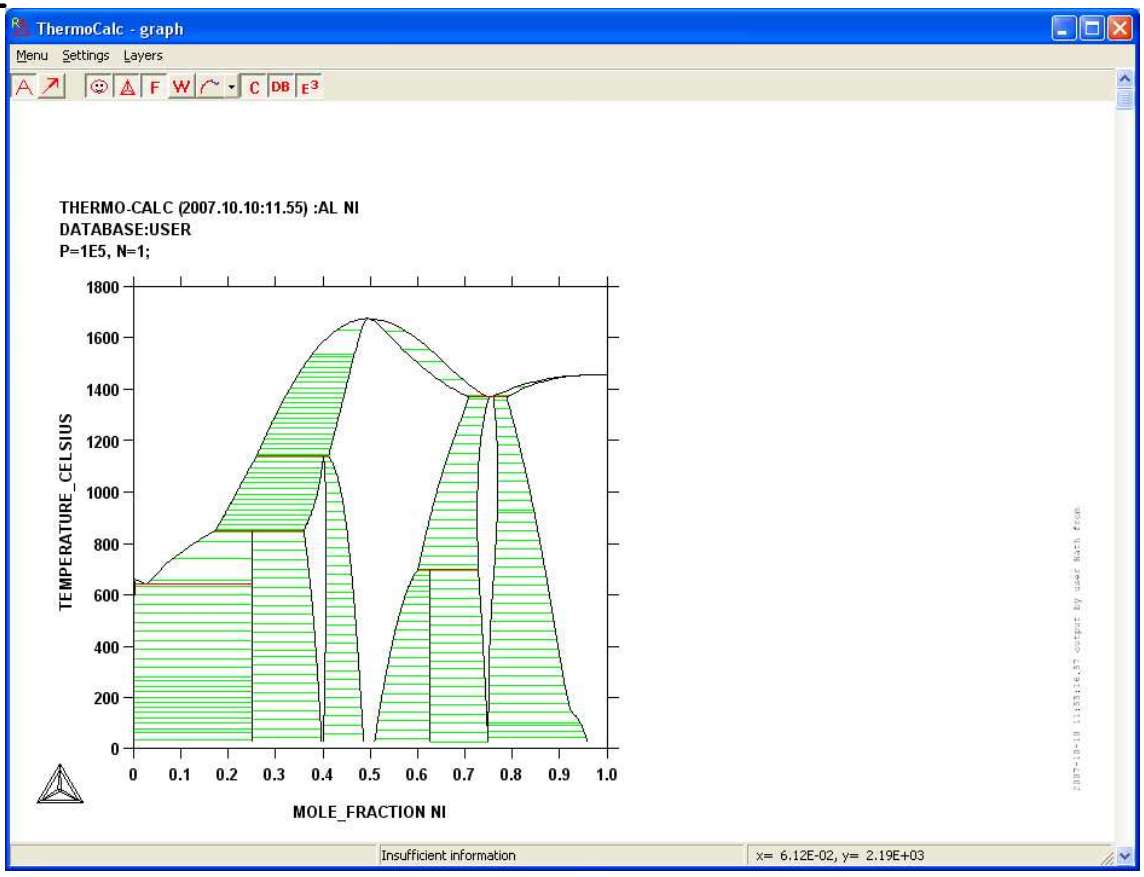
sa
alni
y
add

map
$EXIT -> CPU time          55  seconds
```

Improving tdb

ASSESSED_SYSTEMS AL-NI(;P3 STP:.8/1200/2) !

go bin
U alni
al ni



Improving POST

```
GO D
sw
u
alni.tdb
def-sy al ni
get
go g
a-p-d fcc
COMPOSITION_SETS
2



a-p-d l12
COMPOSITION_SETS
2



a-p-d l12
maj
1
ni
ni
va
a-p-d l12
maj
2
ni
al
va

go p-3
s-c p=1e5 n=1 t=1200 x(ni)=.8
ch-st p l12 l12#2
e
1
s-s-c l12 *
s-s-c l12#2 *
c-e
l-e

nx
s-a-v 1 x(ni) 0 1

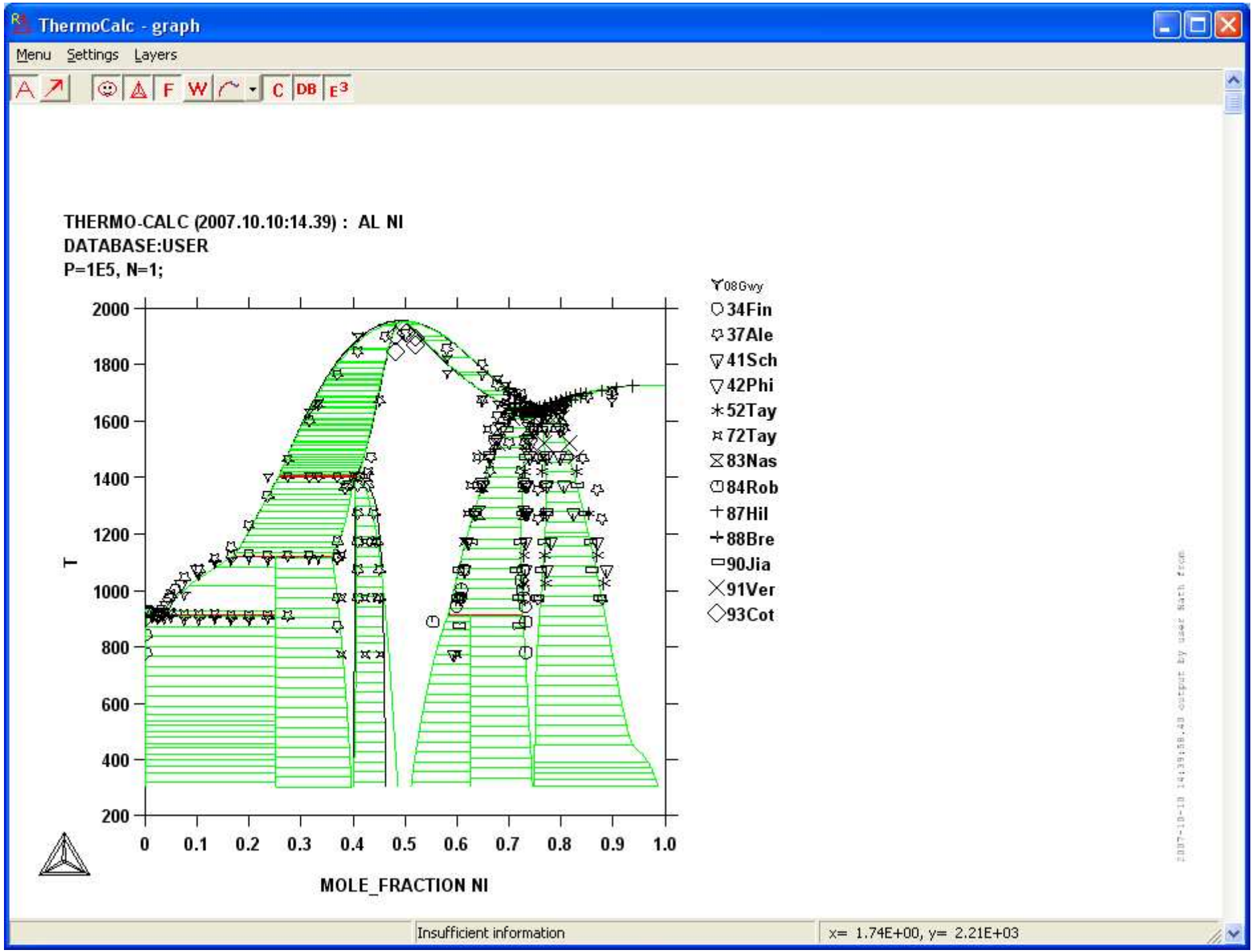
s-a-v 2 t 500 2000

sa
alni
y
add

map
$EXIT -> CPU time          55  seconds
```

```
go bin
U NI15VA
al ni

s_d_a y t
app y alni-k alni-diagdat
1
1
1
1
pl,,
set_int
```


ThermoCalc - graph
Menu Settings Layers
THERMO-CALC (2007.10.10:14.39) : AL NI
DATABASE:USER
P=1E5, N=1;
T
MOLE_FRACTION NI
08Gwy
34Fin
37Ale
41Sch
42Phi
52Tay
72Tay
83Nas
84Rob
87Hil
88Bre
90Jia
91Ver
93Cot
Insufficient information
x= 1.74E+00, y= 2.21E+03

A recent one

```
GO D
sw
u
alni.tdb
def-sy al ni
get
go g
a-p-d fcc
COMPOSITION_SETS
2



a-p-d l12
COMPOSITION_SETS
2



a-p-d l12
maj
1
ni
ni
va
a-p-d l12
maj
2
ni
al
va

go p-3
s-c p=1e5 n=1 t=1200 x(ni)=.8
ch-st p l12 l12#2
e
1
s-s-c l12 *
s-s-c l12#2 *
c-e
l-e

nx
s-a-v 1 x(ni) 0 1

s-a-v 2 t 500 2000

sa
alni
y
add

map
$EXIT -> CPU time          55  seconds
```

```
go bin
U NI
al ni

add .05 1300 N Liquide

add .5 1200 N AlNi

add .85 1200 N (Ni)

add .25 300 N ^RO90Al^DO3$Ni

add .4 300 N ^RO90Al^DO3$Ni^DO2$

add .62 300 N ^RO90Al^DO3$Ni^DO5$

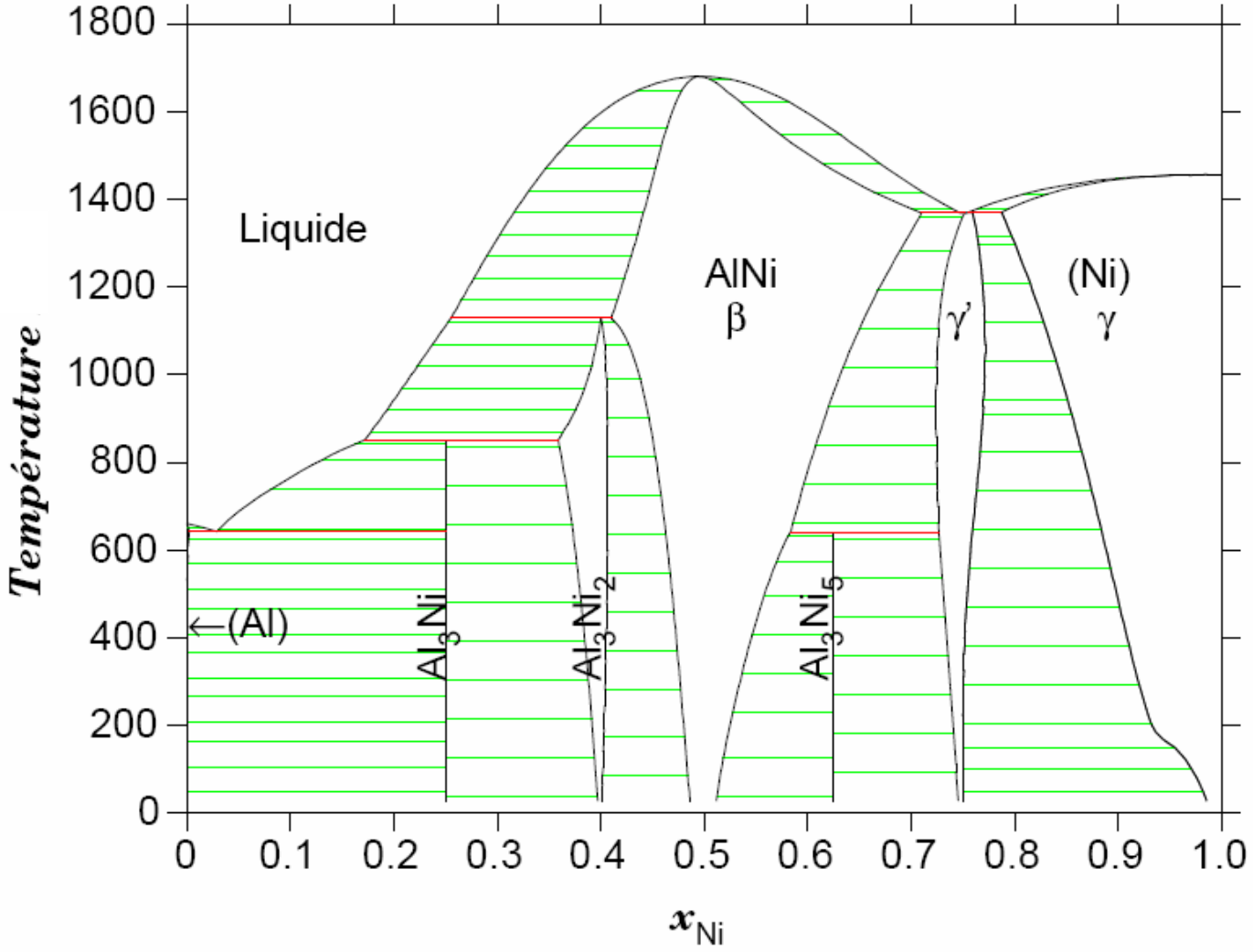
add .52 1100 N ^GRb$

add .88 1100 N ^GRg$

add .735 1100 N ^GRg$'

add 0 400 N ^GRA$(Al)

s_a_te x n ^FO20x^DONi$
s_a_te y n ^FO20Temp^CCearature
s_a_le x 15
s_p_o n n n ,,,,
du pdf m alni
set_int
```


Température
1800
1600
1400
1200
1000
800
600
400
200
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
x_{Ni}
Liquide
AlNi
β
γ'
(Ni)
γ
←(Al)
Al_3Ni
Al_3Ni_2
Al_3Ni_5

F option

5 SUBLATTICES, SITES .25: .25: .25: .25: 1
CONSTITUENTS: AL,NI : AL,NI : AL,NI : AL,NI : VA

G(L12_FCC,AL:AL:AL:AL:VA;0)-H298(FCC_A1,AL;0) = 0.0
G(L12_FCC,NI:AL:AL:AL:VA;0)-0.75 H298(FCC_A1,AL;0)-0.25 H298(
0) = +AL3NI
G(L12_FCC,AL:NI:AL:AL:VA;0)-0.75 H298(FCC_A1,AL;0)-0.25 H298(
0) = +AL3NI
G(L12_FCC,NI:NI:AL:AL:VA;0)-0.5 H298(FCC_A1,AL;0)-0.5 H298(FC
0) = +AL2NI2
G(L12_FCC,AL:AL:NI:AL:VA;0)-0.75 H298(FCC_A1,AL;0)-0.25 H298(
0) = +AL3NI
G(L12_FCC,NI:AL:NI:AL:VA;0)-0.5 H298(FCC_A1,AL;0)-0.5 H298(FC
0) = +AL2NI2
G(L12_FCC,AL:NI:NI:AL:VA;0)-0.5 H298(FCC_A1,AL;0)-0.5 H298(FC
0) = +AL2NI2
G(L12_FCC,NI:NI:NI:AL:VA;0)-0.25 H298(FCC_A1,AL;0)-0.75 H298(F
0) = +ALNI3
G(L12_FCC,AL:AL:AL:NI:VA;0)-0.75 H298(FCC_A1,AL;0)-0.25 H298(
0) = +AL3NI
G(L12_FCC,NI:AL:AL:NI:VA;0)-0.5 H298(FCC_A1,AL;0)-0.5 H298(FC
0) = +AL2NI2
G(L12_FCC,AL:NI:AL:NI:VA;0)-0.5 H298(FCC_A1,AL;0)-0.5 H298(FC
0) = +AL2NI2
G(L12_FCC,NI:NI:AL:NI:VA;0)-0.25 H298(FCC_A1,AL;0)-0.75 H298(F
0) = +ALNI3
G(L12_FCC,AL:AL:NI:NI:VA;0)-0.5 H298(FCC_A1,AL;0)-0.5 H298(FC
0) = +AL2NI2
G(L12_FCC,NI:AL:NI:NI:VA;0)-0.25 H298(FCC_A1,AL;0)-0.75 H298(F
0) = +ALNI3
G(L12_FCC,AL:NI:NI:NI:VA;0)-0.25 H298(FCC_A1,AL;0)-0.75 H298(F
0) = +ALNI3
G(L12_FCC,NI:NI:NI:NI:VA;0)-H298(FCC_A1,NI;0) = 0.0

2^4 = 16 compounds
actually for symmetry reason
only 5 ≠ (A, A_3B, AB, AB_3, B)

-> F Option

5 SUBLATTICES, SITES .25: .25: .25: .25: 1
CONSTITUENTS: AL,NI : AL,NI : AL,NI : AL,NI : VA

G(L12_FCC,AL:AL:AL:AL:VA;0)-H298(FCC_A1,AL;0) = 0.0
G(L12_FCC,NI:AL:AL:AL:VA;0)-0.75 H298(FCC_A1,AL;0)-(
0) = +AL3NI
G(L12_FCC,NI:NI:AL:AL:VA;0)-0.5 H298(FCC_A1,AL;0)-0.
0) = +AL2NI2
G(L12_FCC,NI:NI:NI:AL:VA;0)-0.25 H298(FCC_A1,AL;0)-0
0) = +ALNI3
G(L12_FCC,NI:NI:NI:NI:VA;0)-H298(FCC_A1,NI;0) = 0.0

faster calculations and
automatic naming

F option

OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWNS/: c
Output from POLY-3, equilibrium = 1, label A0 , database: USER

Conditions:
P=1E5, N=1, T=1200, X(NI)=0.8
DEGREES OF FREEDOM 0

Temperature 1200.00 K (926.85 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass 5.23484E+01
Total Gibbs energy -8.76558E+04, Enthalpy -5.68209E+03, Volume 0.00000E+00

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
AL	2.0000E-01	1.0309E-01	4.7628E-09	-1.9119E+05	SER
NI	8.0000E-01	8.9691E-01	2.0474E-03	-6.1772E+04	SER

L12_FCC_A1#1 Status ENTERED Driving force 0.0000E+00
Number of moles 3.3201E-01, Mass 1.7948E+01 Mass fractions:
NI 9.27091E-01 AL 7.29091E-02

L12_FCC_L12#2 Status ENTERED Driving force 0.0000E+00
Number of moles 6.6799E-01, Mass 3.4401E+01 Mass fractions:
NI 8.81169E-01 AL 1.18831E-01

B option

B Option for BCC ordering

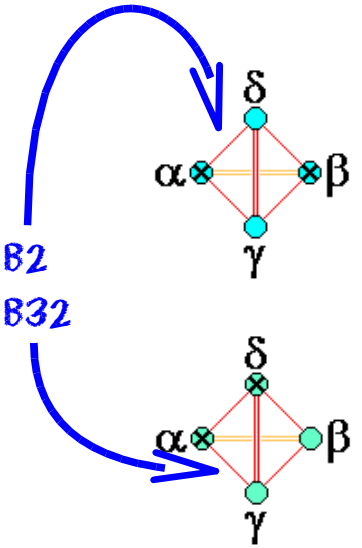
6 different compounds (irregular tetraedra)

```
DO3_BCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
  4 SUBLATTICES, SITES  .25:  .25:  .25:  .25
    CONSTITUENTS: A,B : A,B : A,B : A,B

      G(DO3_BCC,A:A:A:A;0)-H298(BCC_A2,A;0) = 0.0
      G(DO3_BCC,A:A:A:B;0)-0.75 H298(BCC_A2,A;0)-0.25 H298(BCC_A2,B;0) =
          +2*UAB+1.5*VAB
      G(DO3_BCC,A:A:B:B;0)-0.5 H298(BCC_A2,A;0)-0.5 H298(BCC_A2,B;0) = +4*UAB
      G(DO3_BCC,A:B:A:B;0)-0.5 H298(BCC_A2,A;0)-0.5 H298(BCC_A2,B;0) =
          +2*UAB+3*VAB
      G(DO3_BCC,A:B:B:B;0)-0.25 H298(BCC_A2,A;0)-0.75 H298(BCC_A2,B;0) =
          +2*UAB+1.5*VAB
      G(DO3_BCC,B:B:B:B;0)-H298(BCC_A2,B;0) = 0.0
      L(DO3_BCC,A,B:A,B:*:*;0) = +W2AB
      L(DO3_BCC,A,B:*:A,B:*;0) = +W1AB
      L(DO3_BCC,A,B:*:*:*;0) = +L0AB
      L(DO3_BCC,A,B:*:*:*;1) = +L1AB
```

B2

B32



B option

DO3_BCC_B2#1 Status ENTERED Driving force 0.0000E+00
Moles 6.9670E-01, Mass 2.8188E-02, Volume fraction 0.0000E+00 Mass fractions:
B 5.80637E-01 A 3.55522E-01 C 6.38416E-02
Constitution:
Sublattice 1, Number of sites 2.5000E-01
B 8.40680E-01 A 9.07195E-02 C 6.86001E-02
Sublattice 2, Number of sites 2.5000E-01
B 8.40680E-01 A 9.07195E-02 C 6.86001E-02
Sublattice 3, Number of sites 2.5000E-01
A 9.75479E-01 C 2.39016E-02 B 6.19076E-04
Sublattice 4, Number of sites 2.5000E-01
A 9.75479E-01 C 2.39016E-02 B 6.19076E-04

DO3_BCC_A2#2 Status ENTERED Driving force 0.0000E+00
Moles 3.0330E-01, Mass 1.6113E-02, Volume fraction 0.0000E+00 Mass fractions:
C 9.28096E-01 A 4.78741E-02 B 2.40301E-02
Constitution:
Sublattice 1, Number of sites 2.5000E-01
C 8.82879E-01 A 9.42616E-02 B 2.28594E-02
Sublattice 2, Number of sites 2.5000E-01
C 8.82879E-01 A 9.42616E-02 B 2.28594E-02
Sublattice 3, Number of sites 2.5000E-01
C 8.82879E-01 A 9.42616E-02 B 2.28594E-02
Sublattice 4, Number of sites 2.5000E-01
C 8.82879E-01 A 9.42616E-02 B 2.28594E-02

B option

DO3_BCC_B32#1 Status ENTERED Driving force 0.0000E+00
Moles 6.9735E-01, Mass 2.8117E-02, Volume fraction 0.0000E+00 Mass fractions:
B 5.91849E-01 A 3.59976E-01 C 4.81748E-02
Constitution:
Sublattice 1, Number of sites 2.5000E-01
B 8.53085E-01 A 8.69925E-02 C 5.99220E-02
Sublattice 2, Number of sites 2.5000E-01
A 9.88850E-01 C 9.63968E-03 B 1.51047E-03
Sublattice 3, Number of sites 2.5000E-01
B 8.53085E-01 A 8.69925E-02 C 5.99220E-02
Sublattice 4, Number of sites 2.5000E-01
A 9.88850E-01 C 9.63968E-03 B 1.51047E-03

DO3_BCC_A2#2 Status ENTERED Driving force 0.0000E+00
Moles 3.0265E-01, Mass 1.6184E-02, Volume fraction 0.0000E+00 Mass fractions:
C 9.51546E-01 A 4.14774E-02 B 6.97643E-03
Constitution:
Sublattice 1, Number of sites 2.5000E-01
C 9.11118E-01 A 8.22020E-02 B 6.68003E-03
Sublattice 2, Number of sites 2.5000E-01
C 9.11118E-01 A 8.22020E-02 B 6.68003E-03
Sublattice 3, Number of sites 2.5000E-01
C 9.11118E-01 A 8.22020E-02 B 6.68003E-03
Sublattice 4, Number of sites 2.5000E-01
C 9.11118E-01 A 8.22020E-02 B 6.68003E-03

B option

DO3_BCC_D03#1 Status ENTERED Driving force 0.0000E+00
Moles 6.0089E-01, Mass 2.7238E-02, Volume fraction 0.0000E+00 Mass fractions:
B 5.71839E-01 A 2.16894E-01 C 2.11267E-01
Constitution:
Sublattice 1, Number of sites 2.5000E-01
B 9.27911E-01 C 5.66469E-02 A 1.54418E-02
Sublattice 2, Number of sites 2.5000E-01
B 9.27911E-01 C 5.66469E-02 A 1.54418E-02
Sublattice 3, Number of sites 2.5000E-01
C 5.67945E-01 A 4.31394E-01 B 6.61458E-04
Sublattice 4, Number of sites 2.5000E-01
A 9.95233E-01 C 4.67599E-03 B 9.12916E-05

DO3_BCC_B32#2 Status ENTERED Driving force 0.0000E+00
Moles 3.9911E-01, Mass 1.7063E-02, Volume fraction 0.0000E+00 Mass fractions:
C 6.44646E-01 A 2.86294E-01 B 6.90601E-02
Constitution:
Sublattice 1, Number of sites 2.5000E-01
C 9.63331E-01 B 3.29438E-02 A 3.72549E-03
Sublattice 2, Number of sites 2.5000E-01
A 9.03540E-01 B 7.27922E-02 C 2.36682E-02
Sublattice 3, Number of sites 2.5000E-01
C 9.63331E-01 B 3.29438E-02 A 3.72549E-03
Sublattice 4, Number of sites 2.5000E-01
A 9.03540E-01 B 7.27922E-02 C 2.36682E-02

Many thanks