Thermo-Calc Software

Simulating interdiffusion in NiAl / Ni-base superalloy systems

Anders Engström[a], Henrik Larsson[b], Lars Höglund[a,c] and Paul Mason[d]

[a] *Thermo-Calc Software AB, Stockholm Technology Park, SE-113 47 Stockholm, Sweden*
[b] *Sandvik Tooling AB, Stockholm, Sweden*
[c] *Division of Physical Metallurgy, Department of Materials Science and Engineering, The Royal Institute of Technology (KTH), SE-100 44 Stockholm, Sweden*
[d] *Thermo-Calc Software Inc., 4160 Washington Road, McMurray PA 15317, USA*

NIST Diffusion Workshop March 25-26, 2009

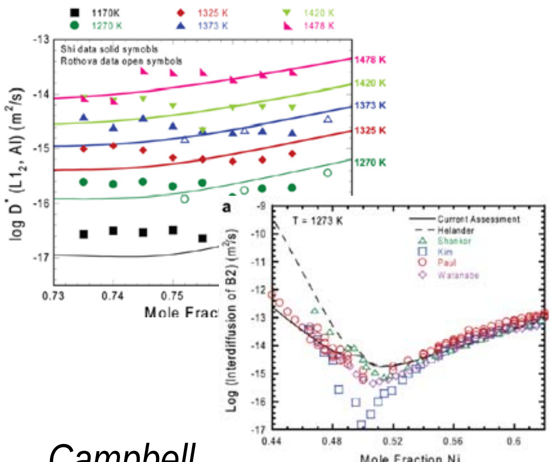
http://www.thermocalc.com
E-mail: info@thermocalc.se

Phone: +46 8 545 959 30
Fax: +46 8 673 3718

Introduction

DATA

Assessed difusional mobilities
In the γ' and B2 phases



Campbell,
Acta Mat 56(2008), p. 4277

MODEL

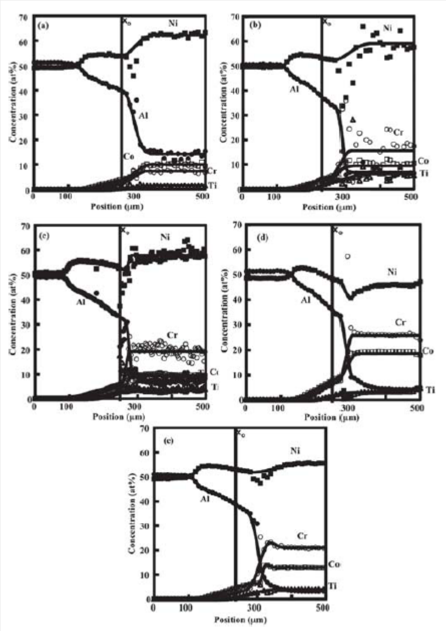
Homogenization approach available in DICTRA for diffusion simulations in multi-phase systems

$$J_k = \frac{-1}{V_m}\sqrt{[M_k x_k]_{n-1}^{eff}[M_k x_k]_n^{eff}}\,\frac{\Delta \mu_k}{\Delta z}$$

Larsson and Engström,
Acta Mat 54(2006), p. 2431

APPLICATION

Interdiffusion in NiAl / Ni-base superalloy diffusion couples



Perez et al.,
J. Phase Eq. 27(2006), p. 659

Thermodynamic Data

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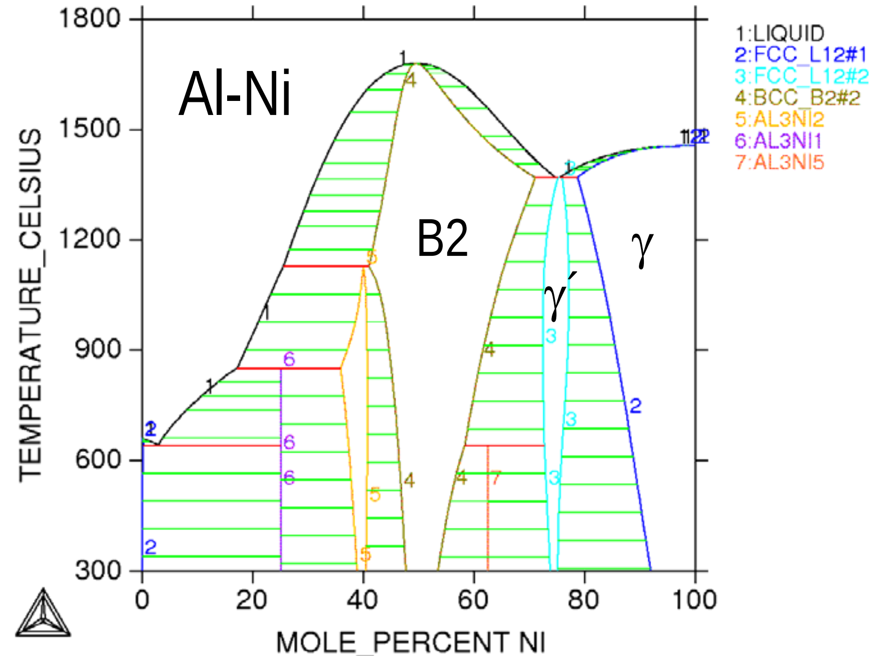
- TCNi1 – A thermodynamic database for Ni-base superalloys

Dupin and Sundman,
Scand J Metal 30(2001), p. 184



Two-sublattice order-disorder description used to model both B2 and $L1_2$,

e.g. for Al-Cr-Ni

FCC_A1 :AL CR NI: VA:
FCC_L12 :AL CR NI: AL CR NI: VA:

BCC_A2 :AL CR NI VA: VA:
BCC_B2 :AL CR NI VA: AL CR NI VA: VA:

Kinetic Data

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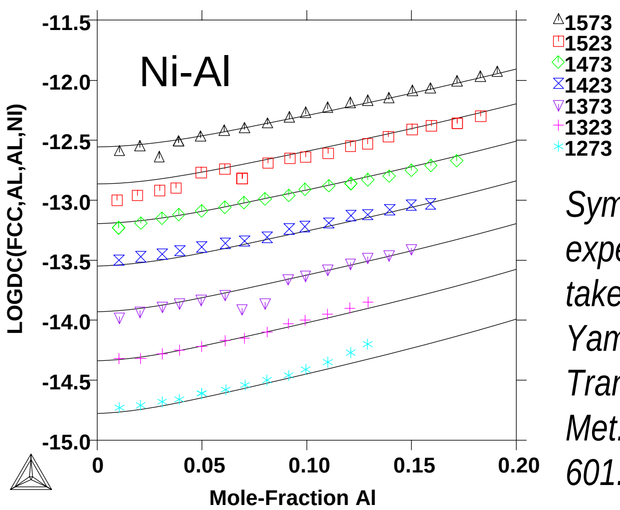
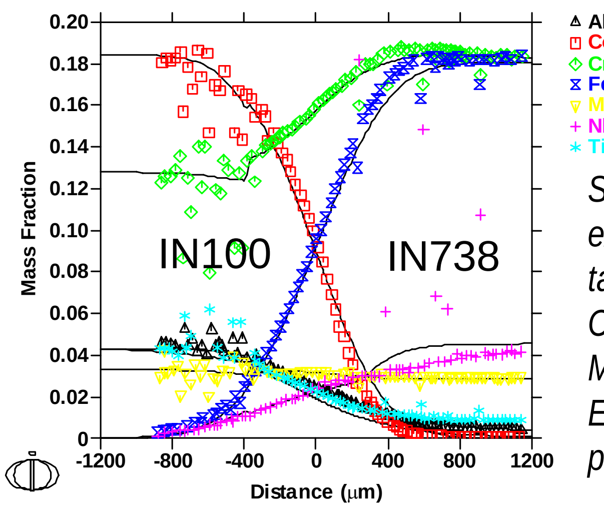
❑ Extended version of MobNi1 – A mobility DB for Ni-base superalloys

Mobilities in the γ-phase (disordered FCC), are well described on the basis of several published assessments, e.g.

- *Jönsson, Z. Metallkde. 85(1994) 502.* Ni-Cr-Fe
- Engström and Ågren, Z. Metallkde. 86(1995) 92. Ni-Al-Cr
- Matan et al., Acta mater., 46(1998) 4587. Ni-Al-Ti
- Campbell et al., Acta Mat. 50(2002) 775. Ni-Co, Ni-Hf, Ni-Mo, Ni-Ta, Ni-W, Ni-Re
- *Campbell et al., J. Phase Eq. and Diff. 25(2004) 6.* Fe-Al, Fe-Co



Symbols are experimental data taken from Yamamoto et al, Trans. Jpn. Inst. Met. 21(1980), p. 601.



Symbols are experimental data taken from Campbell et al, Materials Sci & Eng A 407(2005), pp. 135-146.

Kinetic Data

Extension consist of adding a description for the mobilities in the B2 and L12 (γ') phases.

Chemical ordering handled using a phenomenological model suggested by Helander and Ågren, Acta Mater. 47(1999), pp. 1141-52.

$$Q_B = Q_B^{dis} + \Delta Q_B^{ord}$$

Contribution to the activation energy from chemical ordering

$$\Delta Q_B^{ord} = \sum_i \sum_{i \neq j} \Delta Q_{Bij}^{order} \left[y_i^{\alpha} y_j^{\beta} - x_i x_j \right]$$

Contribution to the activation energy from chemical ordering of i-j atoms

Ni-Al-Cr taken from a recent paper by Campbell, Acta Mat. **56**(2008), p. 4277.

Preliminary description for remaining elements, e.g. Co, Ti and W.

Homogenization model

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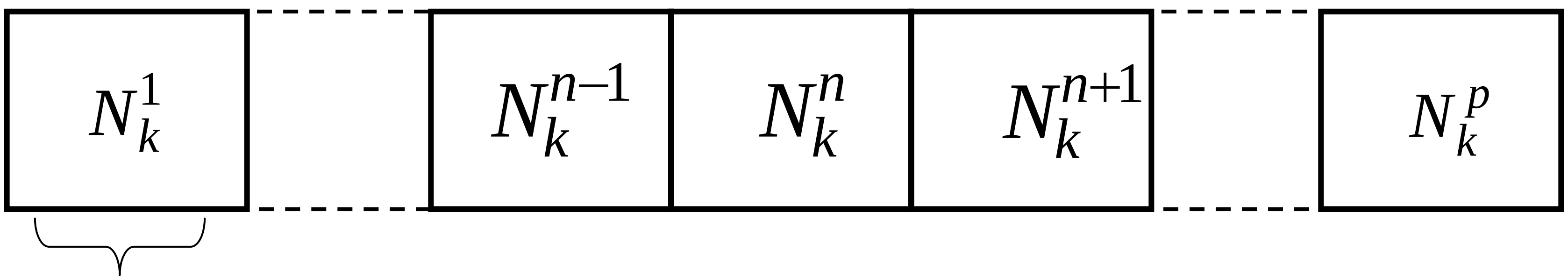
New approach allow us to account for diffusion in more than one phase



Flux between slices “n-1” and “n”

Equilibrium calculation
For each slice

$$J_k = \frac{-1}{V_m}\sqrt{[M_k x_k]_{n-1}^{eff}[M_k x_k]_{n}^{eff}}\,\frac{\Delta\mu_k}{\Delta z}$$

Phase fractions
Phase compositions
Chemical potentials
Mobilities

“Effective” $[M_k x_k]$ from combining rules

Larsson and Engström, Acta Mat 54(2006), p. 2431

Calculating effective [$M_k x_k$]

Combining rules are frequently used for determining an "effective" transport property in a multi-phase mixture, from:

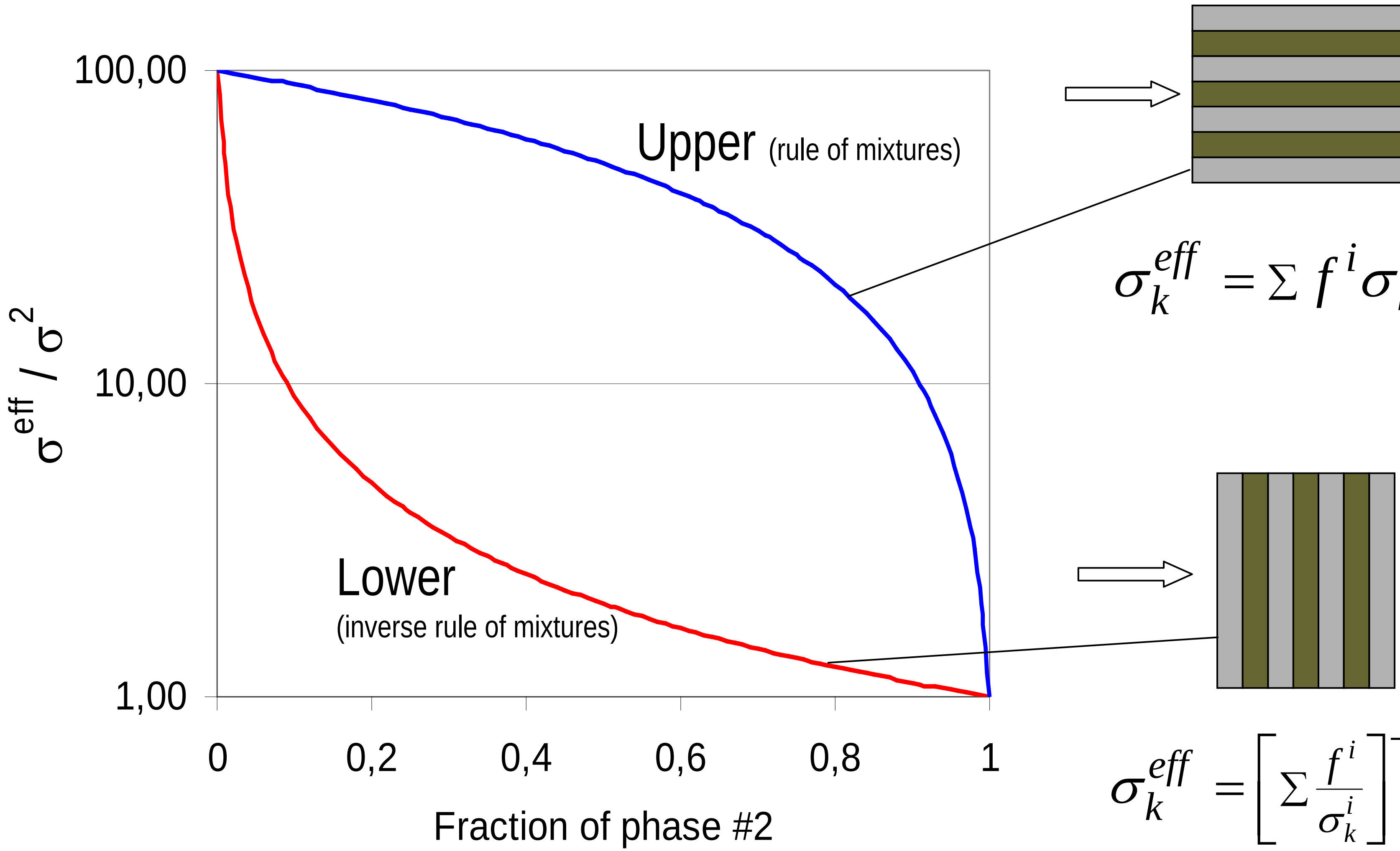
1) the transport properties in the individual phases,
2) the fraction of phases,
3) and sometimes also from their geometrical distribution.

Exact knowledge of the geometrical distribution is rarely known for a real case and it may be useful to study limiting cases or bounds.

Larsson and Engström, Acta Mat 54(2006), p. 2431

Absolute bounds

Wiener bounds are derived only on basis of the fraction of the various phases under consideration.

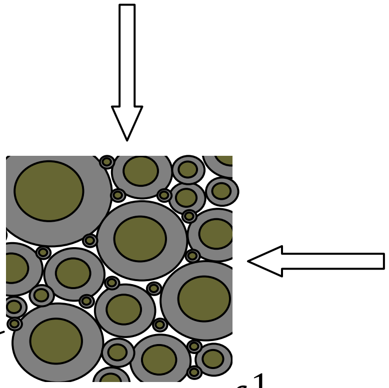


$$\sigma_k^{eff} = \Sigma f^i \sigma_k^i$$

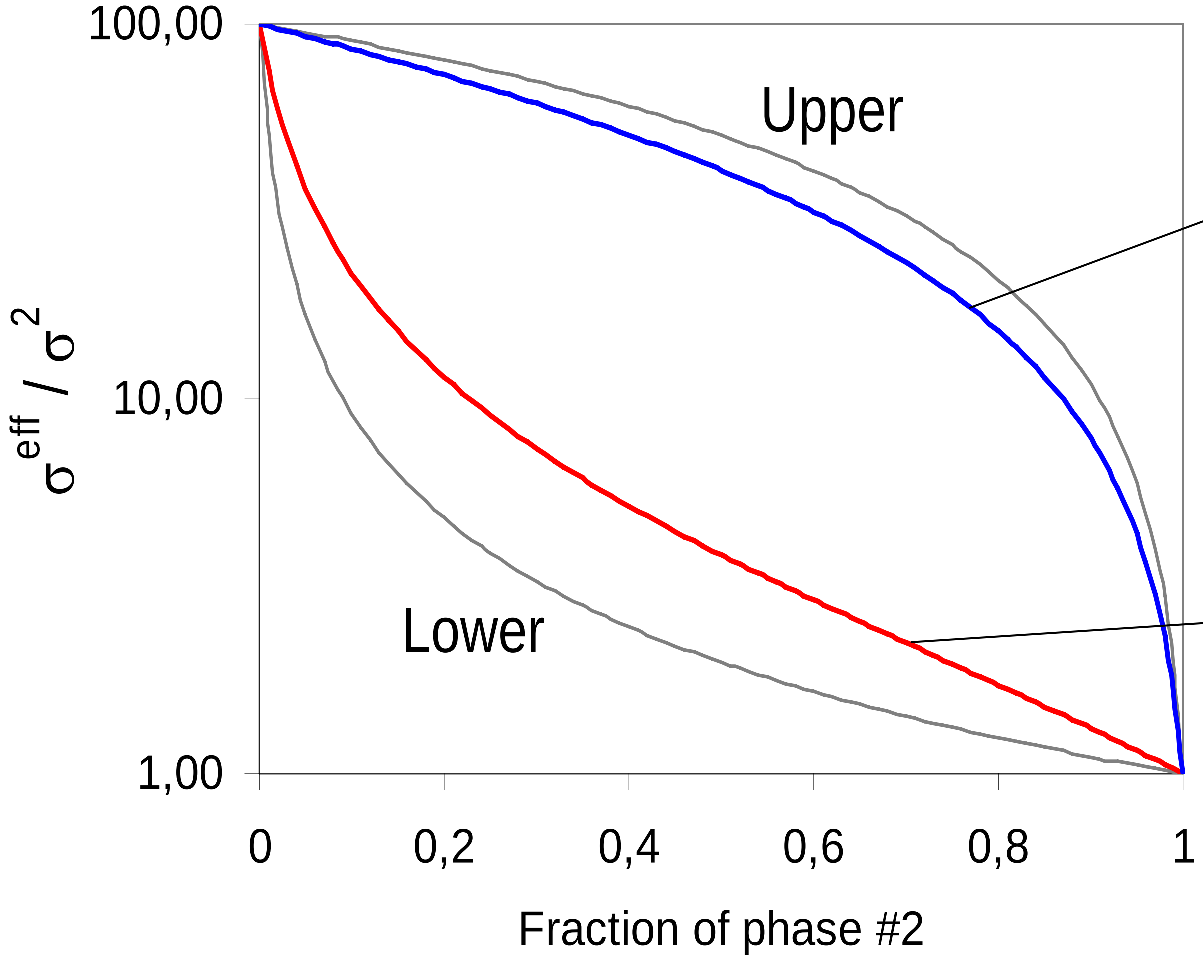
$$\sigma_k^{eff} = \left[\Sigma \frac{f^i}{\sigma_k^i} \right]^{-1}$$

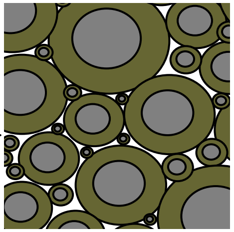
Hashin-Shtrikman bounds

More narrow bounds can be obtained by assuming the compound is in a statistical sense, isotropic and homogeneous.



$$\sigma_k^{eff} = \sigma_k^1 + \frac{f^1}{\frac{1}{\sigma_k^2 - \sigma_k^1} + \frac{f^2}{3\sigma_k^1}}$$

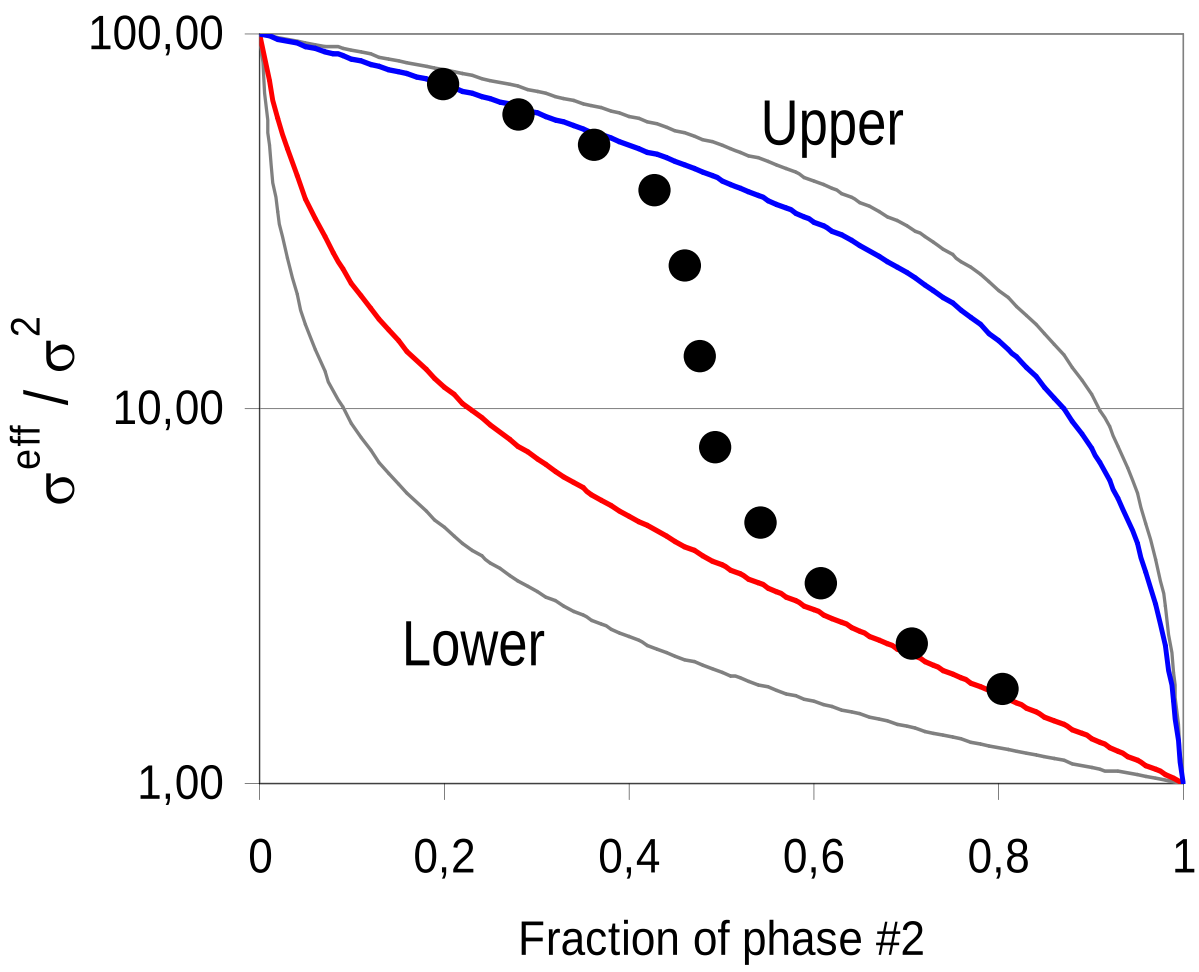




$$\sigma_k^{eff} = \sigma_k^2 + \frac{f^2}{\frac{1}{\sigma_k^1 - \sigma_k^2} + \frac{f^1}{3\sigma_k^2}}$$

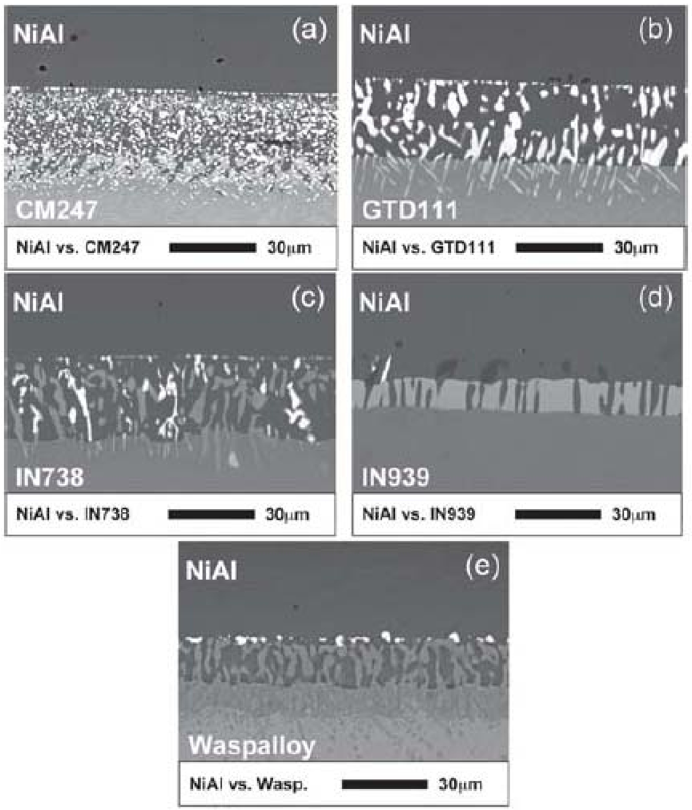
Percolation

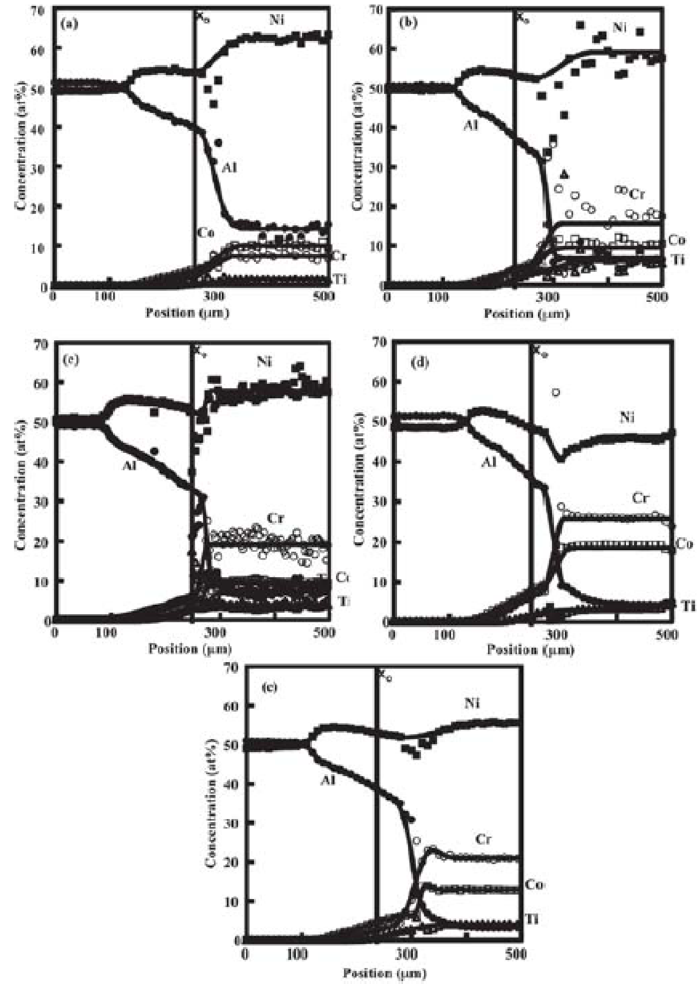
In reality one can not expect the same phase is continuous throughout the whole interval.



For practical calculations one could use e.g. the upper bound below a certain volume fraction of the low mobility phase and the lower bound above the same volume fraction.

NiAl-coating / Ni-base superalloy system





E. Perez, T. Patterson and Y. Sohn,
J. Phase Equilibria and Diffusion 27(2006), pp. 659-64.

NiAl-coating / Ni-base superalloy system

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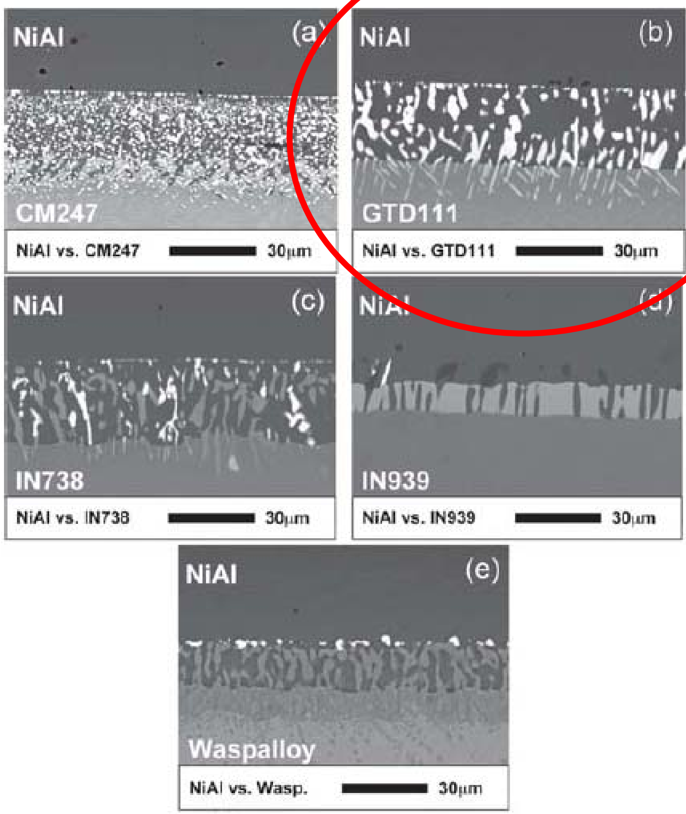

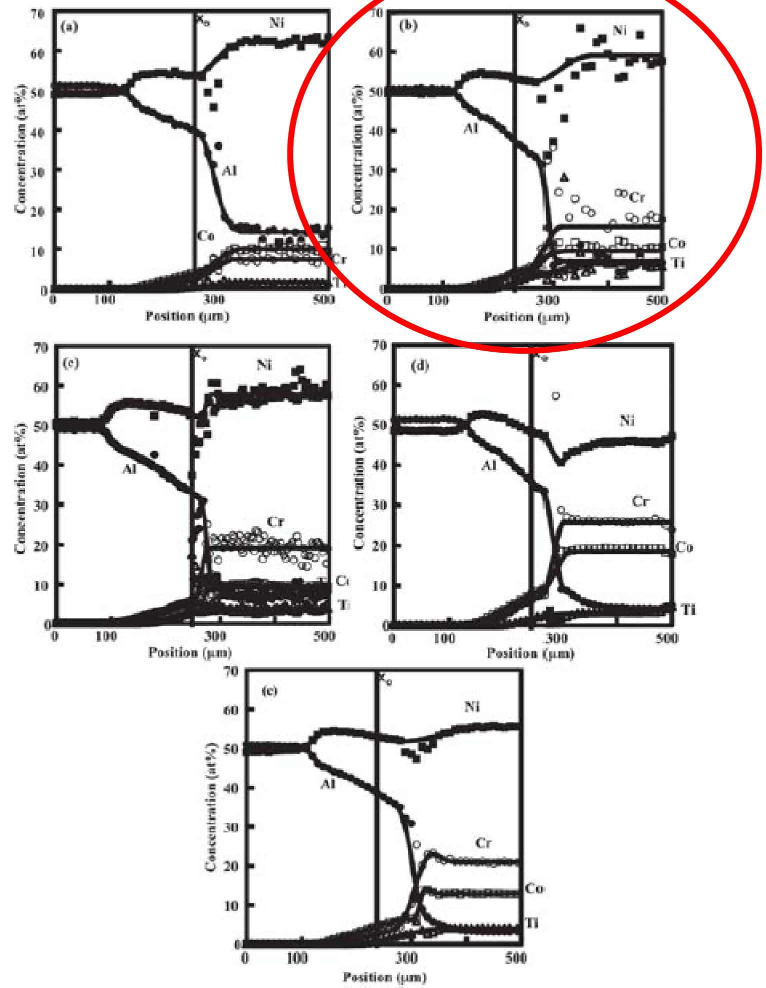

E. Perez, T. Patterson and Y. Sohn,

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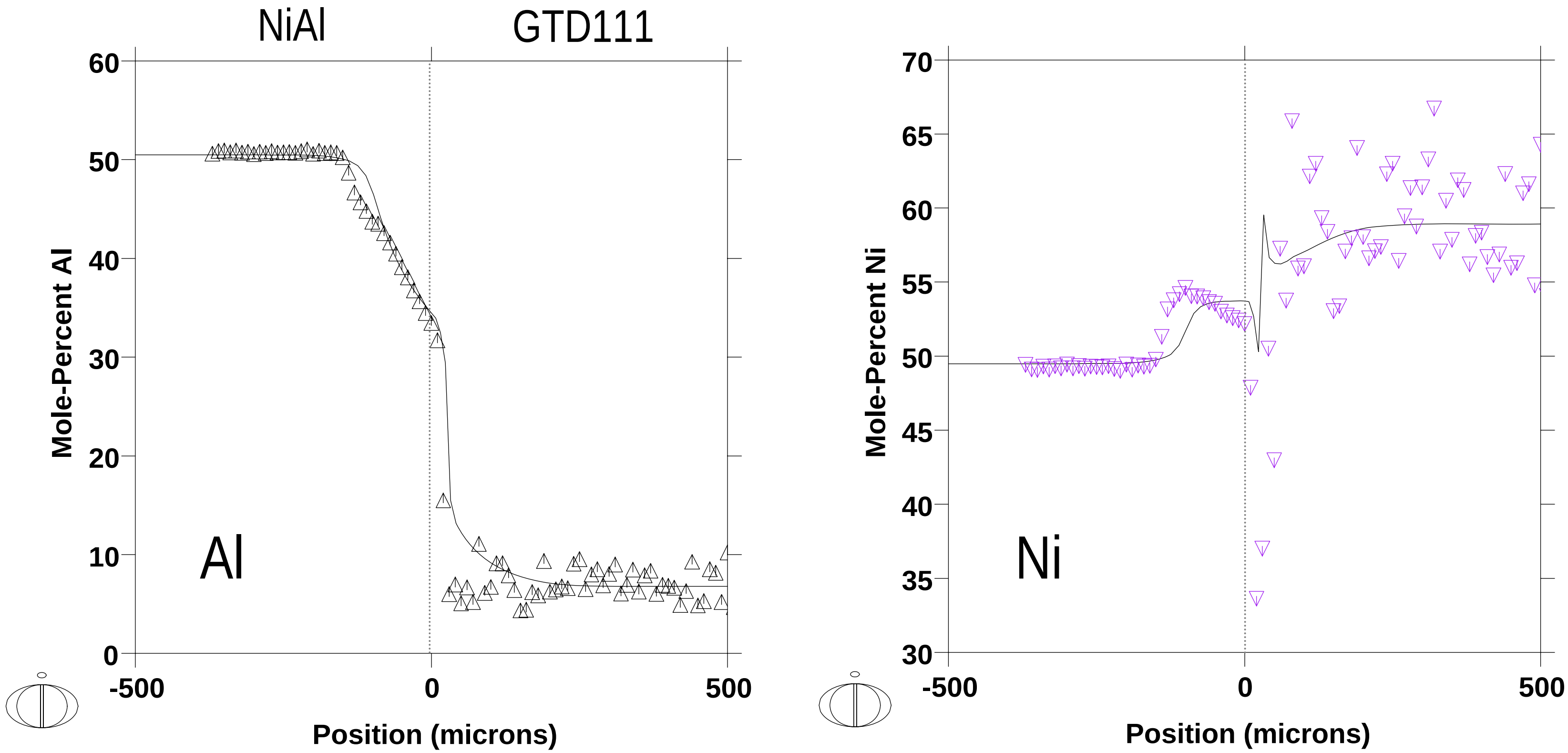
NiAl-coating / GTD111

Thermo-Calc Software

	Ni	Al	C	Co	Cr	Mo	Ta	Ti	W
NiAl-Coating	Bal	50.5	-	-	-	-	-	-	-
GTD111	Bal	6.9	0.48	9.5	16.6	0.97	0.89	6.24	0.97

Temp. 1050°C
Time 96h

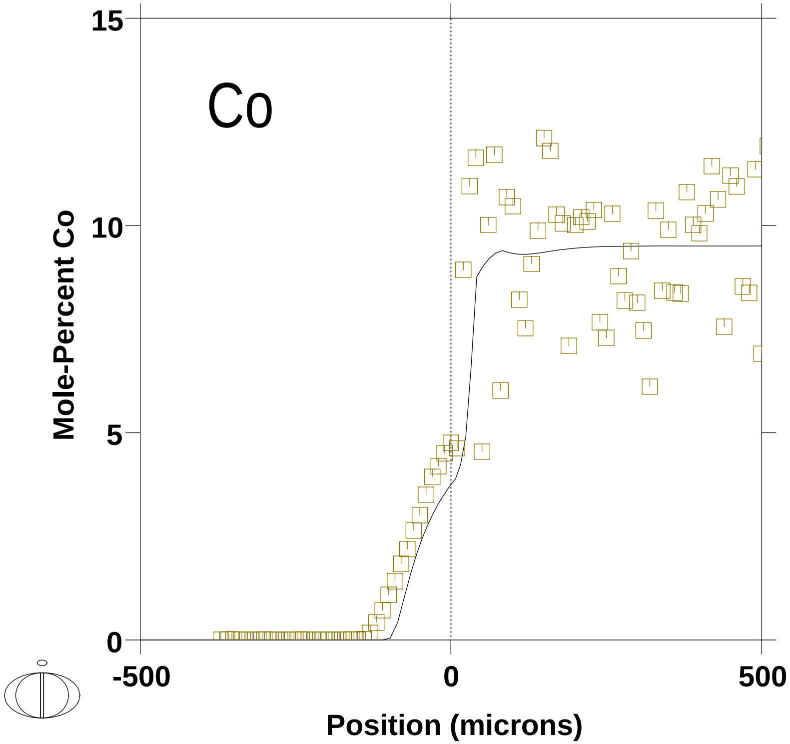
Rule of mixtures

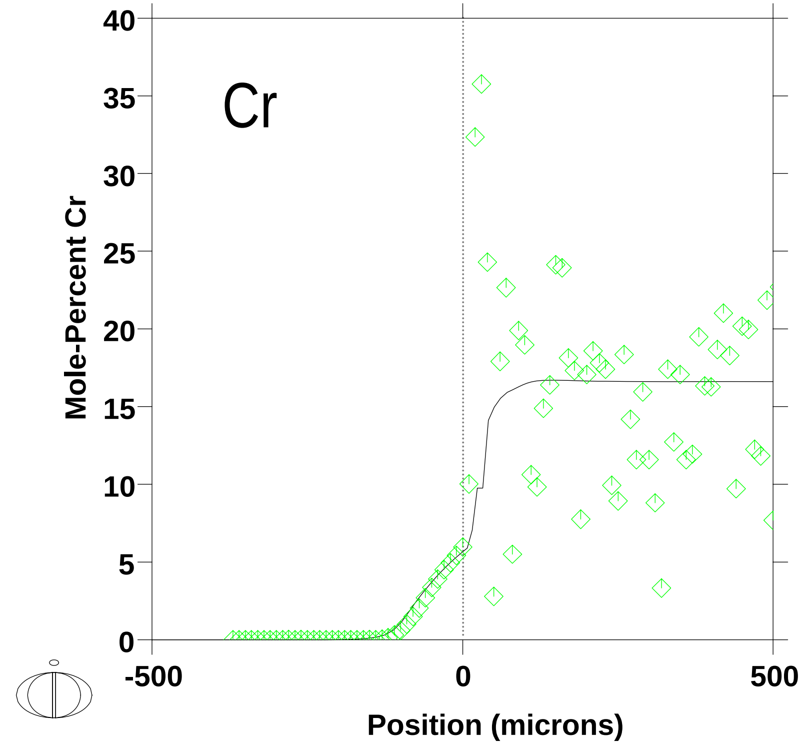


Symbols are experimental data from E. Perez, T. Patterson and Y. Sohn, J. Phase Equilibria and Diffusion 27(2006), pp. 659-64.

NiAl-coating / GTD111

Thermo-Calc Software





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NiAl-coating / GTD111

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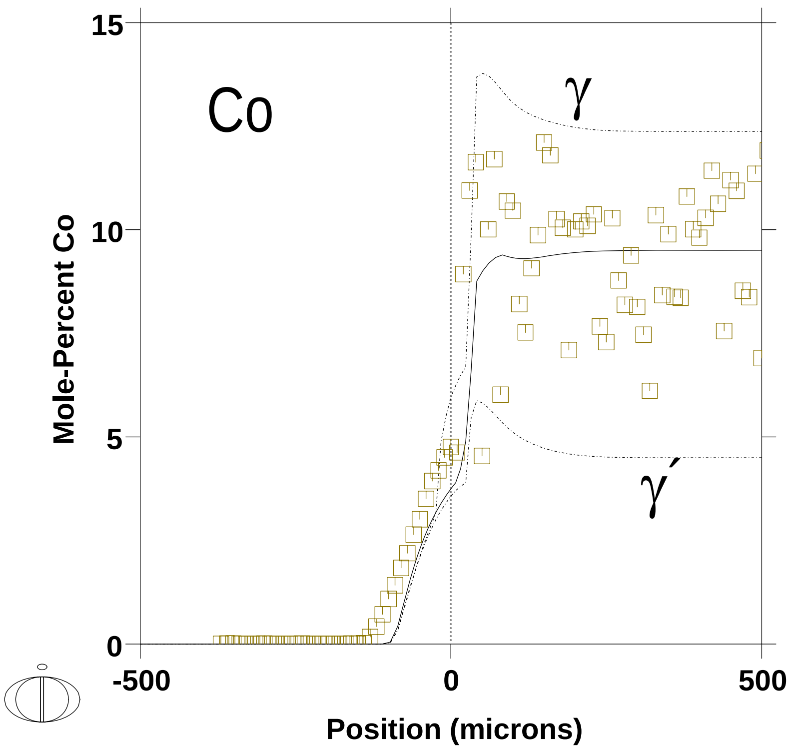

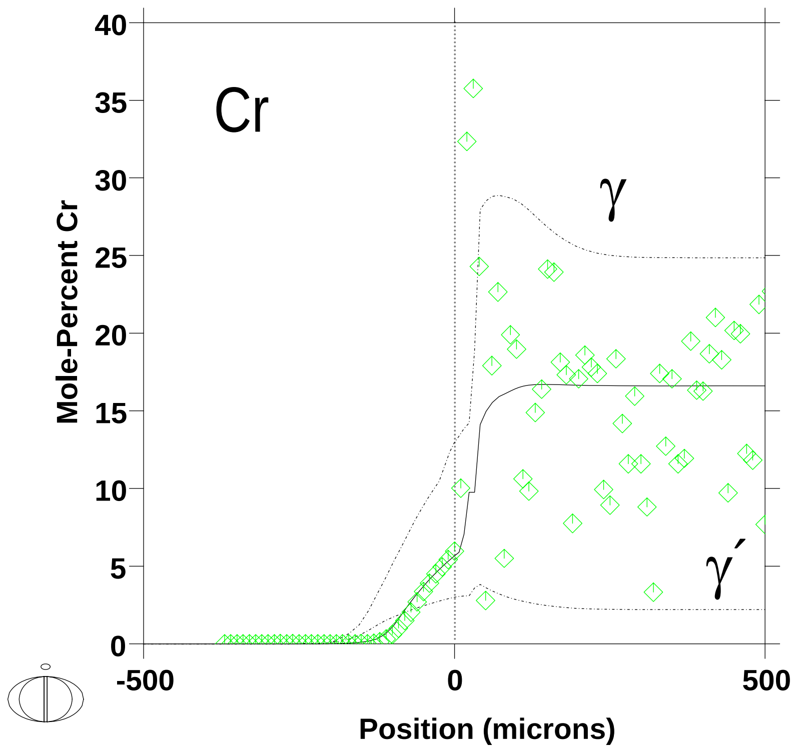

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NiAl-coating / GTD111

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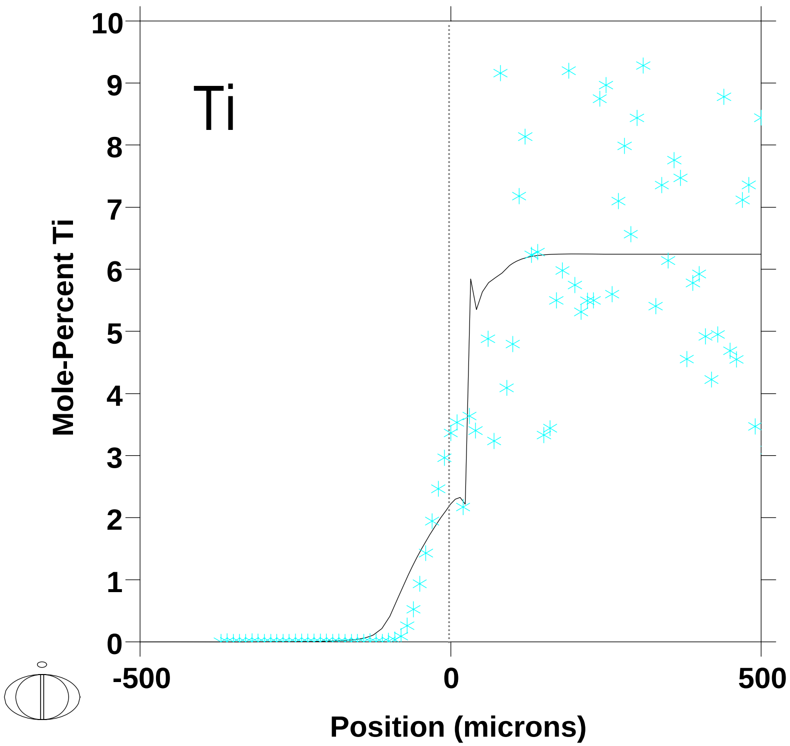

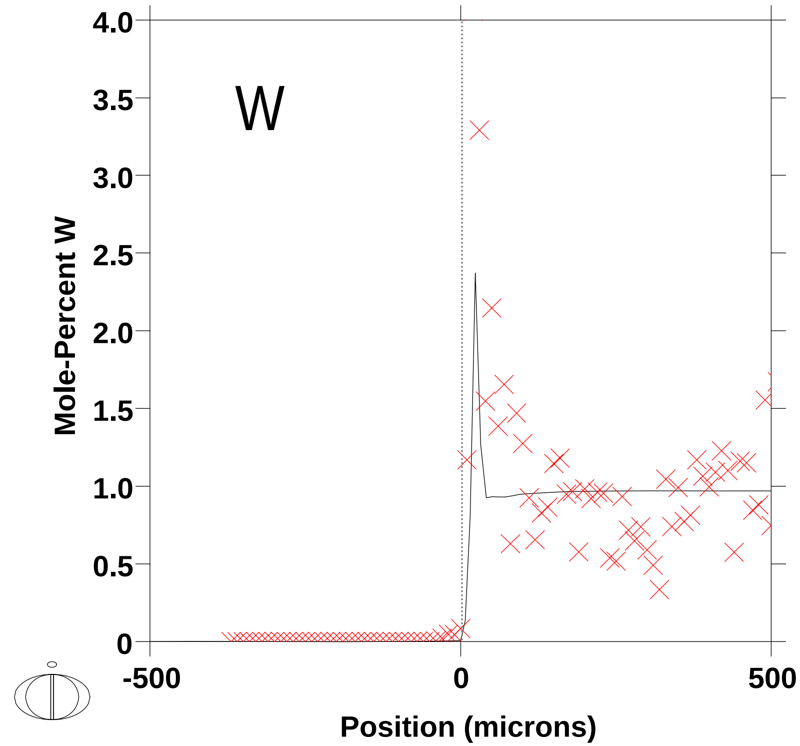

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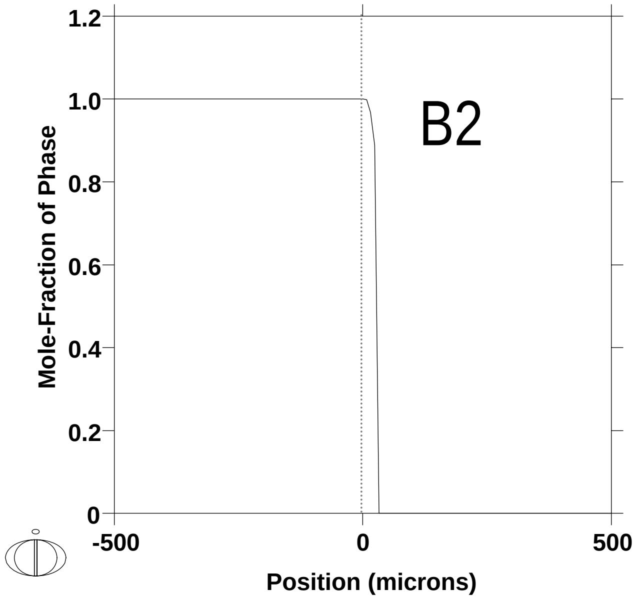
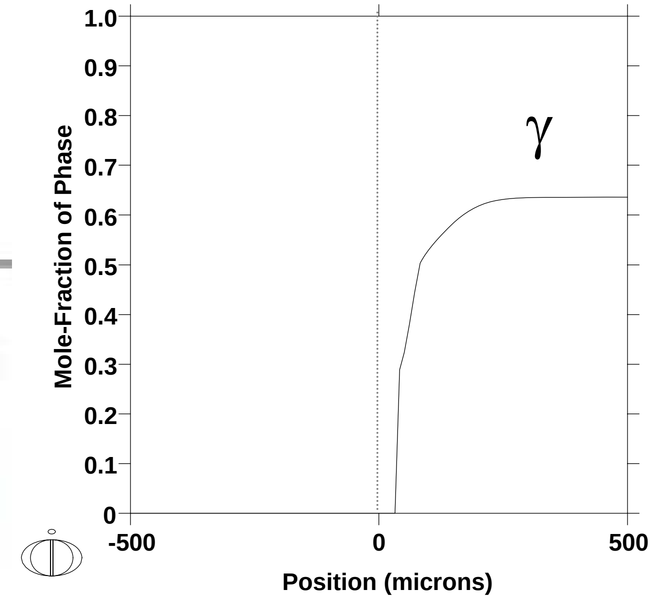
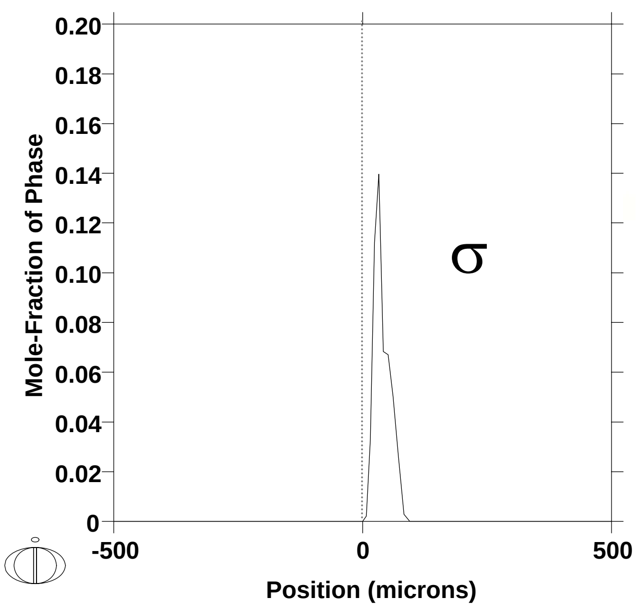
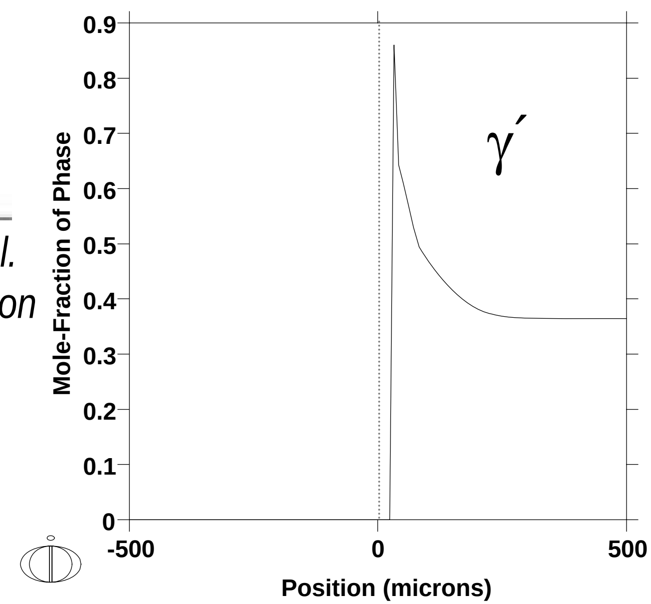




Micrograph from E. Perez et al. J. Phase Equilibria and Diffusion 27(2006), pp. 659-64.





NiAl-coating / Ni-base superalloy system

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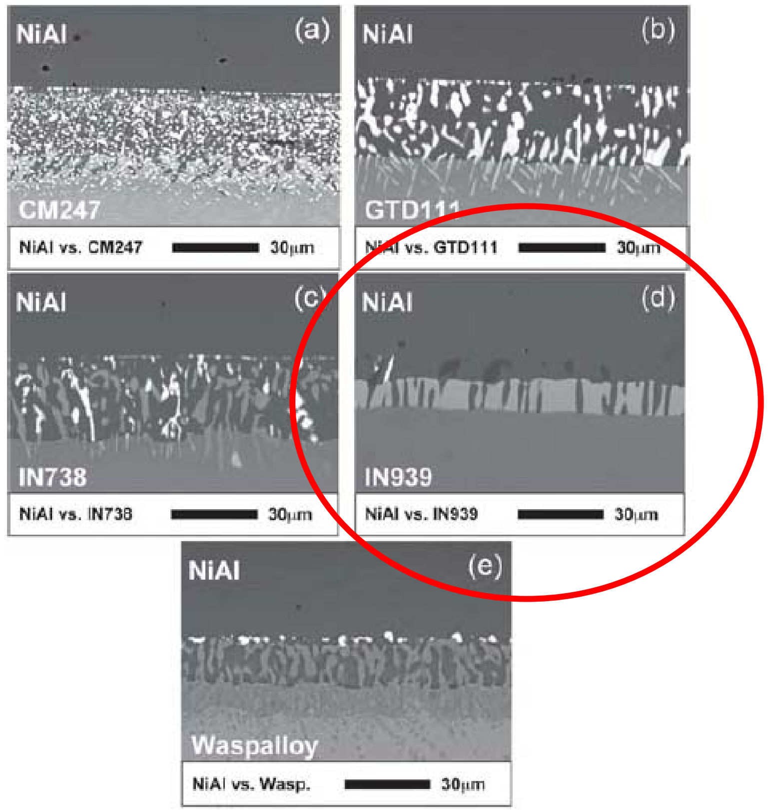
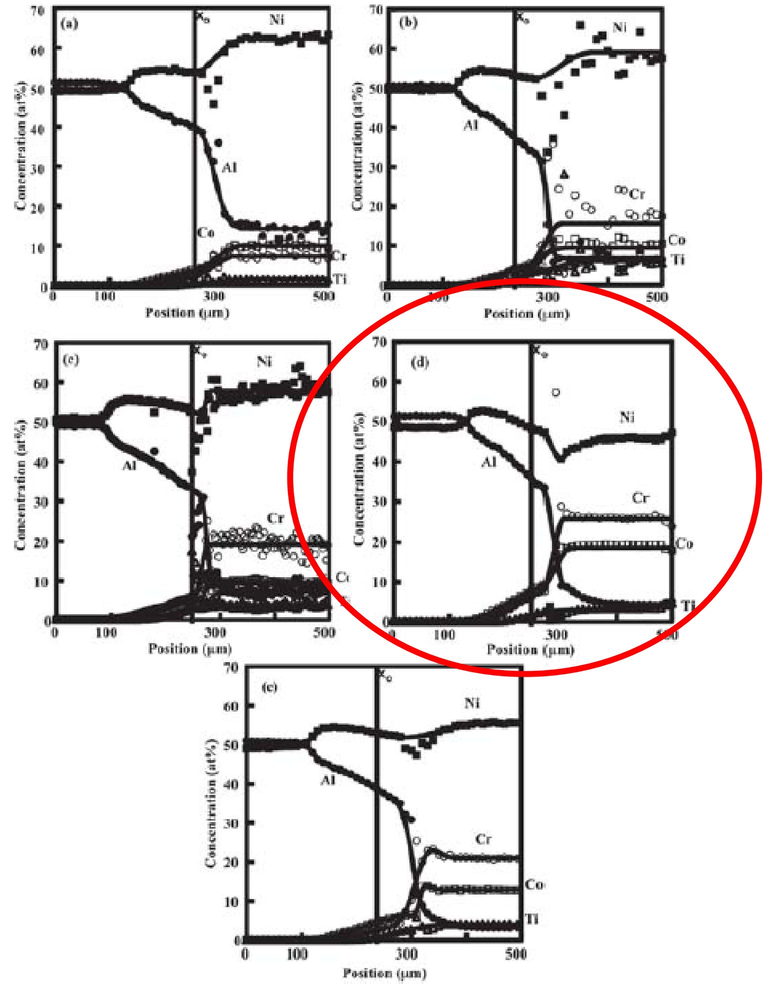




E. Perez, T. Patterson and Y. Sohn,
J. Phase Equilibria and Diffusion 27(2006), pp. 659-64.

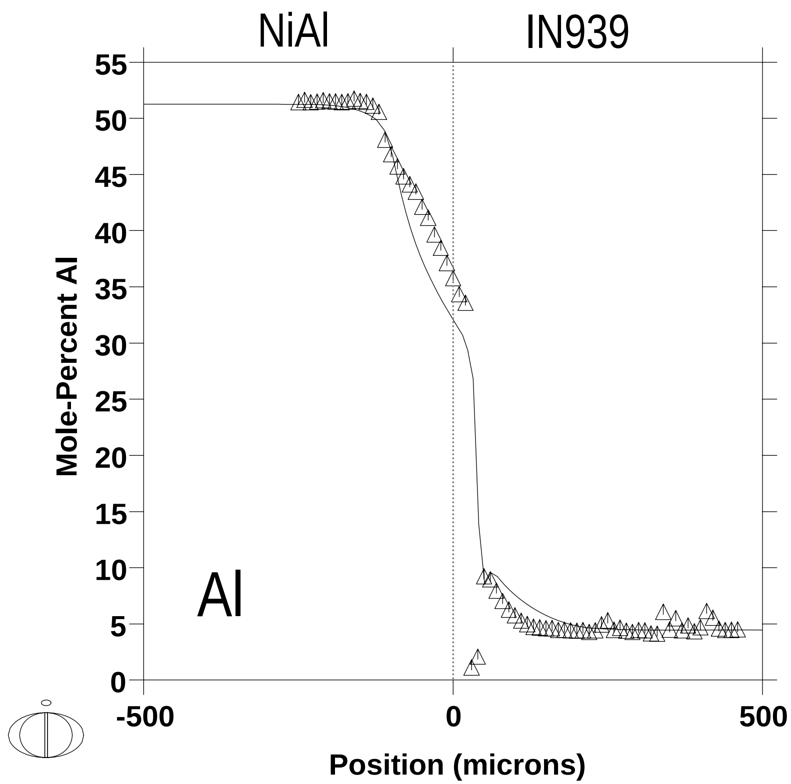
NiAl-coating / IN939

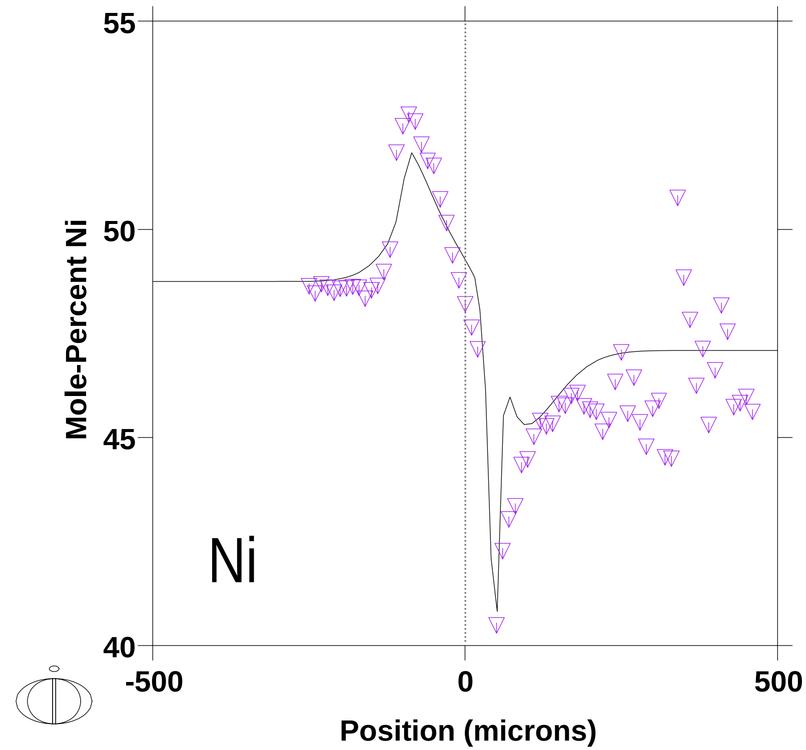
Thermo-Calc Software

	Ni	Al	C	Co	Cr	Nb	Ta	Ti	W
NiAl-Coating	Bal	51.2	-	-	-	-	-	-	-
IN939	Bal	4.45	0.71	18.6	25.3	0.43	0.37	4.07	0.51

Temp. 1050°C
Time 96h

Rule of mixtures





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NiAl-coating / IN939

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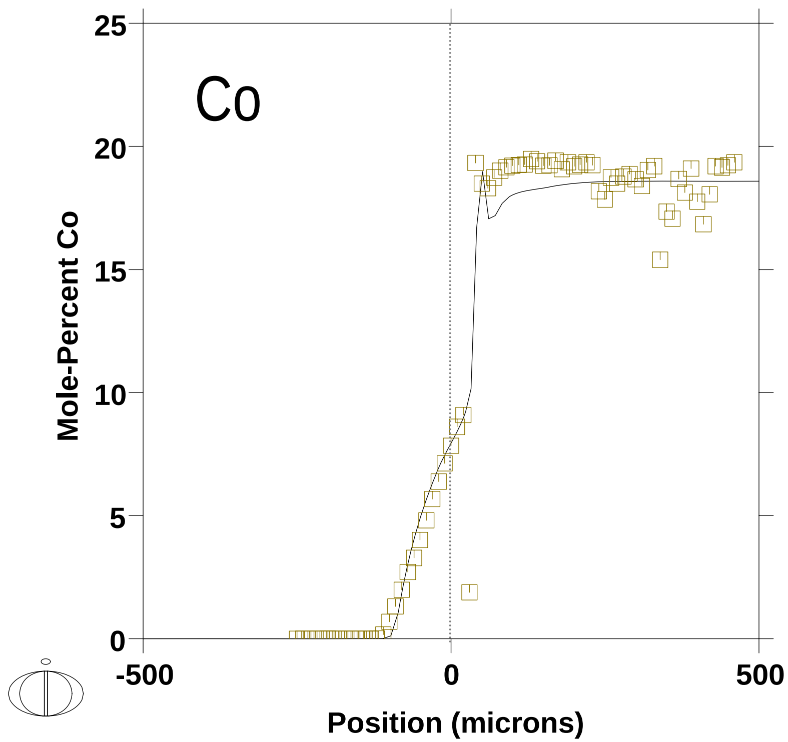

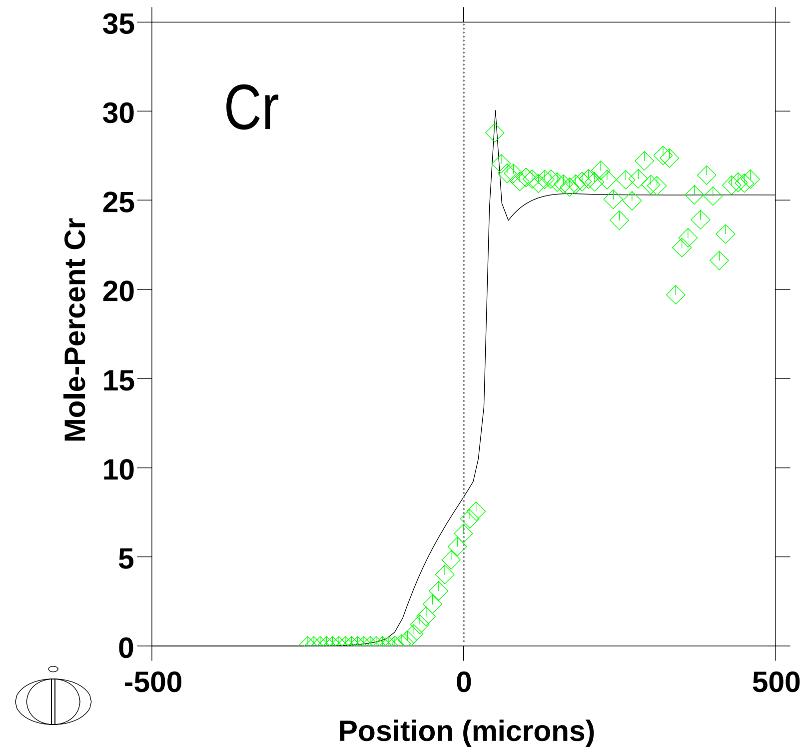

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NiAl-coating / IN939

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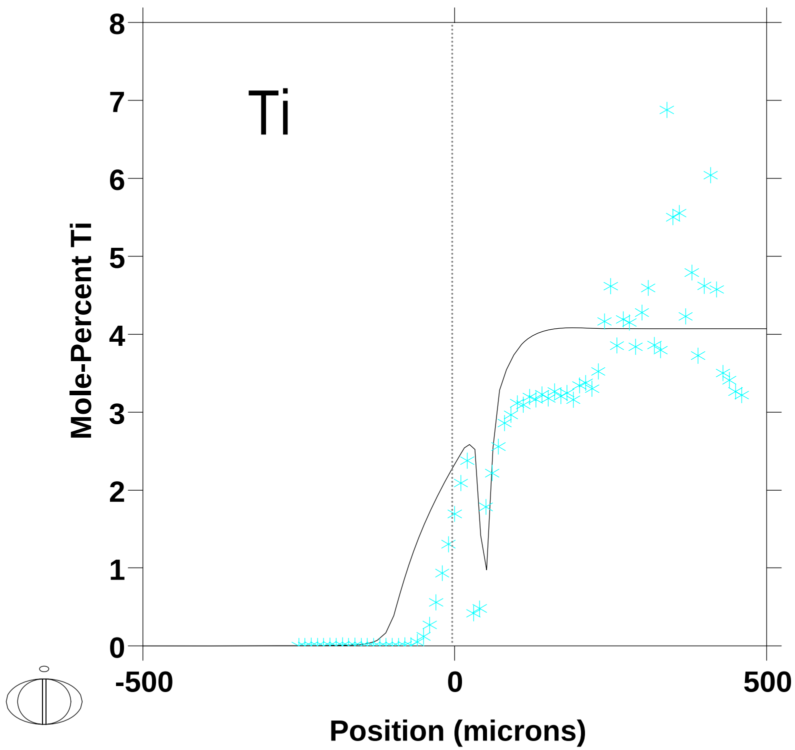

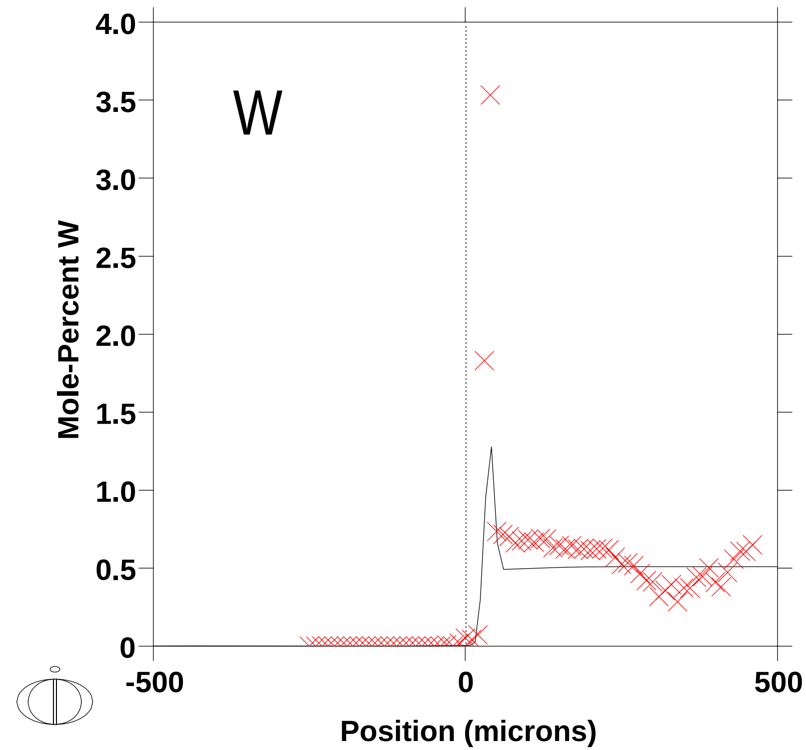

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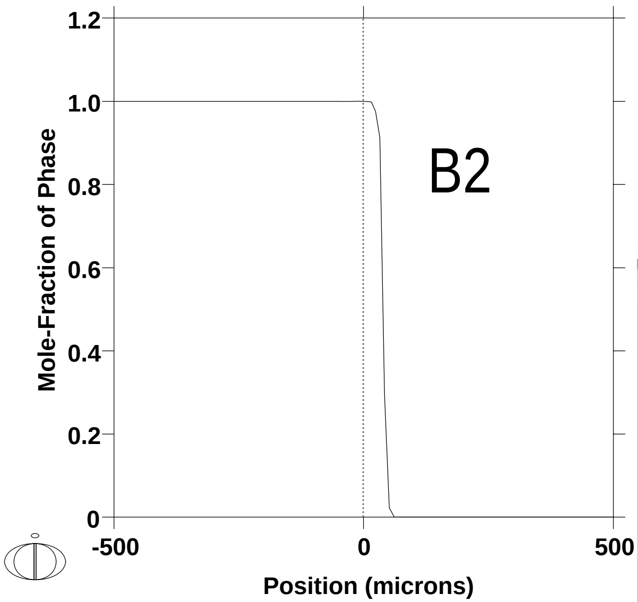

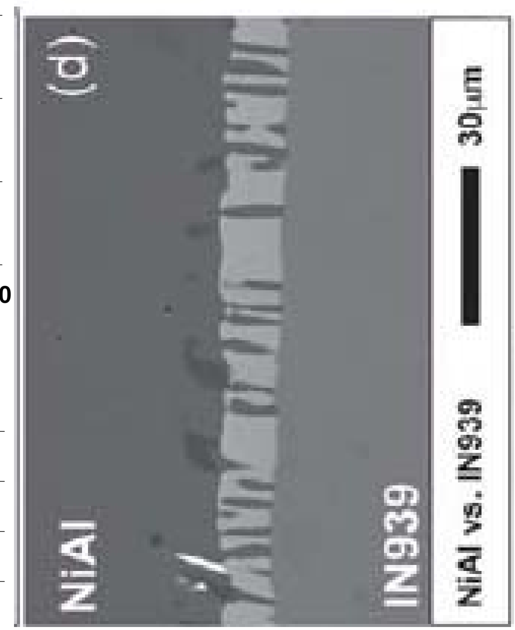

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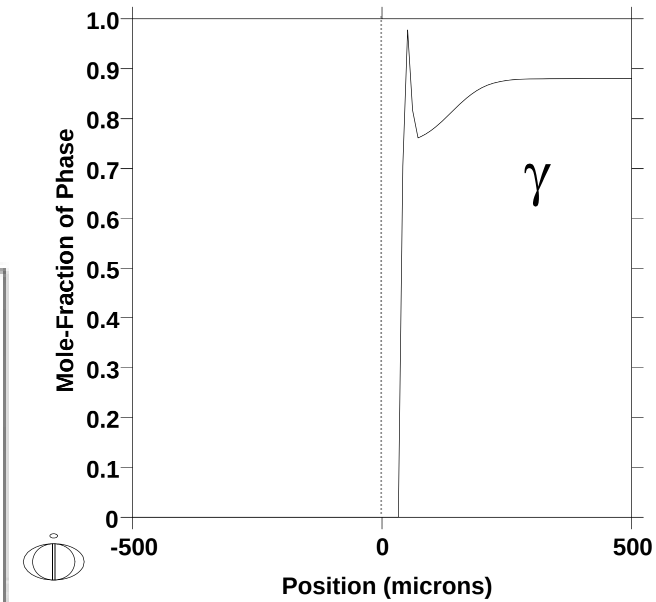

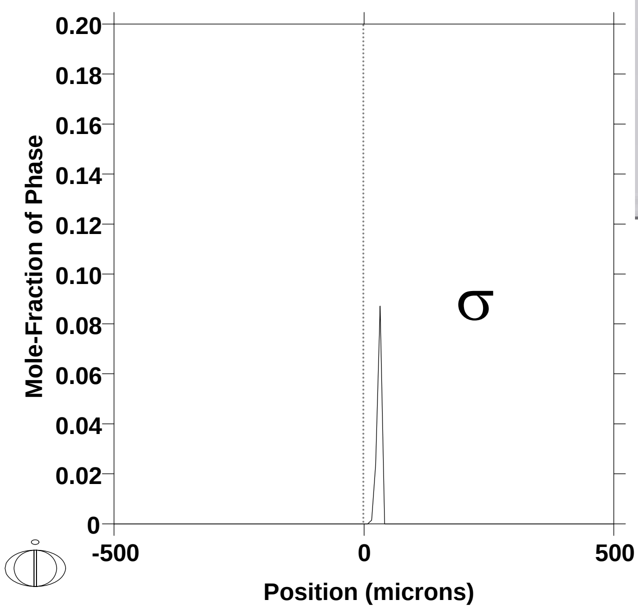

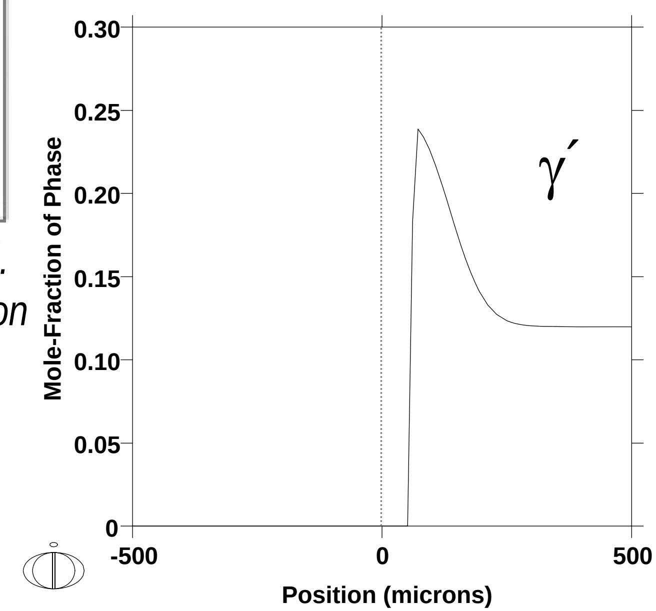

Thermo-Calc Software

CALCULATING THERMODYNAMIC PROPERTIES

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http://www.thermocalc.com
E-mail: info@thermocalc.se

Phone: +46 8 545 959 30
Fax: +46 8 673 3718