Dictra 1D multiphase moving phase boundary simulations under local equilibrium conditions

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DICTRA

- Software package for simulation of diffusion controlled reactions in multi-component alloys.
- Simulation on geometries, which may be reduced to one spatial coordinate (planar, cylindrical or spherical)
- Linked to Thermo-Calc, which provides all necessary thermodynamic properties.
- The result of more than 20 years and 60 man-years R&D at:

  Royal Institute of Technology in Stockholm, Sweden

  Max-Planck Institute für Eisenforschung in Düsseldorf, Germany

  Thermo-Calc Software

Thermo-Calc Software

Outline

- Multiphase simulations
- Moving phase boundary simulations
- Combining the above

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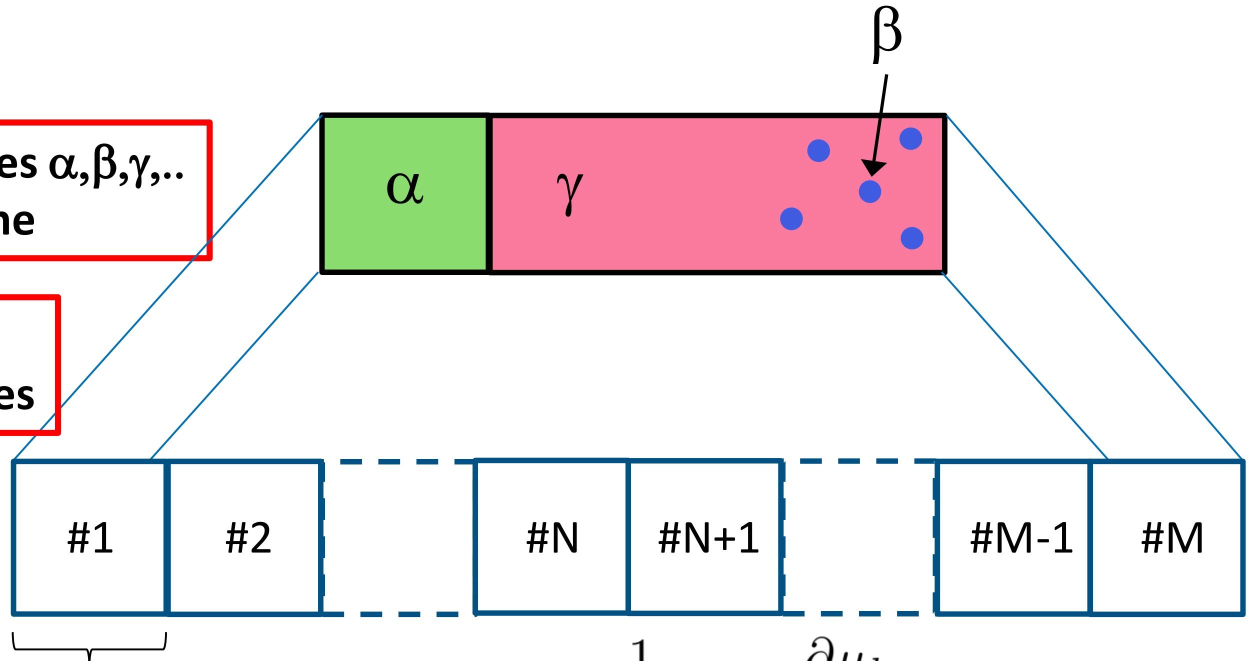
Multiphase simulations

Allow a set of phases α,β,γ,.. in each finite volume

No front-tracking
No explicit interfaces



Equilibrium calculation

- Phase fractions
- Phase compositions
- Chemical potentials
- Mobilities

$$J_k = \frac{-1}{V_m} M_k x_k \frac{\partial \mu_k}{\partial z}$$

$$\simeq \frac{-1}{V_m} \sqrt{[M_k x_k]^{\text{eff}}_{\#N} \, [M_k x_k]^{\text{eff}}_{\#N+1}} \frac{\Delta \mu_k}{\Delta z}$$

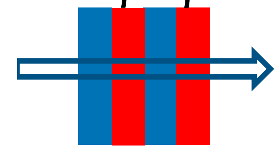
Engström, Thesis, KTH, 1996
Larsson, Engström, Acta Mater 54(2006)2431
Larsson, Höglund, Calphad 33(2009)495

Multiphase simulations

Estimates of $[M_k x_k]^{\text{eff}} = \Gamma_k^\star$

What are the kinetics of a Multiphase mixture?

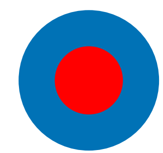
αβαβ

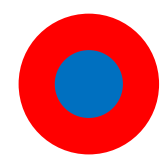


$$\Gamma_k^\star = \left[\sum_\phi \frac{f^\phi}{\Gamma_k^\phi}\right]^{-1}$$

$$\Gamma_k^\star = \sum_\phi f^\phi \Gamma_k^\phi$$

Wiener bounds, rule-of-mixtures





$$\Gamma_k^\star = \Gamma_k^\alpha + \frac{A_k^\alpha}{1 - \frac{A_k^\alpha}{3\Gamma_k^\alpha}}$$

$$A_k^\alpha = \sum_{\phi \neq \alpha} \frac{f^\phi}{\frac{1}{\Gamma_k^\phi - \Gamma_k^\alpha} + \frac{1}{3\Gamma_k^\alpha}}$$

$$\begin{cases} \Gamma_k^\alpha = \min\left[\Gamma_k^\beta, \Gamma_k^\gamma, \Gamma_k^\delta, \ldots\right] \\ \Gamma_k^\alpha = \max\left[\Gamma_k^\beta, \Gamma_k^\gamma, \Gamma_k^\delta, \ldots\right] \end{cases}$$

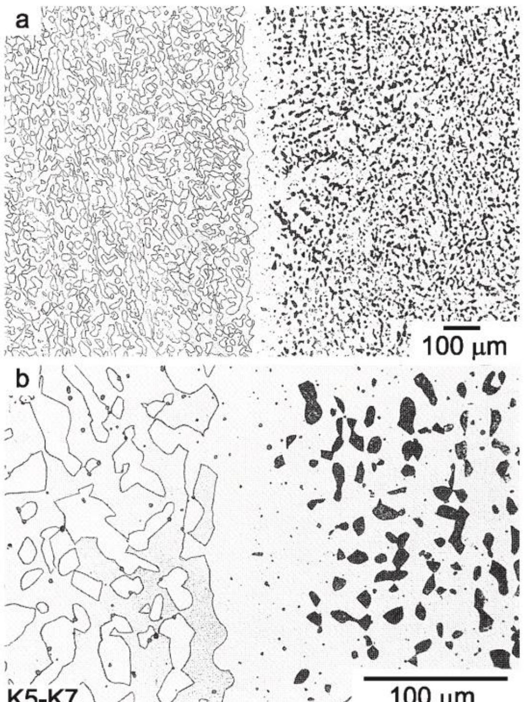
Hashin-Shtrikman bounds

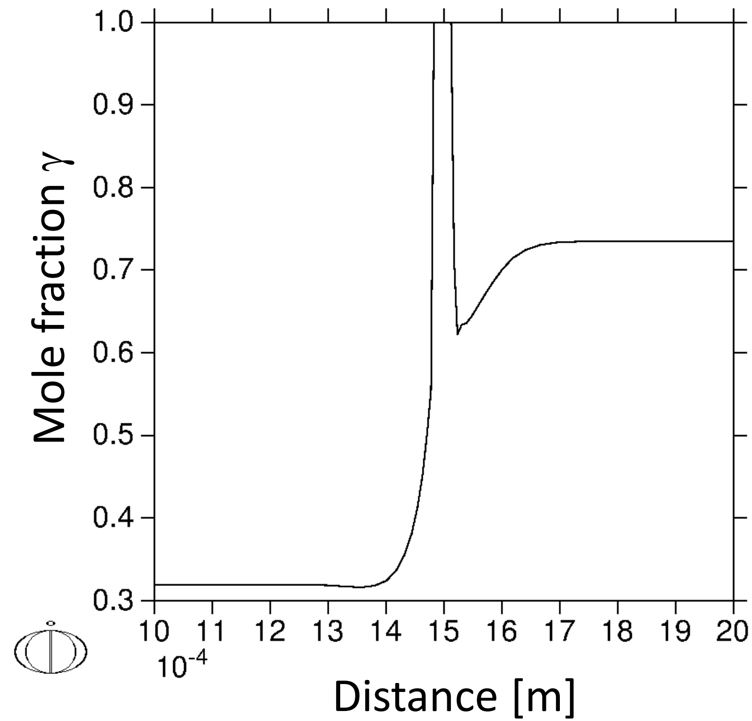
Wiener, Thesis, Königl Sächs Gesell Wissen, 1912
Rayleigh, Phil Mag 34(1892)481
Hashin, Shtrikman, J Appl Phys 33(1962)3125

Multiphase simulations

Example: Fe-Cr-Ni $\alpha+\gamma$ diffusion couple

- 25.7 Cr 6.5 Ni - 42.3 Cr 27.6 Ni (at-%)
- 100 h, 1100°C
- Experiment by Engström



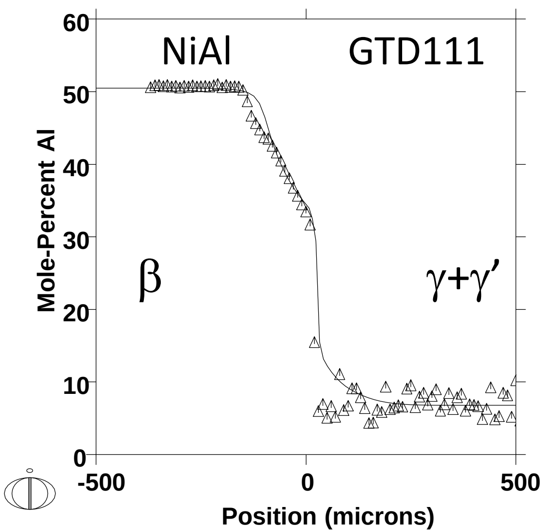


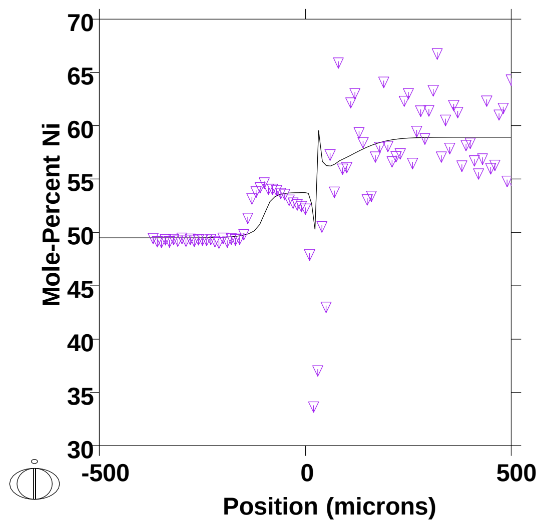
Engström, Scand J Metall 24(1995)12
Larsson, Engström, Acta Mater 54(2006)2431

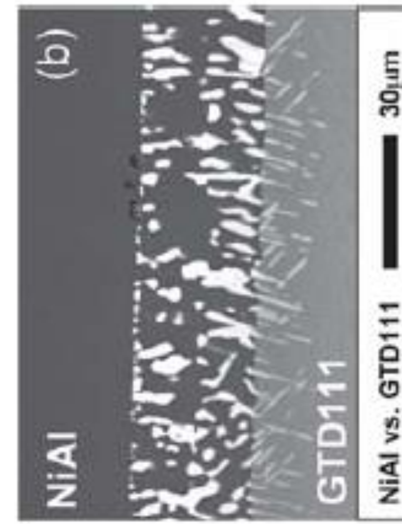
Multiphase simulations

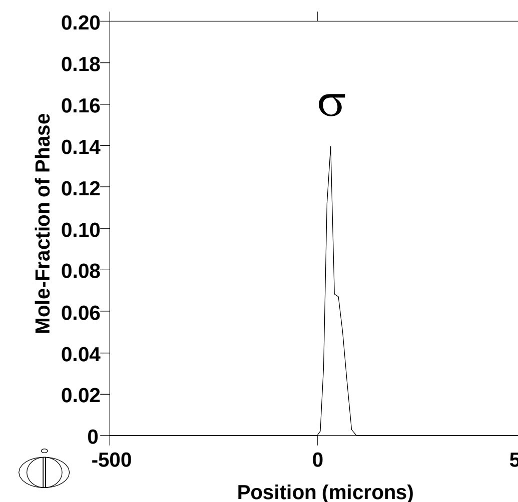
Example: NiAl-coating / Ni superalloy diffusion couple

- 50.5 Al - 6.9 Al 9.5 Co 16.6 Cr 6.2 Ti (at-%, bal. Ni)
- 96 h, 1050°C
- Experiment by Perez, Patterson, Sohn









Perez, Patterson, Sohn, J Phase Equilibria Diffusion 27(2006)659

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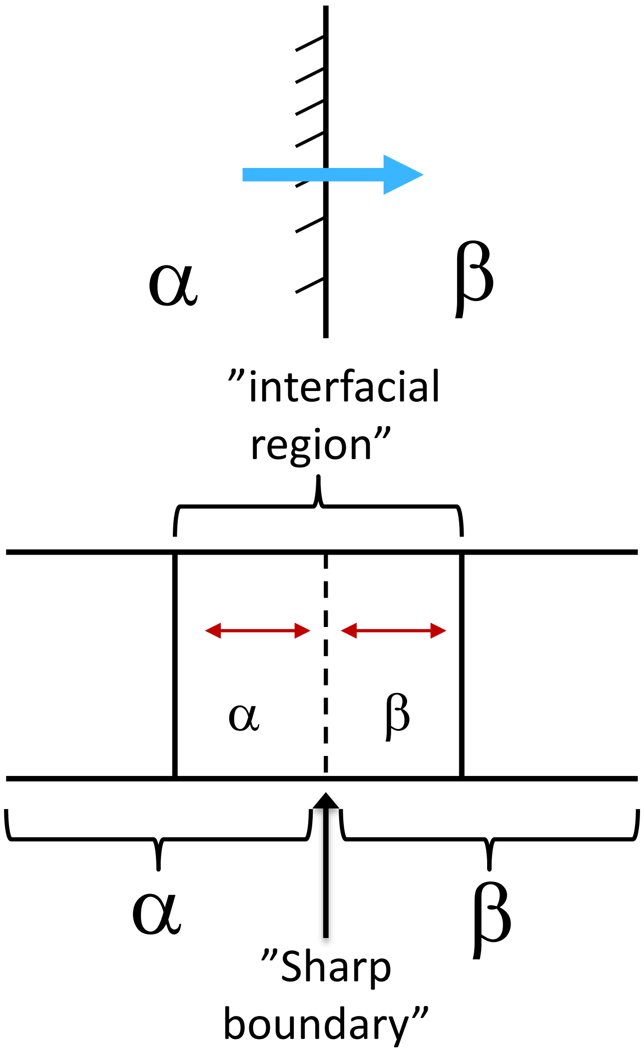
Local equilibrium – finite width interface



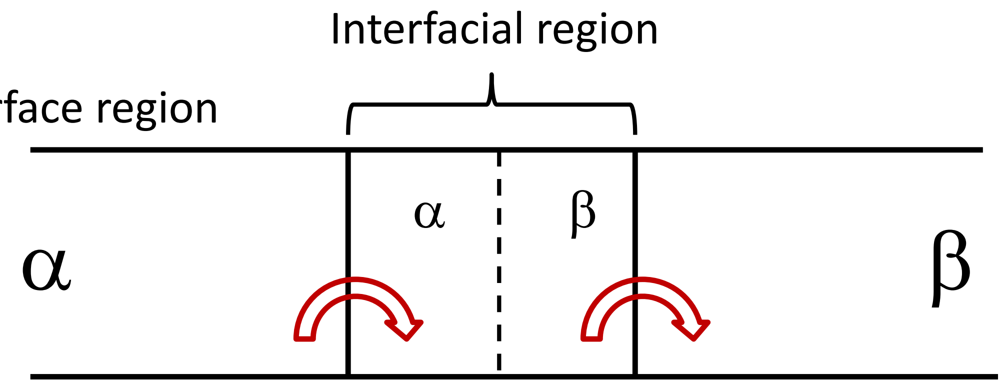
A recently added model in Dictra in addition to the originally implemented Sharp interface model

Assume

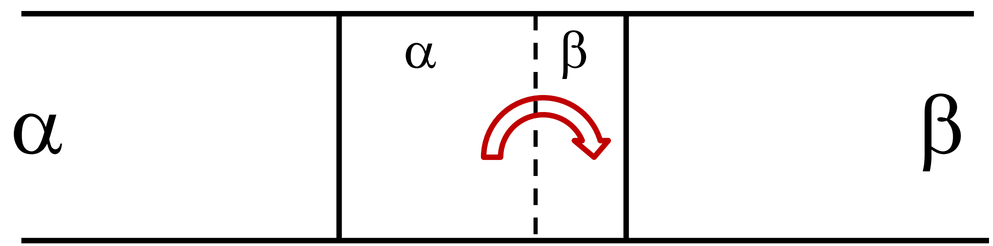
- An interfacial region of constant, finite width
- Local equilibrium holds inside the interfacial region
- Kinetics is infinitely fast in the interfacial region
- A sharp boundary in the middle of the interfacial region separate the phases
- Interface migration is caused by mass transfer over the sharp boundary $v^{\alpha/\beta} = -\overset{\curvearrowright}{J} V_m$

Conceived sequence of events leading to interface migration

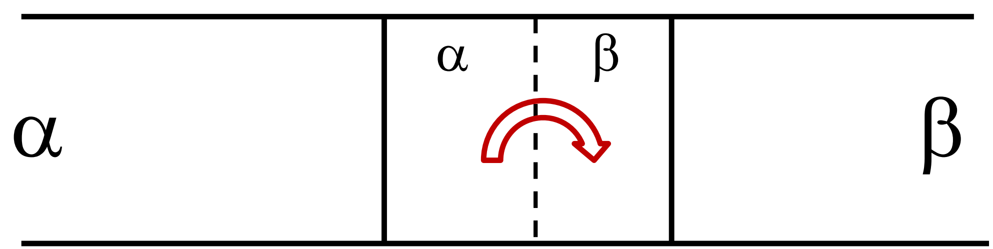
Fluxes into interface region



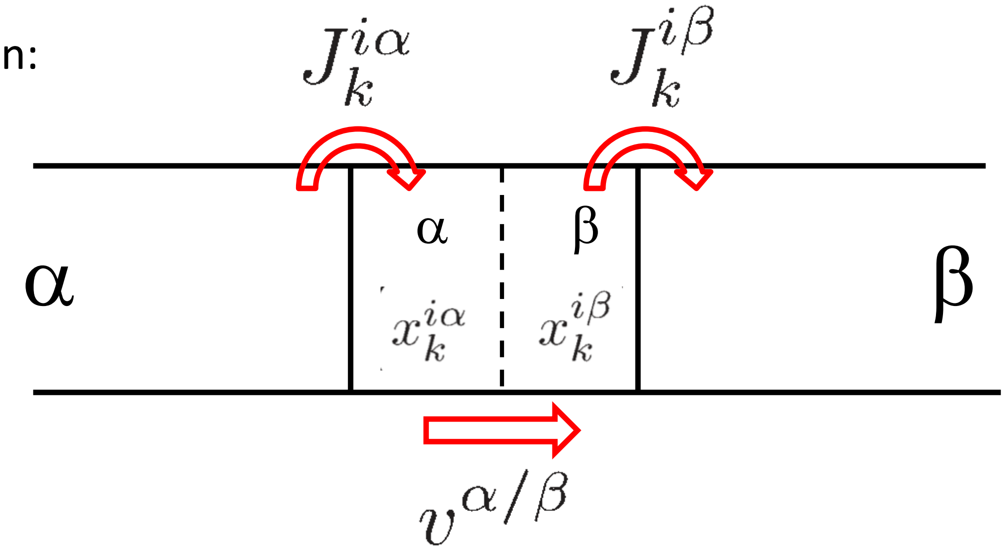
Instantaneous redistribution inside interface to maintain equilibrium



The interfacial region is dragged along convectively



Fluxes into interfacial region:



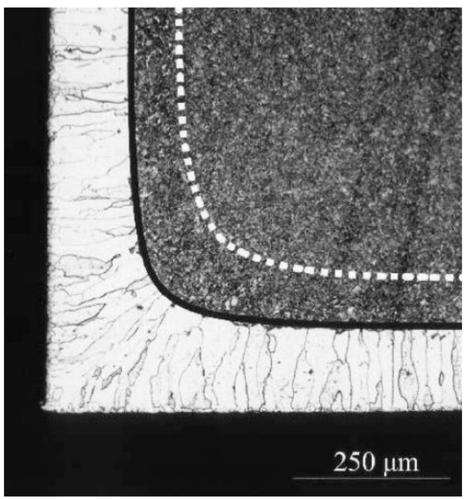
Interface velocity given by:

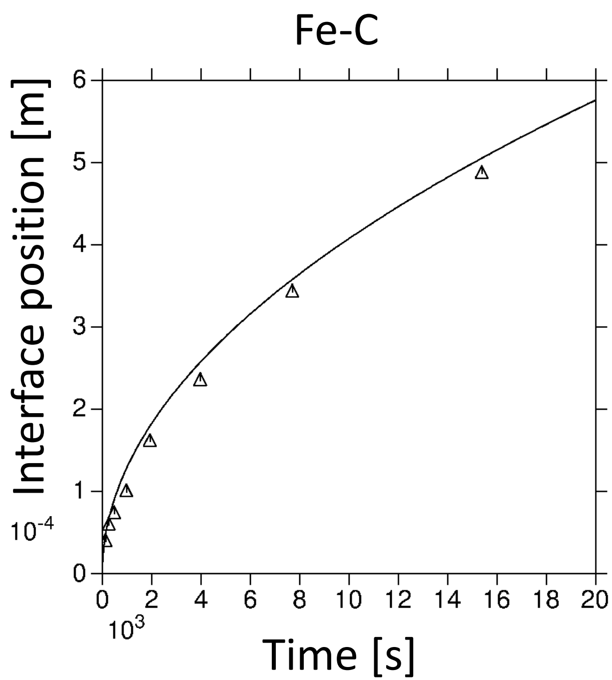
$$v^{\alpha/\beta} = V_m \frac{\sum \frac{\partial f^\alpha}{\partial N_k}\left(J_k^{i\alpha} - J_k^{i\beta}\right)}{\sum \frac{\partial f^\alpha}{\partial N_k}\left(x_k^{i\alpha} - x_k^{i\beta}\right)}$$

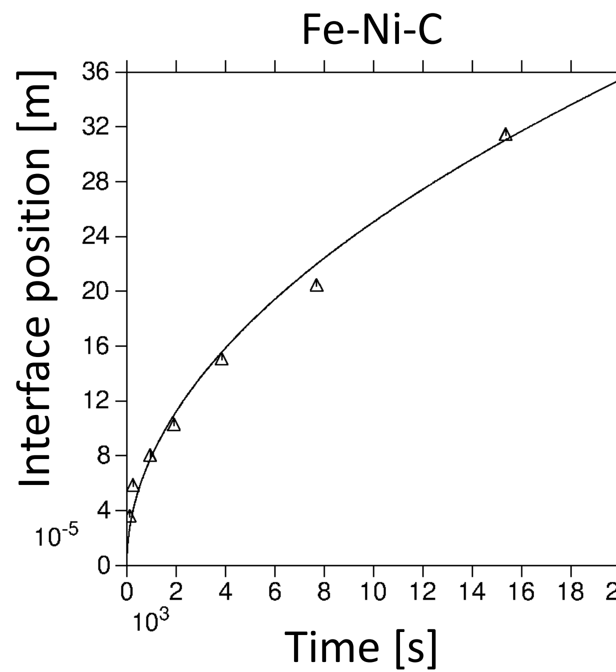
Larsson, Reed, Acta Mater 56(2008)3754

Example: Ferrite growth during decarburization

- $\gamma \rightarrow \alpha$
- Experiments by Phillion et al.
- Fe-Ni-C: Ferrite growth under NPLE conditions (no long-range Ni diffusion)







Phillion et al., Metall Mater Trans A 35A(2004)1237

Local equilibrium, sharp vs finite width interface

The original moving boundary model in Dictra

Local equilibrium – sharp interface

Interface velocity found by solving
Set of flux balance equations

$$v\left(c_k^{\alpha} - c_k^{\gamma}\right) = J_k^{\alpha} - J_k^{\gamma}$$

$$k = 1, \ldots, n-1$$

Fast and efficient

First implemented in Dictra v27

Local equilibrium – finite interface

Explicit expression for interface velocity

$$v^{\alpha/\beta} = V_m \frac{\sum \frac{\partial f^{\alpha}}{\partial N_k}\left(J_k^{i\alpha} - J_k^{i\beta}\right)}{\sum \frac{\partial f^{\alpha}}{\partial N_k}\left(x_k^{i\alpha} - x_k^{i\beta}\right)}$$

Robust

Both methods are available in the Dictra software

Höglund, Thesis, KTH, 1997
Crusius, Inden, Knoop, Höglund, Ågren, Z Metallkd 83(1992)9

Larsson, Reed, Acta Mater 56(2008)3754

Thermo-Calc Software

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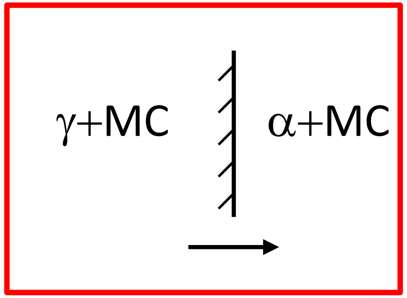
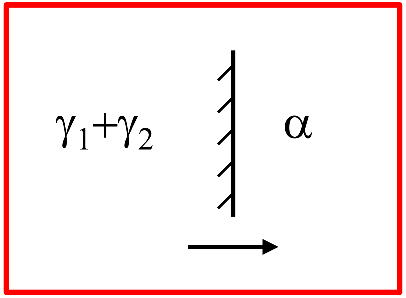
Combining a moving phase boundary model with the multiphase approach

Why?

Phase(s) present on both sides of an interface



Reaction product inside spinodal



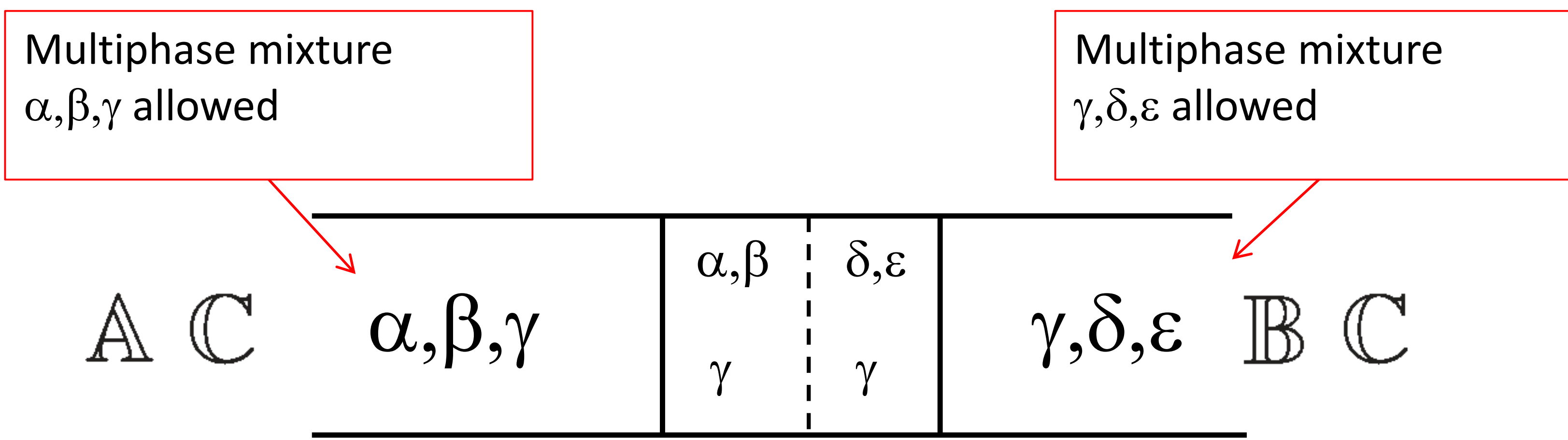
Combined multiphase – finite width-local eq.

Three sets of phases:

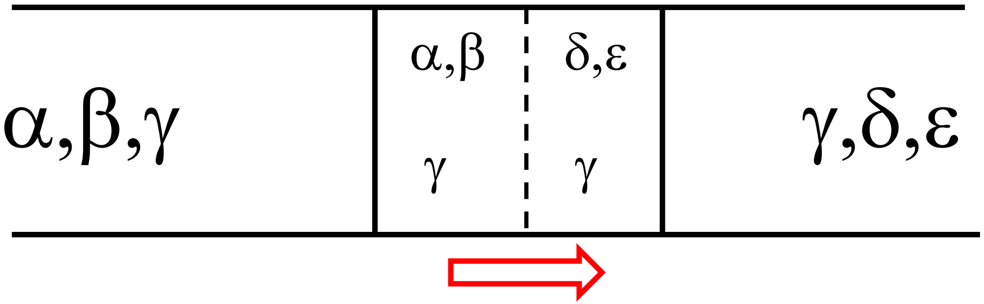
$\mathbb{A}$: α,β Allowed only on the left side of the interface

$\mathbb{B}$: δ,ε Allowed only on the right side of the interface

$\mathbb{C}$: γ Allowed on both sides of the interface



Combined multiphase – finite width-local eq.

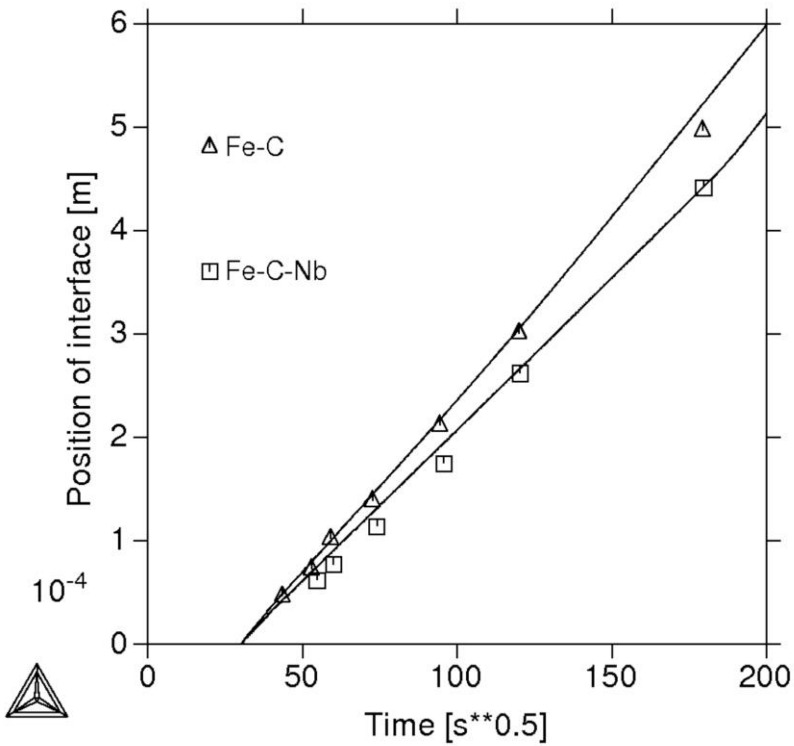


Interface velocity given by: $v^{\mathbb{A}/\mathbb{B}}$

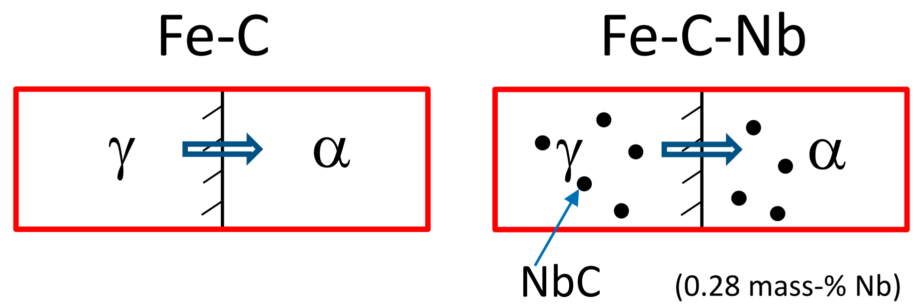
$$v^{\mathbb{A}/\mathbb{B}} = V_m \frac{\sum_{\alpha\in\mathbb{A}} \sum_{k} \frac{\partial f^{\alpha}}{\partial N_k} \left(J_k^{i\mathbb{A}} - J_k^{i\mathbb{B}}\right) - \sum_{\delta\in\mathbb{B}} \sum_{k} \frac{\partial f^{\delta}}{\partial N_k} \left(J_k^{i\mathbb{A}} - J_k^{i\mathbb{B}}\right)}{\sum_{\alpha\in\mathbb{A}} \sum_{k} \frac{\partial f^{\alpha}}{\partial N_k} \left(x_k^{i\mathbb{A}} - x_k^{i\mathbb{B}}\right) - \sum_{\delta\in\mathbb{B}} \sum_{k} \frac{\partial f^{\delta}}{\partial N_k} \left(x_k^{i\mathbb{A}} - x_k^{i\mathbb{B}}\right)}$$

Larsson, Calphad 47(2014)1

Combined multiphase – finite width-local eq.
Example: Carburization of Fe-C and Fe-C-Nb



Togashi, Nishizawa, J Japan Inst Met 40(1976)2

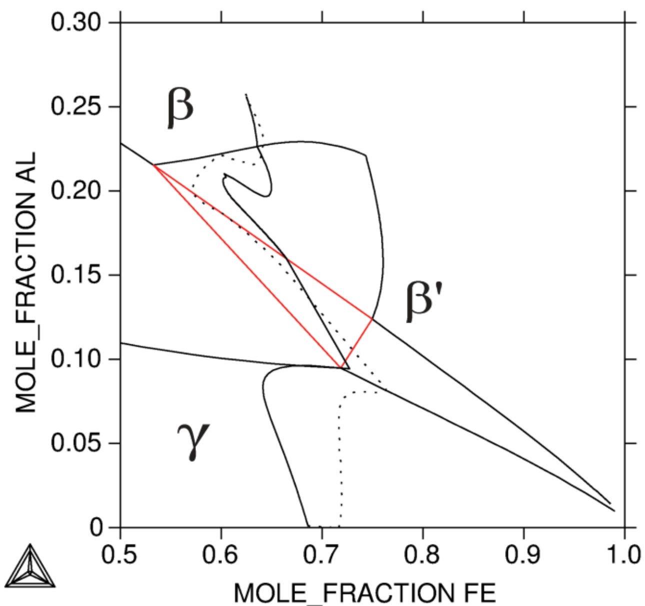


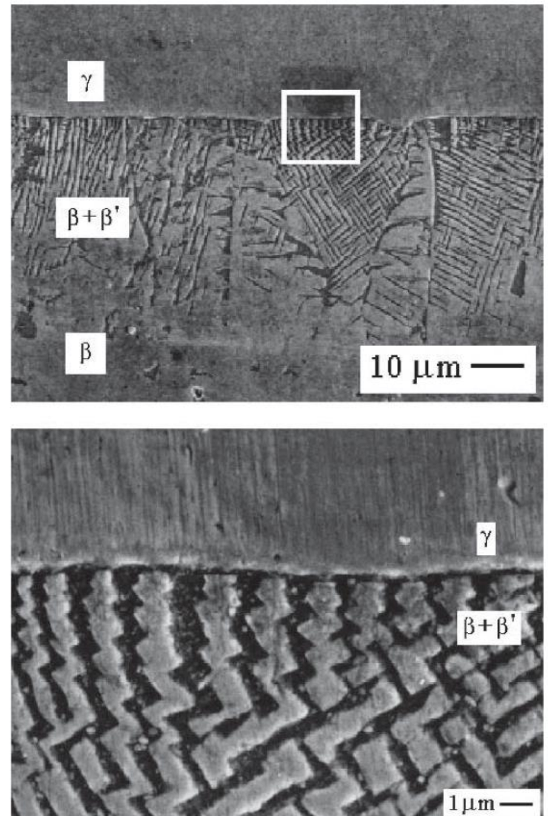
Exp. by Togashi and Nishizawa
Carburization at 1073 K

Carbon mobilities fitted to binary case

Combined multiphase – finite width-local eq.
Example: Al-Fe-Ni Diffusion couple

Diffusion path
Dotted: Experiment
Solid: Simulation





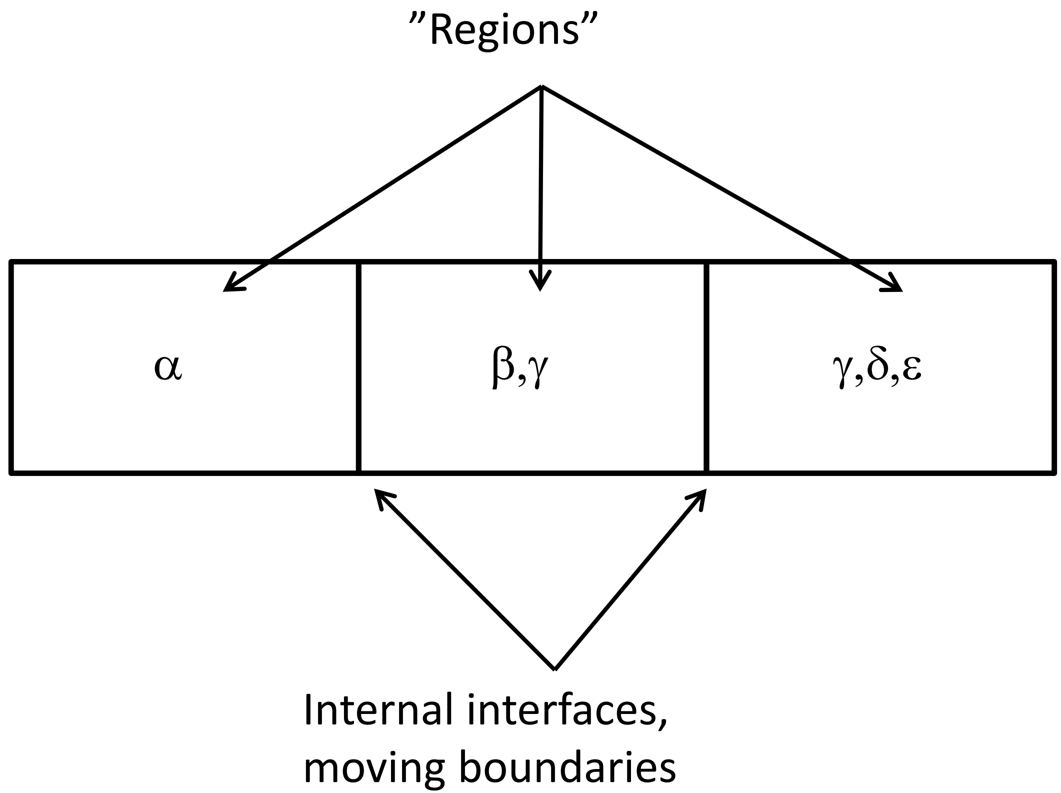
Experiment by Sohn, Puccio,Dayananda

1273 K
48 h

Al mobilities of database
Increased by a factor two

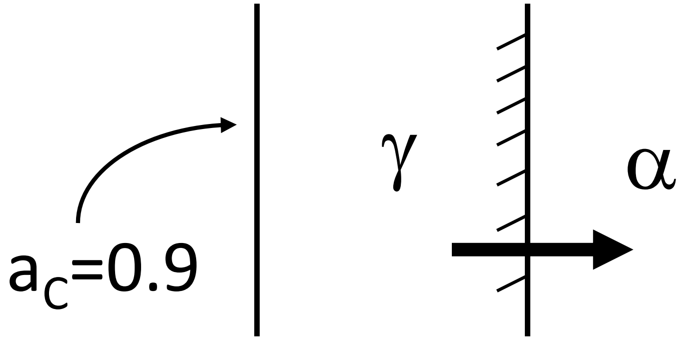
Sohn, Puccio, Dayananda, Metall Mater Trans A 36A(2005)2361

Dictra set-up using new model



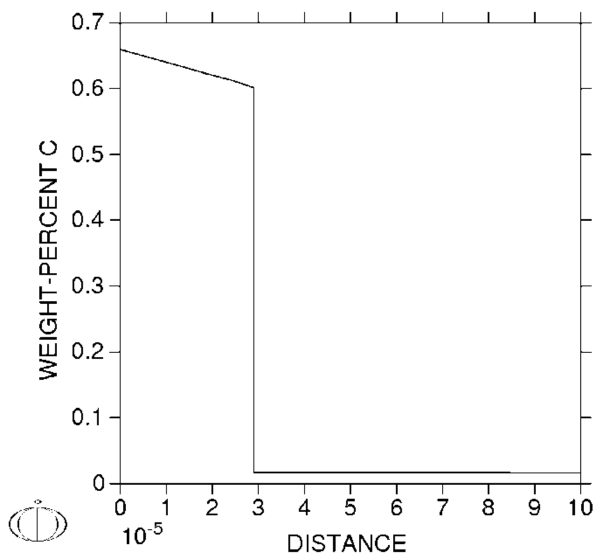
Arbitrary set of phases in each region

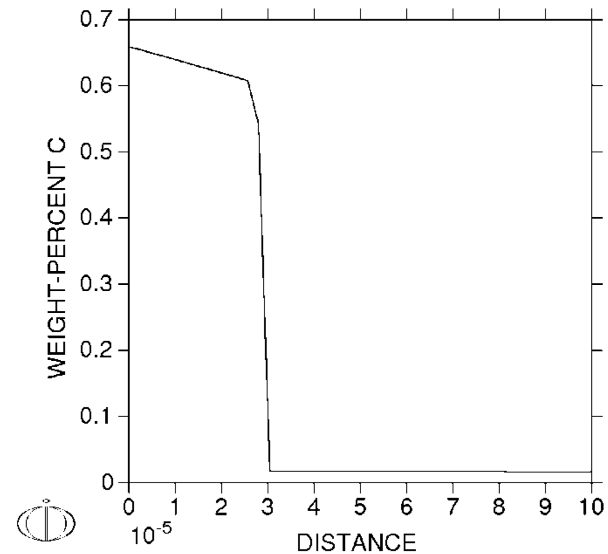
Remaining requirement: one unique phase in each region

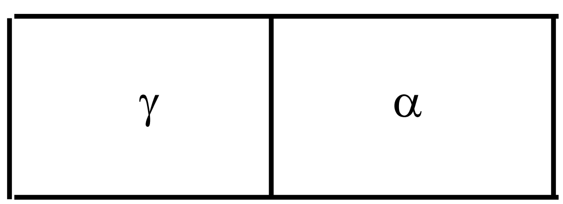


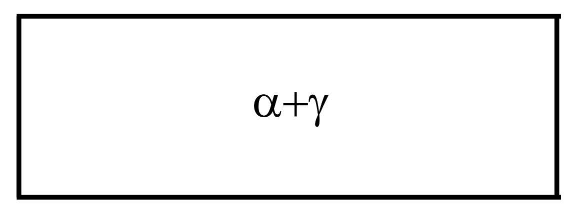
Different set-ups, same results

Carburizing plain carbon steel
at 750°C









Summary

- Two alternative models for moving phase boundary simulations in Dictra
- Dictra diffusion simulations can now be set up in a very general manner
- More important than ever to carefully consider all assumptions when setting up a simulation

Thank you!