



## DICTRA On-line Training

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## Diffusion Module (DICTRA)

### Day 2

9:00	Home assignment 1
9:10	<b>Example</b> - Solidification using Scheil
9:30	<b>Example</b> - Scheil with real back-diffusion in the solid.
9:50	<b>Example</b> – DICTRA solidification (Moving phase boundary)
10:30	Q&A
10:45	Diffusion theory and numerics
11:15	<b>Example</b> – Homogenisation model: Diffusion couple
11:45	Q&A
12:00	Home assignment 2

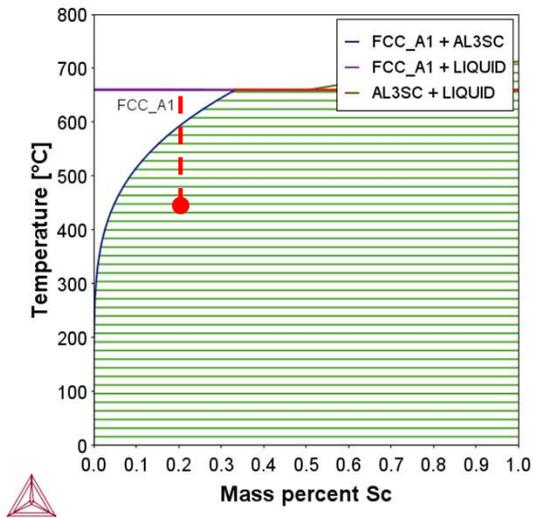
Today's download:

<https://download.thermocalc.com/courses/DICTRA/DICT-Day2/>

# Home assignment 1

# Home assignment 1: Particle growth

Al – 0.2 wt-% Sc



Try to make the Al-Sc simulation we just performed more realistic by adding the cooling from single-phase FCC at 600 °C to 450 °C.

Let's assume this cooling takes 2 seconds.

Does this change how much the phase interface has moved after 1 hour?

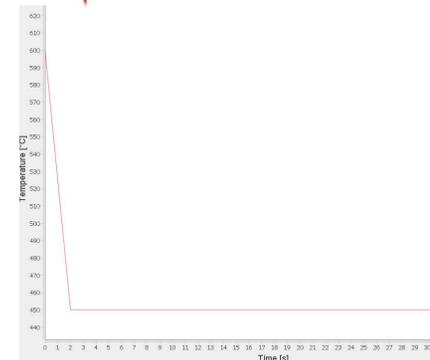
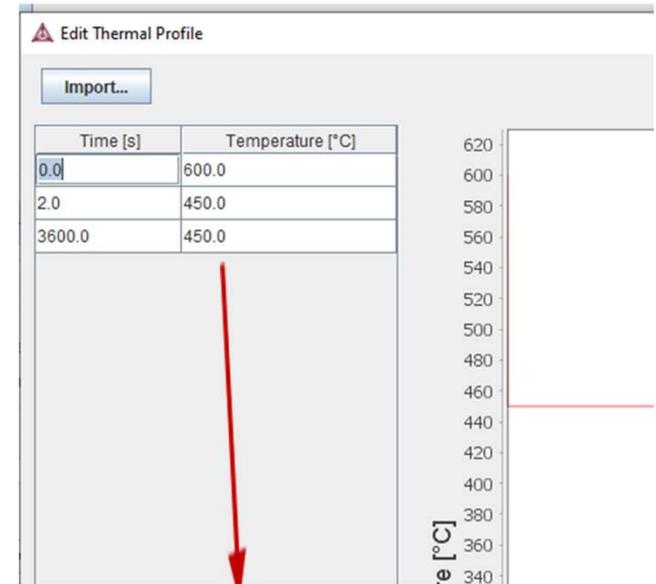
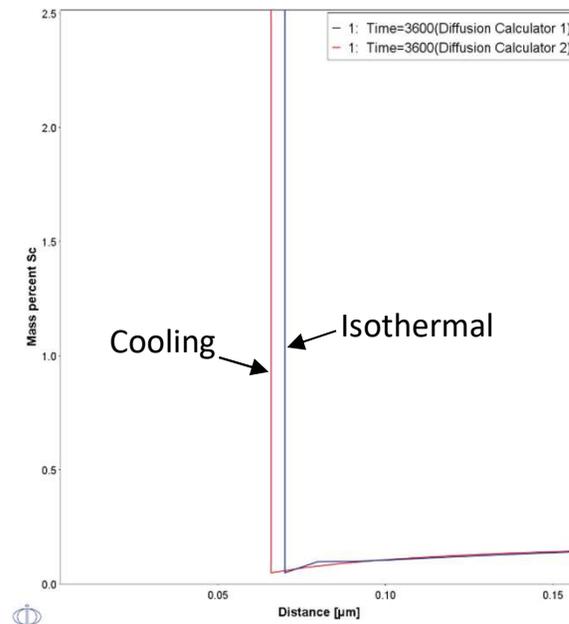
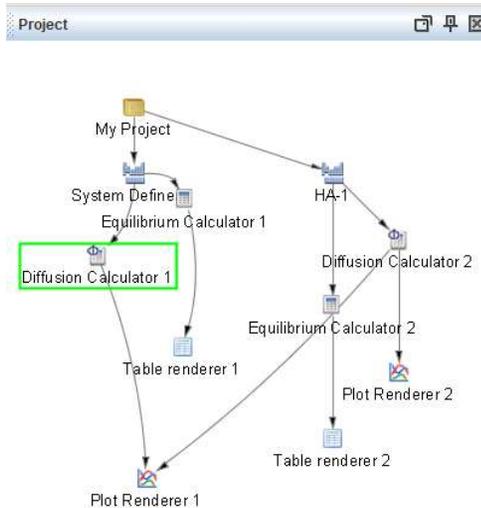
- 1) You have to change the setting to non-isothermal.
- 2) Also consider how you can compare the two results after time=3600 s.

# Home assignment 1: Particle growth

Al – 0.2 wt-% Sc

- 1) You have to change the setting to non-isothermal. →
- 2) Also consider how you can compare the two results after time=3600 s.

Clone the isothermal Project tree in order to keep the results also from the old simulation.



# Solidification – different methods

# Solidification simulations



## Equilibrium methods (lever-rule)

Solute diffusion is rapid, i.e. complete solute back diffusion → uniform composition in both solids and liquid.

## Non equilibrium methods (SCHEIL)

Negligible diffusion in solids, i.e. no solute back diffusion → solids retain same composition through solidification.

## Partial equilibrium methods/ Fast diffusing species

Complete interstitial but negligible substitutional solute back diffusion. No diffusion calculation – equilibration of chemical potential for fast diffusing species.

## Back diffusion calculated in the Primary Phase

Scheil with a simultaneous diffusion calculation in the primary phase. Requires additional kinetic database and takes dendrite spacing and cooling rate into account.

## Scheil with Solute Trapping

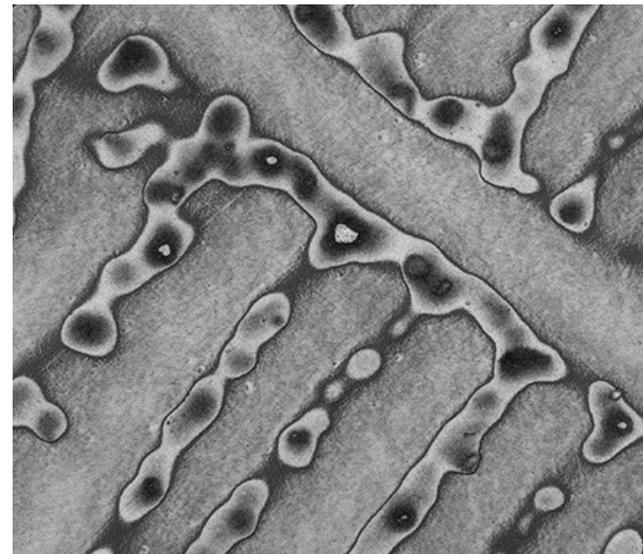
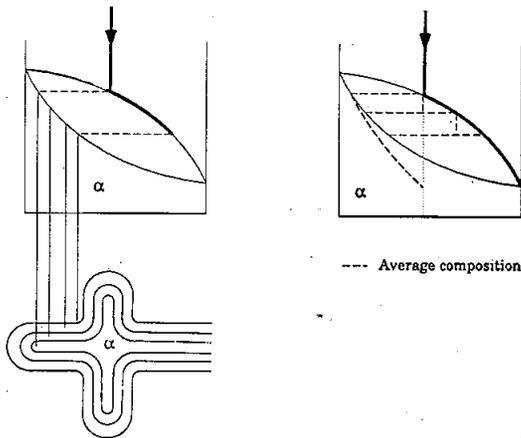
Intended for simulation of very fast cooling, e.g. during Additive Manufacturing. Requires assumption about scanning speed and angle.

## Moving phase boundary methods (DICTRA)

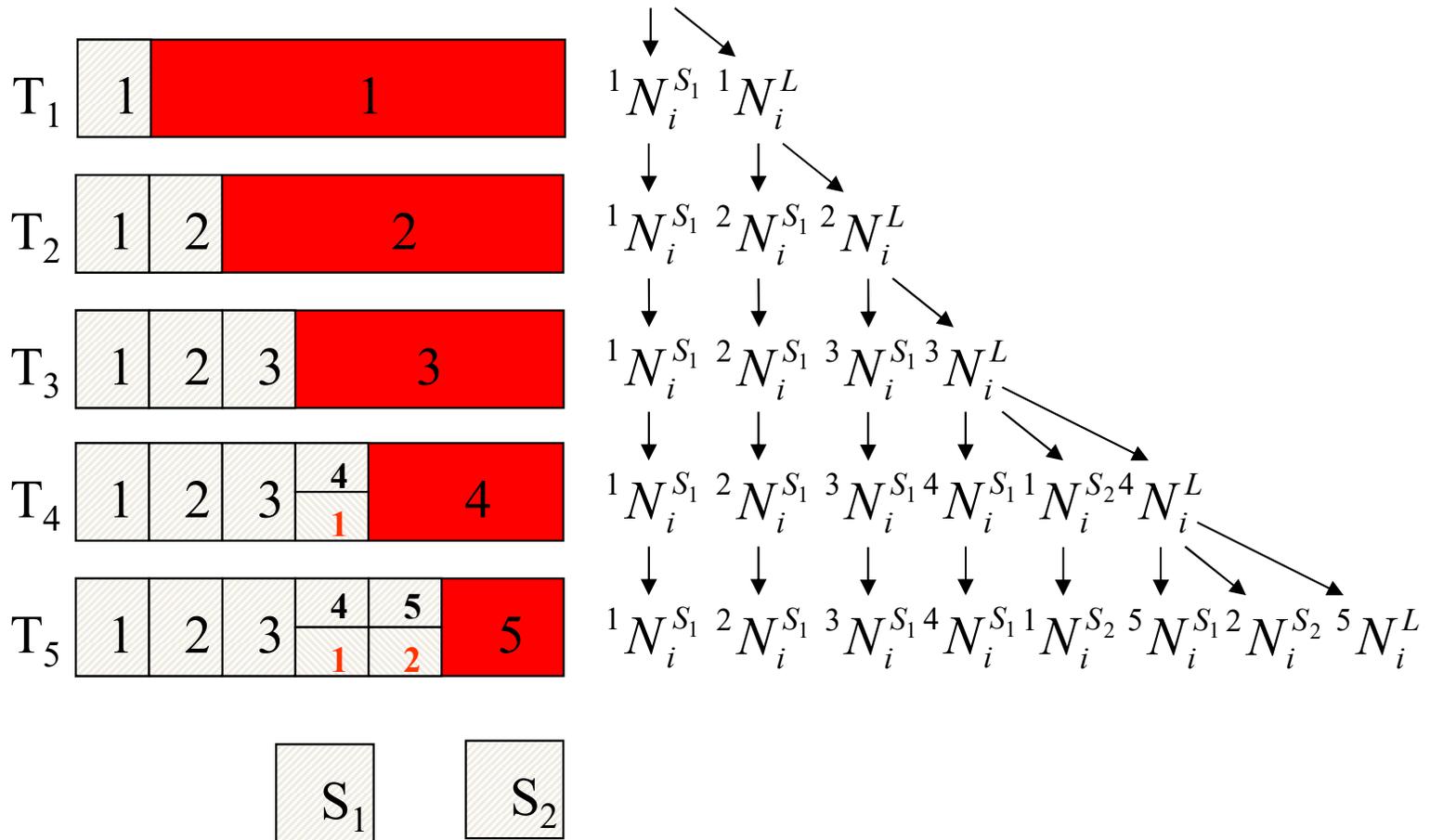
Full integration of thermodynamics and kinetics in all phases. Requires additional kinetic database and takes dendrite spacing and cooling rate into account.

# Scheil model

- Assumptions in traditional Scheil:
  - ❑ Fast diffusion in liquid  $\rightarrow$  homogenous liquid
  - ❑ No diffusion in solid phases  $\rightarrow$  segregations in the solid



# Algorithm in traditional Scheil



# Scheil with back diffusion

- Introduced in Thermo-Calc four years ago.
- It is a real diffusion method where diffusion is simulated in the majority solid phase. Both Thermodynamic and Mobility data is needed.
- This is unlike “Scheil with partial equilibrium” where fast diffusing elements (C, N) are allowed to “move” freely in the solid phases during solidification. In this case the changing concentration of C or N is due to conditions in chemical potential but no diffusion simulation takes place.
- In this example: Use this method and compare with standard Scheil for an Al-alloy AA5005, with the simplified composition **Al – 0.8% Mg – 0.7% Fe – 0.3% Si (wt-%)**. Perform two calculations, one at a low and one at a high cooling rate.

# Scheil and Scheil with back diffusion

Configuration

Scheil2 - 5 K/s

Start temperature: 1600.0

Temperature step: 1.0

Temperature unit: Celsius

Composition unit: Mass percent

Back diffusion in primary phase:

Cooling rate: 5.0 K/s

Secondary dendrite arm spacing: Calculated c: 5.0E-5 n: 0.33 m

Primary phase: BCC\_A2

Composition Fe 67.5  Fast diffuser

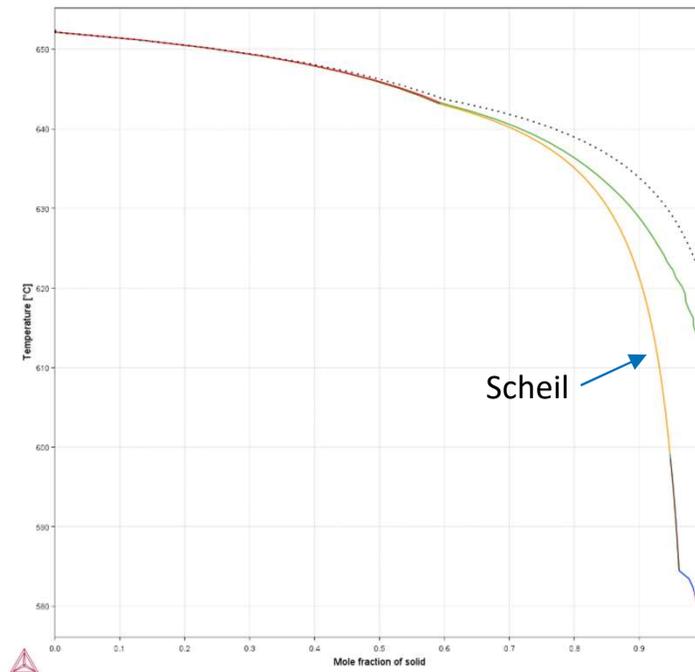
Composition Cr 28.5  Fast diffuser

Composition Mo 4.0  Fast diffuser

Secondary dendrite arm spacing  $\lambda$  can be calculated with an empirical formula:

$$\lambda = c * CR^{-n}$$

where CR is the cooling rate in K/s.



# Moving Phase boundary Example - Solidification

# Solidification simulation using DICTRA



## Assumptions:

- Assumption that equilibrium holds locally at the phase interface.
- Assumption regarding the geometry and size of the system, e.g. the interdendritic spacing.
- Assumption regarding the cooling rate.

## However,

- Full consideration of diffusion in both the liquid and solid phases.

# Example - Solidification

## Solidification of Al-alloy 5005 using DICTRA.

### Composition:

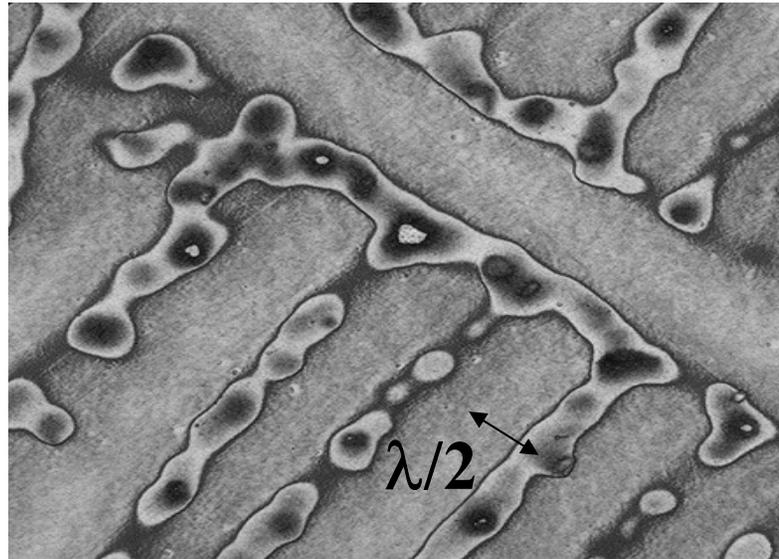
Al – bal.

Mg– 0.8 %

Fe – 0.7 %

Si – 0.3 %

(weight-%, )



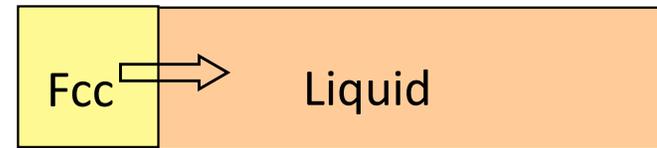
- Secondary dendrite arm spacing – use formula from “Scheil with back diffusion” (see next slide).
- Cooling rate approximately 0.01 °C/s.

# Example - Solidification

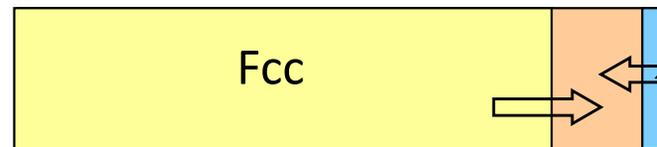
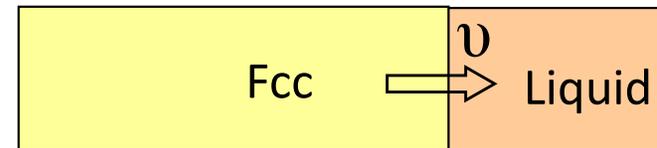
Cooling rate: 0.01°C per second. Start at 653°C, just above  $T_{LIQ}$



Use  $\lambda/2$  as the region size, take  $\lambda$  from "Scheil with back diffusion"- calculation at the same cooling rate.



Scheil calculation shows these are the phases to consider -  
in this case the Equilibrium step is not a good predictor.



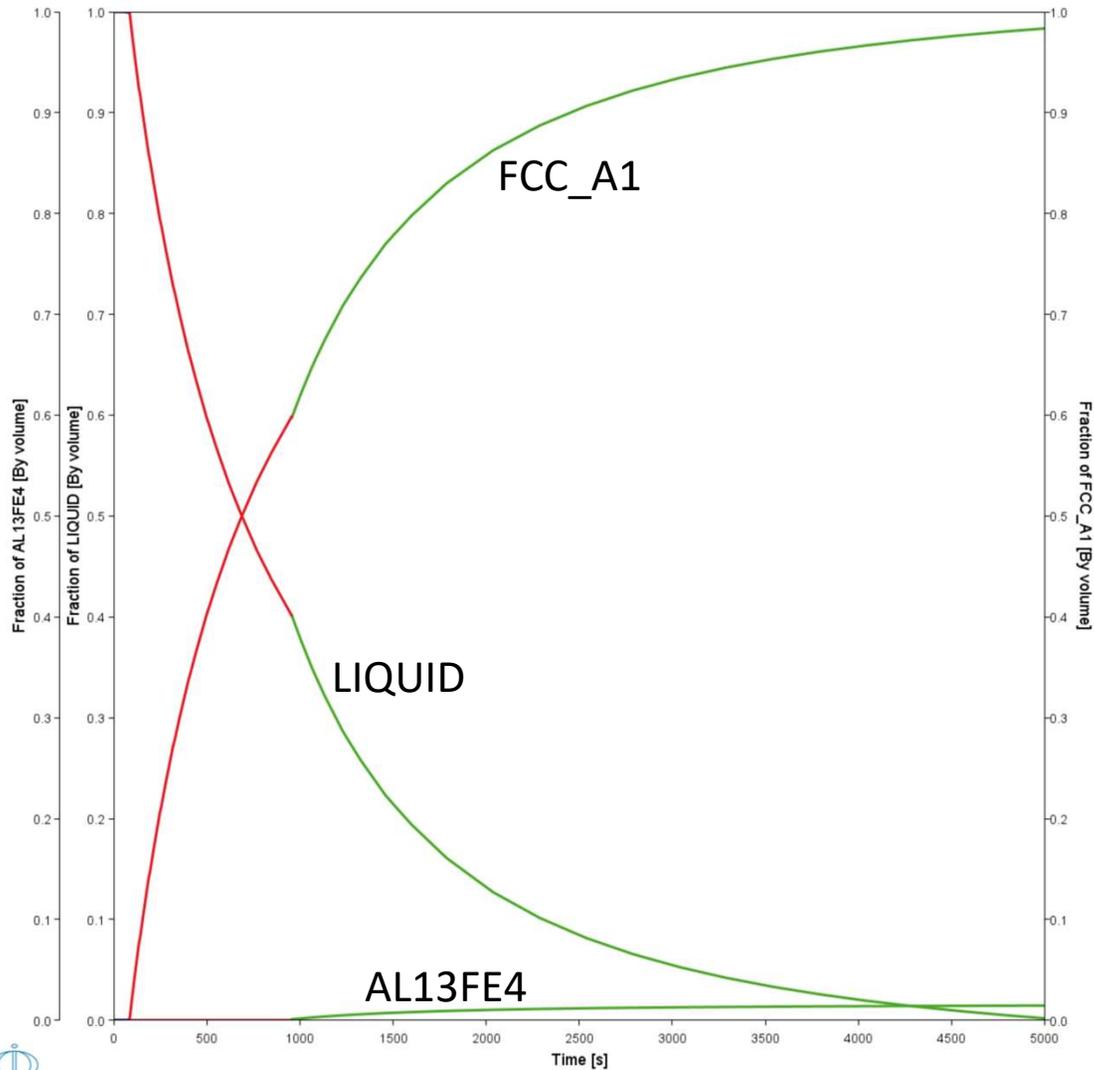
AL13FE4

114.27  $\mu\text{m}$



# Example - Solidification

Cooling rate: 0.01°C per second. Start above  $T_{LIQ}$



# Q & A

# Diffusion theory and numerics

# Multicomponent Diffusion theory

Derivation of expression for the flux  $J_k$  [mol/m<sup>2</sup>s]  
from first principles

Combine the flux expression with mass-balance,  
equation of continuity, to simulate the evolution  
of a concentration field  $c_k(z,t)$  [mol/m<sup>3</sup>]

$$\frac{\partial c_k}{\partial t} = \frac{\partial}{\partial z} \left( - J_k \right) \quad \text{Fick's second law}$$

# Different types of diffusion coefficients



Consider a system with  $C$  components, we have

- $C*(C-1)$  diffusion coefficients in lattice-fixed frame of reference, usually called
  - Individual diffusion coefficients
  - Intrinsic diffusion coefficients
- $(C-1)*(C-1)$  diffusion coefficients in number-fixed frame of reference, called
  - Chemical diffusion coefficients
  - Inter-diffusion coefficients
  - Exchange-diffusion coefficients
- $C$  tracer diffusion coefficients, called self diffusion coefficients if a pure element.

They are all functions of temperature and composition! They are not independent!

# Atomistic treatment of diffusion



For crystalline phases it is generally accepted that diffusion occurs mainly through a vacancy exchange mechanism, i.e. by atoms jumping to adjacent vacant lattice sites.

Assuming that there is a random distribution of vacant sites and that the number of vacancies is everywhere adjusted to equilibrium, it is possible to derive an expression for the flux of  $k$  in a lattice-fixed frame of reference.

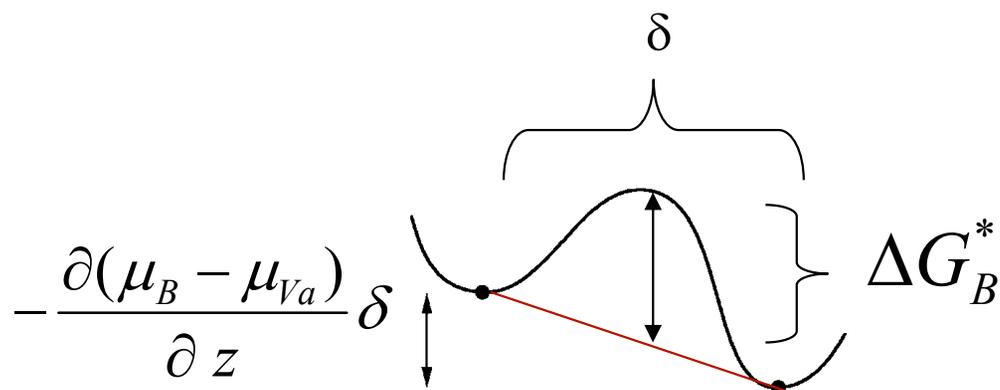
*See, for example,  
Stearn, Eyring, J Phys Chem 44(1940)955  
Bardeen, Phys Rev 76(1949)1403*

# Expressions for the flux

- As said the dominating diffusion mechanism is an atom jumping to an adjacent vacant lattice site.
- The probability for thermally activated "jumps" of an atom to neighboring vacant site is given by

$$p = \exp(-\Delta G / k_B T)$$

where  $\Delta G$  is the change in Gibbs energy caused by jump and  $k_B$  is Boltzmann's constant.



If there is a driving force  $\Delta G$  will be different in the two directions.

$$\Delta \vec{G} = \Delta G_B^* + \frac{1}{2} \frac{\partial(\mu_B - \mu_{Va})}{\partial z} \delta$$

$$\Delta \vec{G} = \Delta G_B^* - \frac{1}{2} \frac{\partial(\mu_B - \mu_{Va})}{\partial z} \delta$$

Assume a random mixture of  $N_{Va}$  mole of vacancies in thermal equilibrium, i.e.

$$\frac{\partial G}{\partial N_{Va}} = 0$$

The quantity  $\partial G / \partial N_{Va}$  may formally be interpreted as the chemical potential of vacancies  $\mu_{Va}$ . However, as vacancies are not conserved, this concept does not have a clear physical meaning.

In a random mixture the probability that a site is vacant is  $y_{Va}$  i.e. the fraction of vacant lattice sites.

Probability for jump in forward direction:

$$\vec{p} = y_{Va} \exp\left(-\frac{1}{kT} \left( \Delta G_B^* + \frac{1}{2} \frac{\partial \mu_B}{\partial z} \delta \right)\right)$$

Probability for jump in backward direction:

$$\vec{p} = y_{Va} \exp\left(-\frac{1}{kT} \left( \Delta G_B^* - \frac{1}{2} \frac{\partial \mu_B}{\partial z} \delta \right)\right)$$

Net flux of atoms (in lattice-fixed frame):

$$J_B = c_B v (\vec{p} - \vec{p}) \delta =$$

$$c_B y_{Va} \delta v \exp\left(-\frac{\Delta G_B^*}{RT}\right) *$$

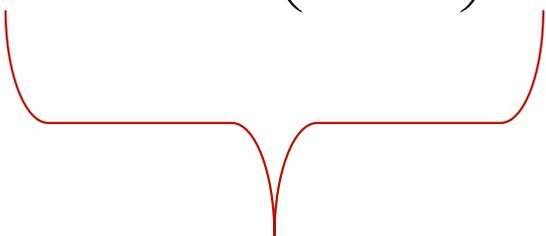
$$\left[ \exp\left(\frac{-1}{2RT} \frac{\partial \mu_B}{\partial z} \delta\right) - \exp\left(\frac{1}{2RT} \frac{\partial \mu_B}{\partial z} \delta\right) \right] =$$

$$= -c_B y_{Va} \delta v \exp\left(-\frac{\Delta G_B^*}{RT}\right) * 2 \sinh\left(\frac{1}{2RT} \frac{\partial \mu_B}{\partial z} \delta\right)$$

$v$  the vibrational frequency in the order of  $10^{13} \text{ s}^{-1}$

$\delta$  in the order of  $10^{-10} \text{ m}$

Net flux of atoms in the limit of low  
Driving forces:

$$J_B \cong -c_B y_{Va} \delta^2 v \exp\left(-\frac{\Delta G_B^*}{RT}\right) \frac{1}{RT} \frac{\partial \mu_B}{\partial z} = -c_B M_B \frac{\partial \mu_B}{\partial z}$$

$$M_B$$

For interstitial B the fraction of vacancies is usually large and known from composition

$$J_B \cong -c_B y_{Va} \delta^2 v \exp\left(-\frac{\Delta G_B^*}{RT}\right) \frac{1}{RT} \frac{\partial \mu_B}{\partial z} = -c_B y_{Va} M_{BVa} \frac{\partial \mu_B}{\partial z}$$

$$M_{BVa}$$

# Fick's equations for $n$ components

$$J_k = -c_k M_k \frac{\partial \mu_k}{\partial z} = -c_k M_k \sum_{j=1}^{n-1} \frac{\partial \mu_k}{\partial c_j} \frac{\partial c_j}{\partial z}$$

$$D_{kj}^n = c_k M_k \frac{\partial \mu_k}{\partial c_j}$$

$$\frac{\partial c_k}{\partial t} = \frac{\partial \left( \sum_{j=1}^{n-1} D_{kj}^n \frac{\partial c_j}{\partial z} \right)}{\partial z}$$

Using matrix-vector notation Fick's equation reads:

$$\mathbf{J} = -\mathbf{D} \frac{\partial \mathbf{c}}{\partial z}$$

$$\mathbf{J} = \begin{bmatrix} J_1 \\ J_2 \\ \vdots \\ J_{n-1} \end{bmatrix}$$

$$\mathbf{c} = \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_{n-1} \end{bmatrix}$$

$$\mathbf{D} = \begin{bmatrix} D_{1,1} & D_{1,2} & \cdots & D_{1,n-1} \\ \vdots & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ D_{n-1,1} & \cdots & \cdots & D_{n-1,n-1} \end{bmatrix}$$

## Example: Fe-Si-C system

*Flux of carbon:*

$$J_C = -D_{CC}^{Fe} \frac{\partial c_C}{\partial z} - D_{CSi}^{Fe} \frac{\partial c_{Si}}{\partial z}$$

*Flux of silicon:*

$$J_{Si} = -D_{SiC}^{Fe} \frac{\partial c_C}{\partial z} - D_{SiSi}^{Fe} \frac{\partial c_{Si}}{\partial z}$$

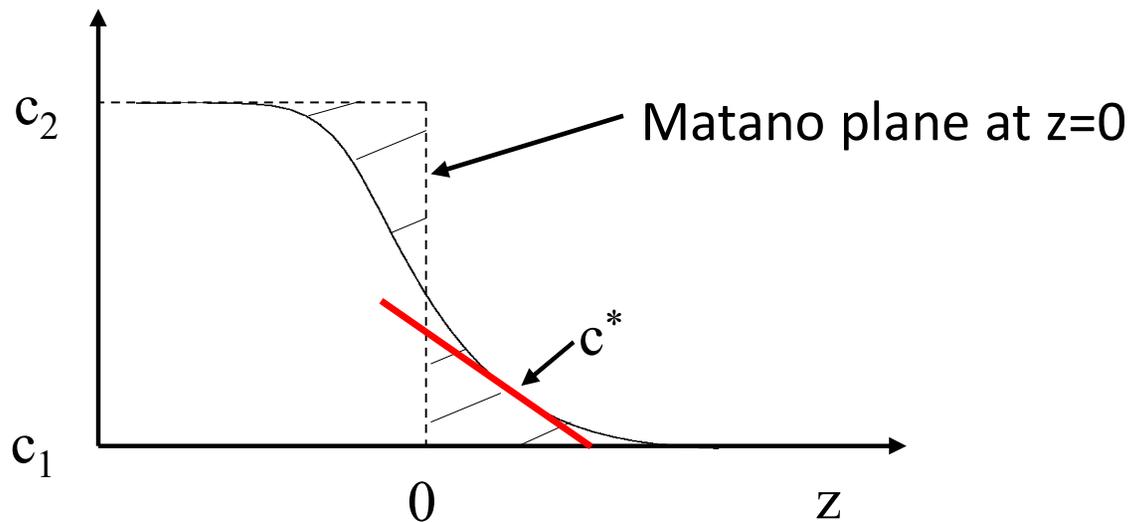
## Fick's second equation

Combining the continuity equation with Fick's equation gives us the fundamental differential equation of diffusion, sometimes referred to as Fick's second equation.

$$\frac{\partial \mathbf{c}}{\partial t} = \frac{\partial}{\partial z} \left( \mathbf{D} \frac{\partial \mathbf{c}}{\partial z} \right)$$

# Frames of reference

*Determining  $D$  with diffusion couple technique (Boltzmann-Matano analysis):*



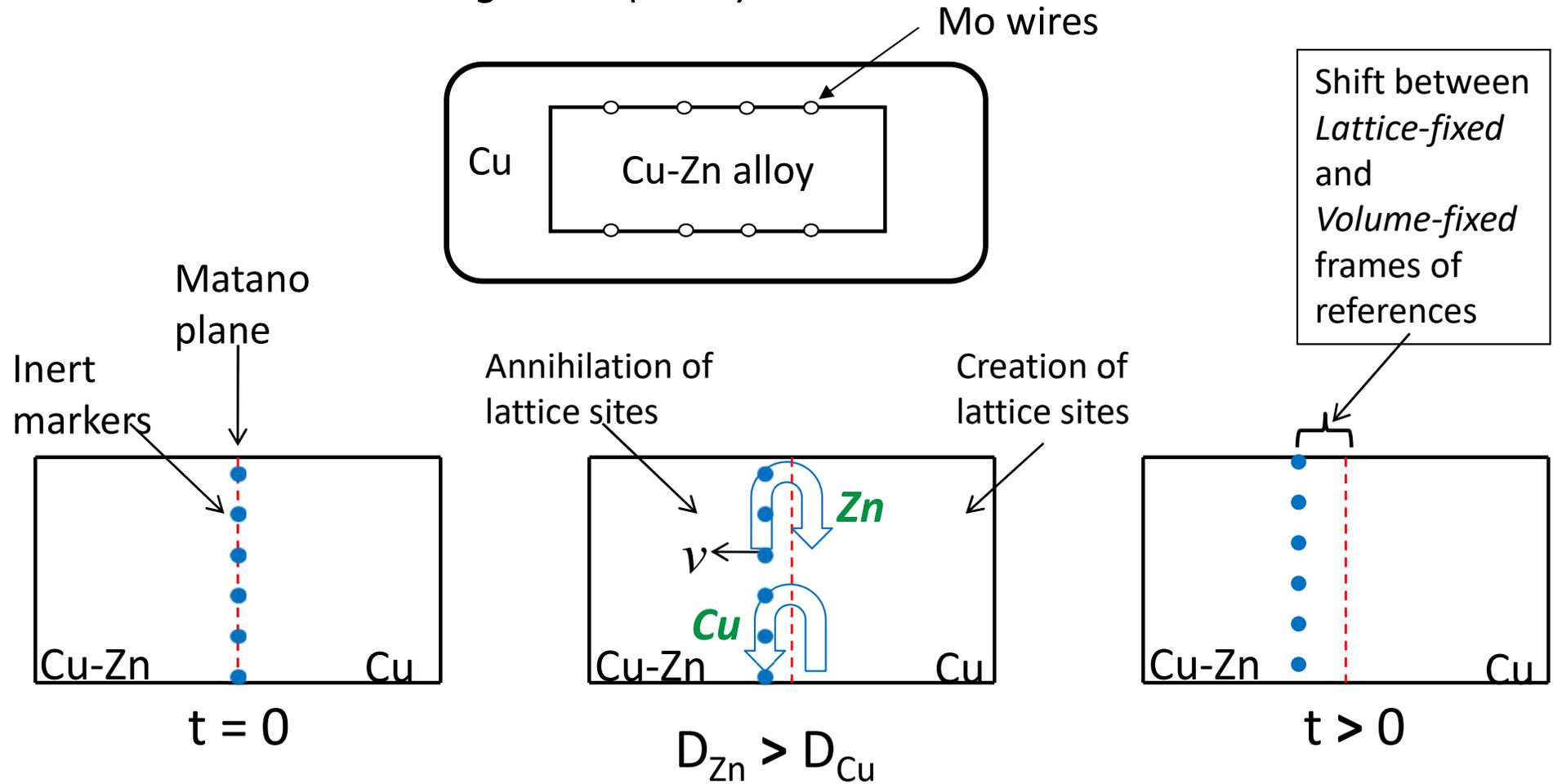
Origin of  $z$   
determined by

$$\int_{c_1}^{c_2} z dc = 0$$

$$\tilde{D}(c^*) = \frac{-1}{2t} \cdot \left( \frac{dz(c^*)}{dc} \right) \cdot \left( \int_{c_1}^{c^*} z dc \right)$$

# Frames of reference

*Kirkendall and Smigelskas (1947):*



# Frames of reference

## Lattice-fixed frame of reference:

- Defined by the inert markers, or that there is no net flow of lattice sites.

$$\sum_{k=1}^n J_k = -J_V a$$

## Volume-fixed frame of reference:

- Defined in such a way that there is no net flow of volume.

$$\sum_{k=1}^n J_k V_k = 0$$

## DICTRA frame of reference:

- Volume-fixed frame, however only the substitutional components are assumed to contribute to the volume.

$$\sum_{k \in S}^n J_k = 0$$

# Frames of reference

The equation for the velocity of the markers in the diffusion zone relative to the ends of the diffusion couple, in the Kirkendall experiment is:

$$v = \sum_{k=1}^n V_k J_k$$

This is the velocity with which the two frames move relative to each other.

We may use this equation in order to transfer the fluxes from the volume-fixed to the lattice-fixed frame, or vice versa:

$$J'_k = J_k - c_k \sum_{k=1}^n V_k J_k$$

# Phenomenological equations

$$J_k^L = - \sum_{i=1}^n L_{ki} \frac{\partial \mu_i}{\partial z} - L_{1T} \frac{\partial T}{\partial z} - L_{1P} \frac{\partial P}{\partial z} - L_{1\phi} \frac{\partial \phi}{\partial z}$$

They are called phenomenological since they stem from no model, but from experimental observations.

For single phase simulations it is possible to perform non-isothermal simulations\*.

If we choose to consider an isothermal, isobaric and isopotential system we have:

$$J_k^L = - \sum_{i=1}^n L_{ki} \frac{\partial \mu_i}{\partial z} \quad \left( J_k^L = -L_{kk} \frac{\partial \mu_k}{\partial z} \right)$$

\* Höglund, Ågren, *J Phase Equil Diffusion* 31(2010)212

# Identification

Assuming that the vacancy exchange mechanism is predominant, and by comparing to the expression derived earlier under this assumption, we may identify:

$$L_{kk} = c_k y_{V_a} M_{kV_a}$$

We have now established a relation between  $M$  and  $L$ .

## Transformation to a volume-fixed frame

$$\begin{aligned} J_k &= J_k^L - c_k v = J_k^L - c_k \sum_{j=1}^n V_j J_j^L \\ &= - \sum_{i=1}^n L_{ki} \frac{\partial \mu_i}{\partial z} + c_k \sum_{j=1}^n V_j \sum_{i=1}^n L_{ji} \frac{\partial \mu_i}{\partial z} \end{aligned}$$

or,

$$J_k = - \sum_{i=1}^n \frac{\partial \mu_i}{\partial z} \sum_{j=1}^n L_{ji} (\delta_{kj} - c_k V_j) = - \sum_{i=1}^n L'_{ki} \frac{\partial \mu_i}{\partial z}$$

where,

$$L'_{ki} = \sum_{j=1}^n (\delta_{kj} - c_k V_j) L_{ji}$$

## Transformation to concentration gradients

Applying the chain-rule of derivation on the previous equation:

$$J_k = - \sum_{i=1}^n L'_{ki} \sum_{j=1}^n \frac{\partial \mu_i}{\partial c_j} \frac{\partial c_j}{\partial z}$$

Or equally if the unreduced diffusivities,  $D_{kj}$  are introduced:

$$J_k = - \sum_{j=1}^n D_{kj} \frac{\partial c_j}{\partial z}$$

where,

$$D_{kj} = \sum_{i=1}^n L'_{ki} \frac{\partial \mu_i}{\partial c_j}$$

# Independent set of driving forces

There is a relation between the  $n$  concentration gradients, and it's possible to eliminate one of them:

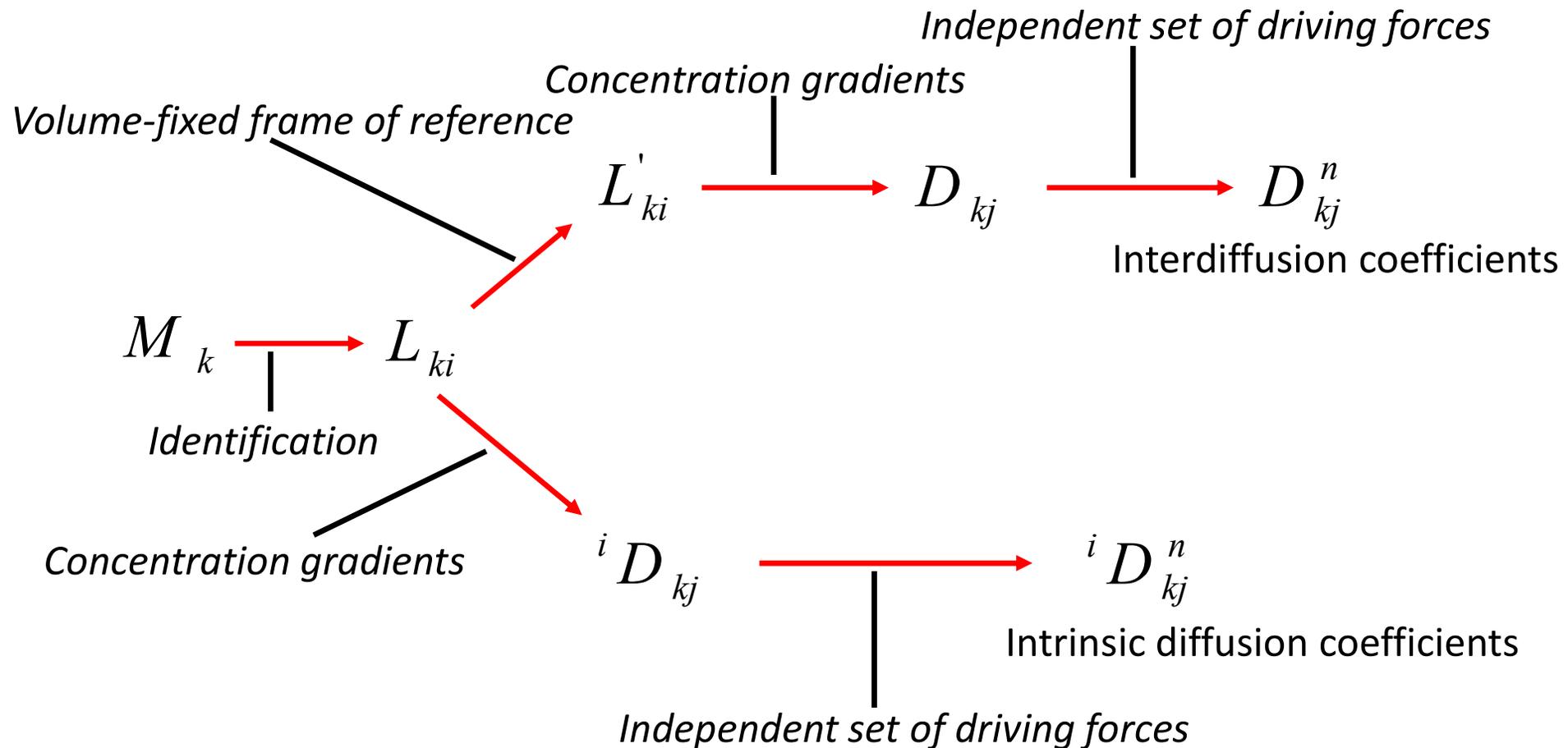
$$\frac{\partial c_n}{\partial z} = -\frac{\partial c_1}{\partial z} - \frac{\partial c_2}{\partial z} - \dots - \frac{\partial c_{n-1}}{\partial z}$$

and thus, the flux is now expressed:  $J_k = -\sum_{j=1}^{n-1} (D_{kj} - D_{kn}) \frac{\partial c_j}{\partial z}$

we may identify:  $D_{kj}^n = D_{kj} - D_{kn}$

and finally obtain:  $J_k = -\sum_{j=1}^{n-1} D_{kj}^n \frac{\partial c_j}{\partial z}$

# Summary of steps taken when transforming from M's to D's



# Combined thermodynamic and mobility databases

## Phase Equilibria & Thermodynamics

**Experiments**  
DTA, Metallography,  
X-ray Diffraction,  
Calorimetry, EMF,  
Vapor Pressure

Physics-based  
**Model Functions**  
with *Adjustable*  
*Parameters*

**Theory**  
Quantum Mechanics,  
Statistical Thermodynamics

Parameter  
**Optimization**  
for *Thermodynamic*  
*Description*

**Thermodynamic**  
**Database**

## Diffusion

**Experiments**  
Tracer, Intrinsic,  
Chemical (Interdiffusion)

**Theory**  
Atomistic  
Calculations

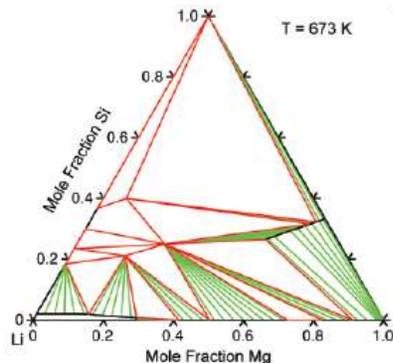
Parameter  
**Optimization**  
for *Diffusion Mobility*  
*Description*

**Diffusion Mobility**  
**Database**

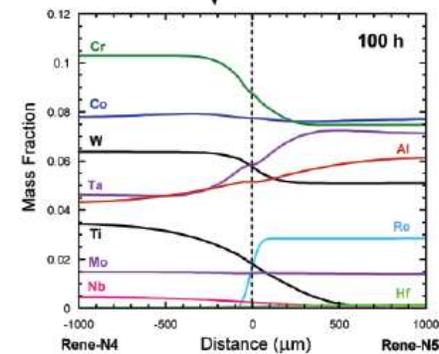
Thermodynamic  
Factor

Thermodynamic  
Factor

**Applications**  
Solidification,  
Phase Transformation Kinetics,  
...



1 Schematic of CALPHAD method



# Numerical models in DICTRA

# Models



## Classic model

(including dispersed system model)

FEM (finite element method)

Computationally efficient

Sensitive to starting values

Crusius, Inden, Knoop, Höglund, Ågren Z Metallkd 83(1992)9  
Engström, Höglund, Ågren, Met Mat Trans A 25A(1994)1127

## Homogenization model

(Also handles moving phase boundary simulations)

FVM (finite volume method)

Robust

Sensitive to grid point spacing

Larsson, Engström, Acta Mater 54(2006)2431  
Larsson, Höglund, Calphad 33(2009)495  
Larsson, Reed, Acta Mater 56(2008)3754  
Larsson, Calphad 47(2014)1

# Models

## Treatment of the interface

### Classic model

Local equilibrium

Sharp (zero width)

Velocity obtained by solving set of flux balance equations

$$v^{\alpha/\beta} \left( c_k^\alpha - c_k^\beta \right) = J_k^\alpha - J_k^\beta$$
$$k = 1, \dots, n - 1$$

### Homogenization model

Local equilibrium

Finite width

Velocity from explicit expression

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

# Defaults



One phase simulations:

Classic model

Moving phase boundary simulations:

Classic model

Cell simulations:

Classic model

Multiphase simulations (more than one phase in any region):

Homogenization model

# Restrictions

## **Only classic model possible**

Simulations involving surface energy contributions

## **Only homogenization model possible**

Simulations with a moving boundary and where at least one region contain multiple phases.

## **Choosing Model:**

In general, try the classic model first, since it is computationally more efficient

# Diffusion theory



*The Role of Diffusion in Materials – A Tutorial.*

This very useful document by Prof. John Ågren was included in the download for Day 1 as pdf. It is also available on our webpage.

Chapter 2 in this guide has a simpler take on the multi-component diffusion than the slides we've just gone through.

## 1 Introduction to Diffusion Simulations

### 1.1 About This Tutorial Guide

This guide is an introduction to some of the concepts and practices used when you set up a diffusion simulation using the Diffusion Module (DICTRA).

The purpose of this tutorial is to make the engineer aware about the type of material issues that are related to diffusion and demonstrate how to solve them. Some problems may be tackled by very simple computations whereas others require more heavy computations based on numerical approaches. Most of the examples concern metallic systems such as steels, super alloys and light metals, but the principles can be applied to many other classes of materials, e.g. ceramics and polymers, provided that appropriate databases are available.

The guide assumes some familiarity with using the Graphical Mode interface of the Thermo-Calc software. However, if you are not familiar you can use the available help and documentation to supplement this guide. See "[Help Resources](#)" on the next page.

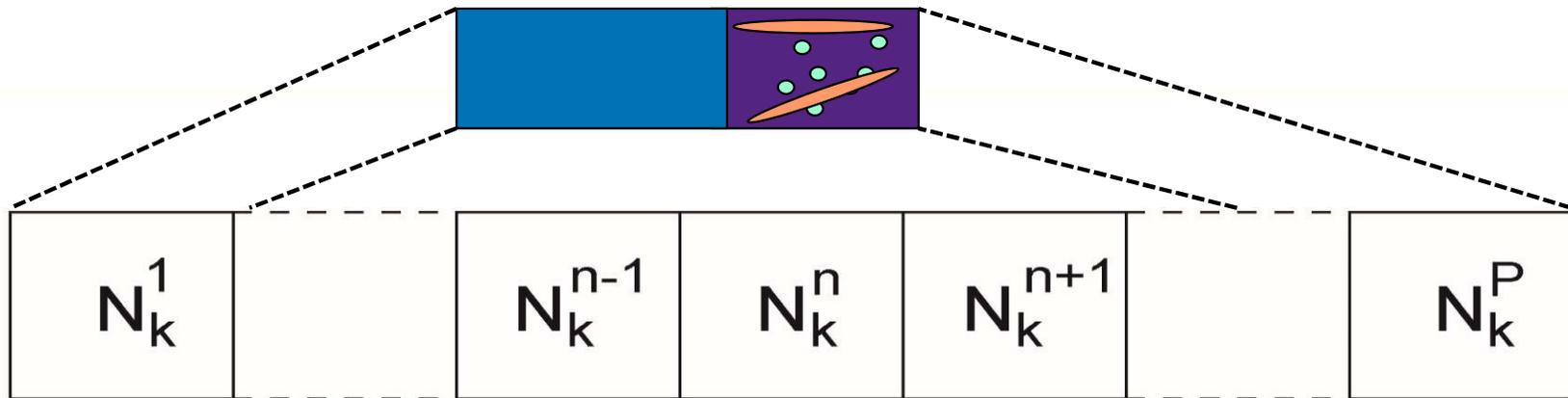
Except for one example at the beginning that includes details about how to recreate the simulation in both Graphical Mode and Console Mode, the exercises in this guide use the Graphical Mode interface. A brief comparison of these modes is included in "[Graphical Mode vs Console Mode](#)" on page 7. It is also useful to read "[An Important Note About Terminology](#)" on page 6.

The training material itself is available at two levels: basic and advanced. At the basic level it

# Homogenization Model

# Homogenization model

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



Equilibrium calculation  
for each slice

Phase fractions  
Phase compositions  
Chemical potentials  
Mobilities

Flux between slices "n-1" and "n"

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

"Effective"  $[M_k x_k]$  from combining rules

# Calculating effective $[M_k x_k]$

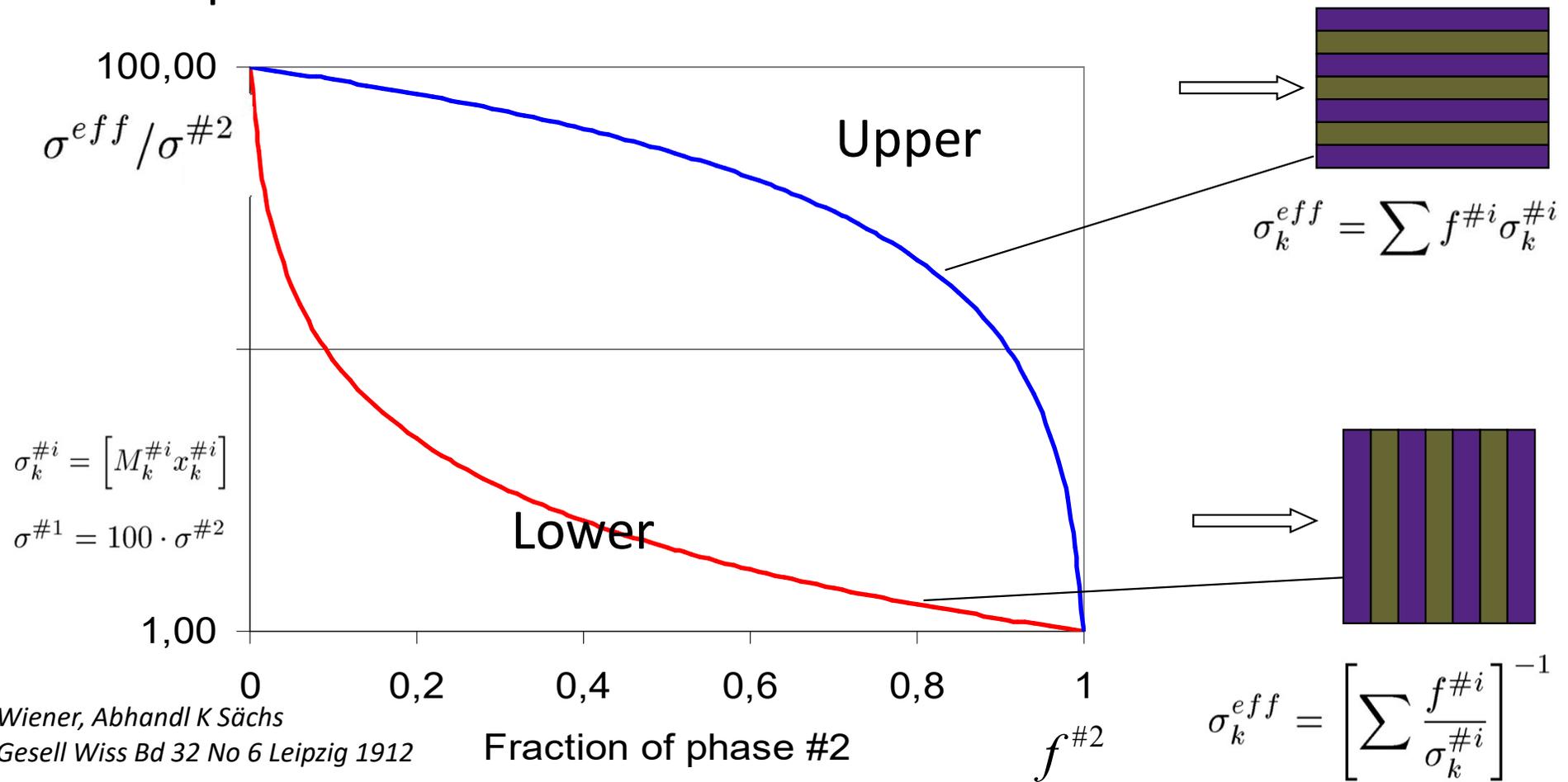
Combining rules are frequently used for determining an “effective” transport property in a multi-phase mixture, from:

- 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.

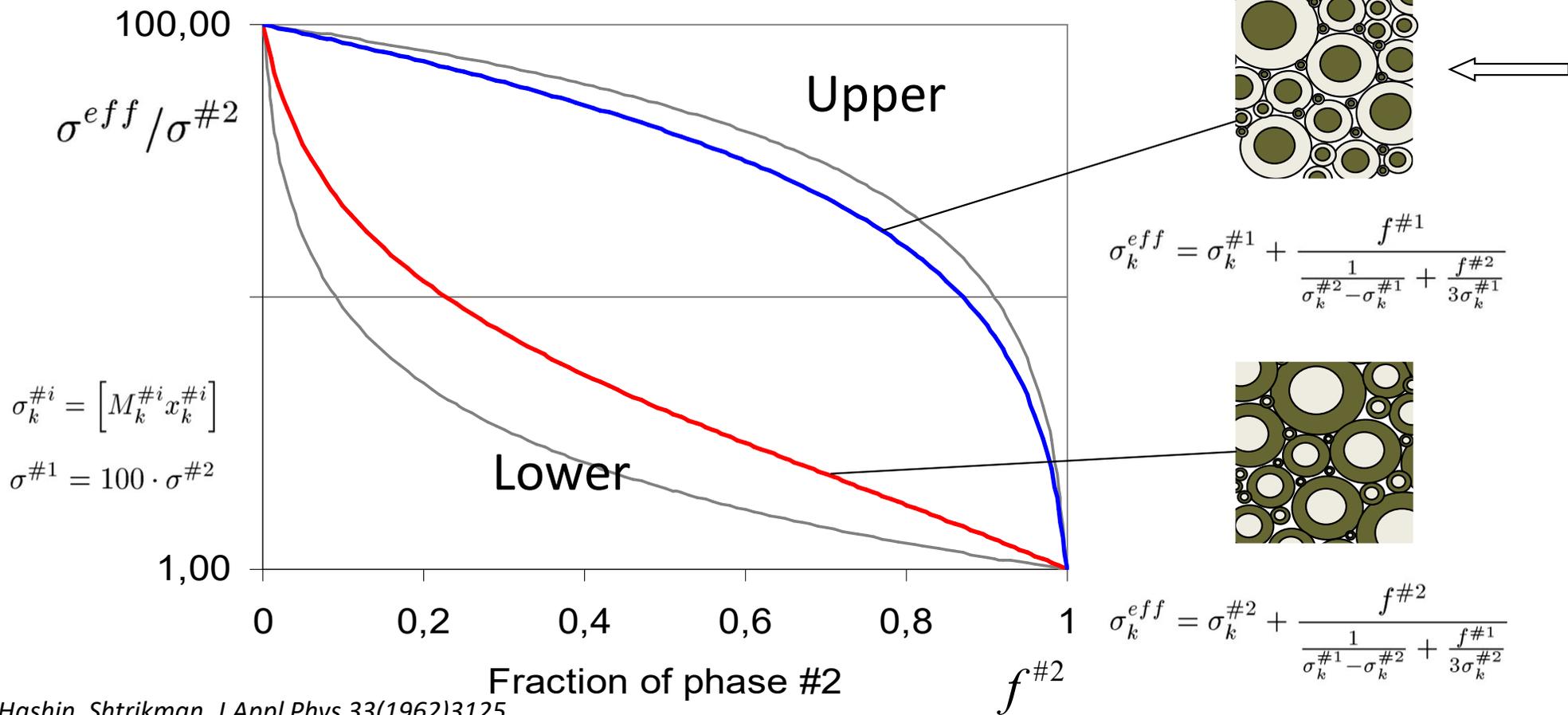
# Absolute bounds

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



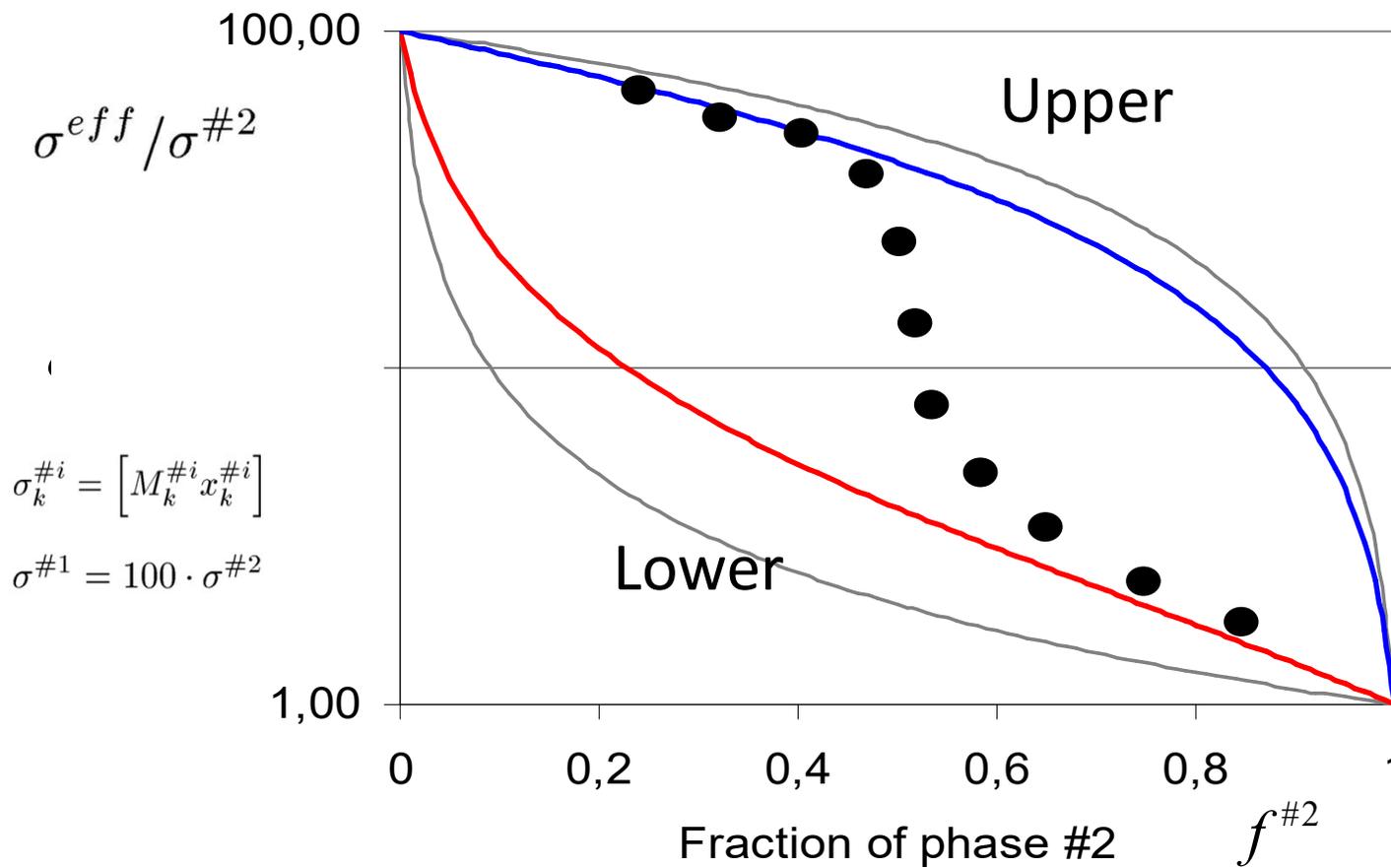
# Hashin-Shtrikman bounds

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



# Percolation

In reality one cannot expect that 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.*

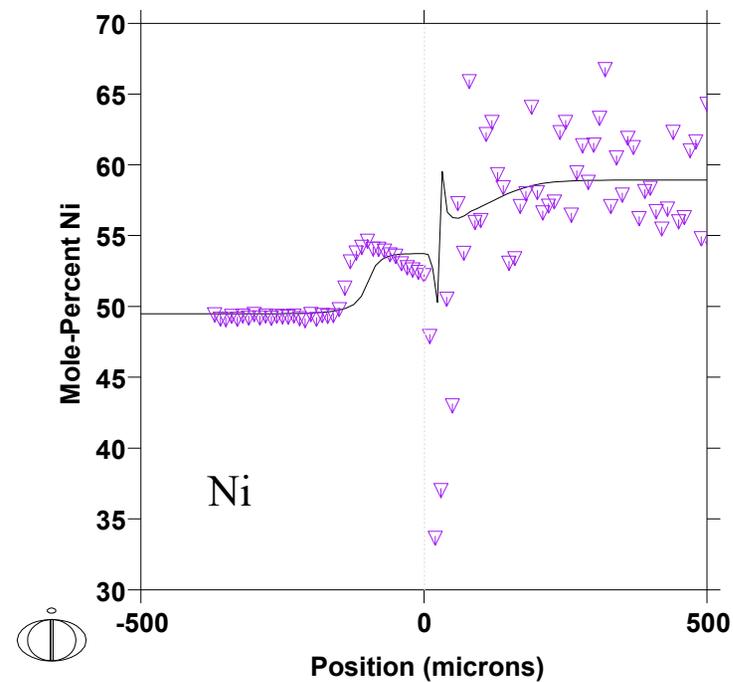
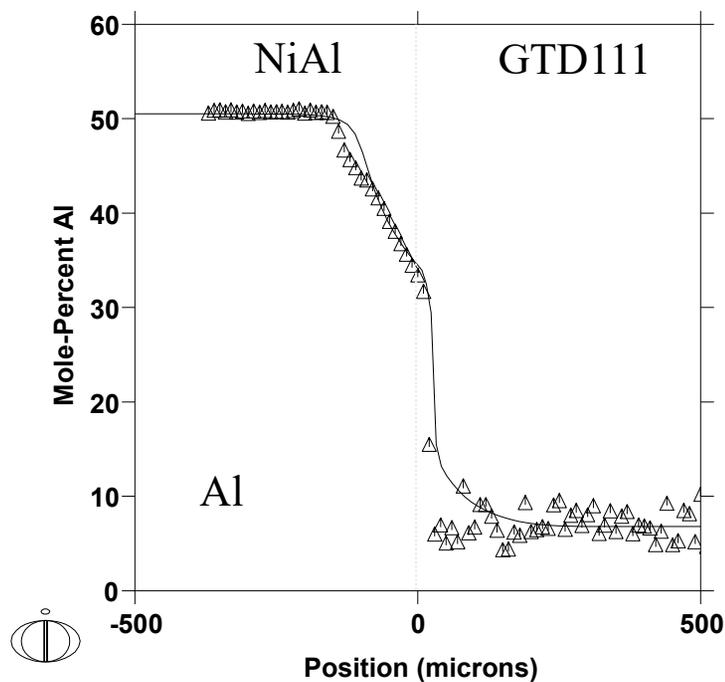
# Homogenization functions in DICTRA

1. General lower Hashin-Shtrikman bound
  2. General upper Hashin-Shtrikman bound
  3. Hashin-Shtrikman bound with prescribed matrix phase
  4. Hashin-Shtrikman bound with majority phase as matrix phase
  5. Rule of mixtures (upper Wiener bound)
  6. Inverse rule of mixtures (lower Wiener bound)
  7. Labyrinth factor  $f$  with prescribed matrix phase
  8. Labyrinth factor  $f^2$  with prescribed matrix phase
  9. General lower Hashin-Shtrikman bound with excluded phase(s)
  10. General upper Hashin-Shtrikman bound with excluded phase(s)
  11. Hashin-Shtrikman bound with prescribed matrix phase & excluded phase(s)
  12. Hashin-Shtrikman bound with majority phase as matrix & excluded phase(s)
  13. Rule of mixtures (upper Wiener bound) with excluded phase(s)
  14. Inverse rule of mixtures (lower Wiener bound) with excluded phase(s)
- Color red = available in Graphical mode

# NiAl coating on superalloy GTD111

	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

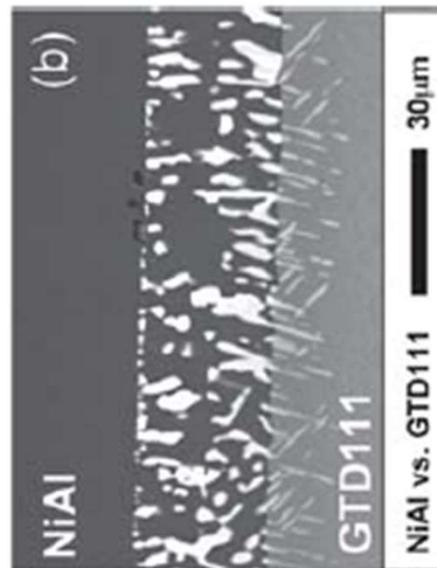
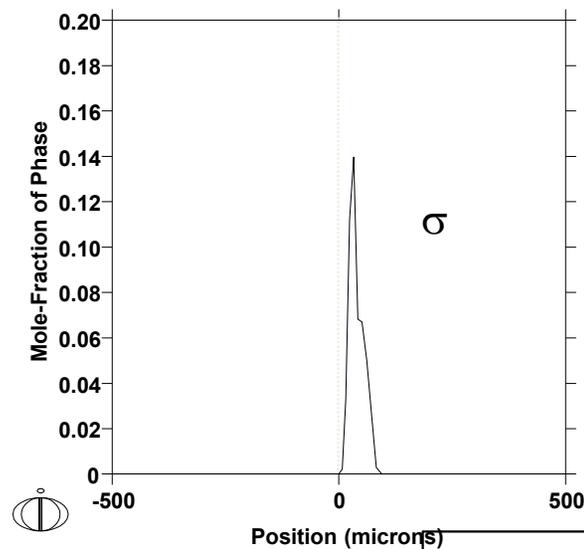
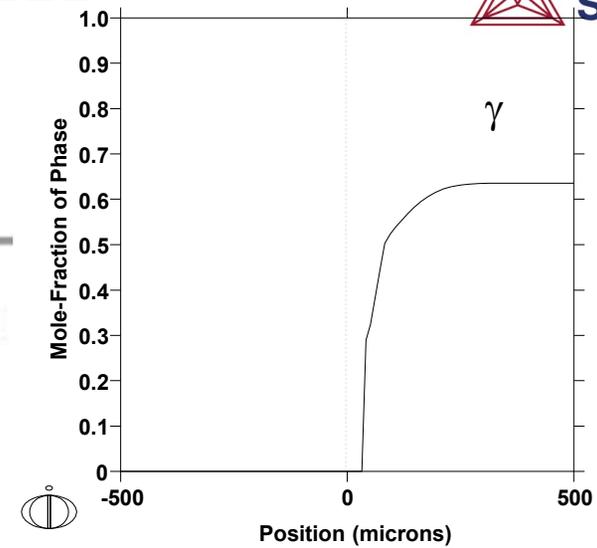
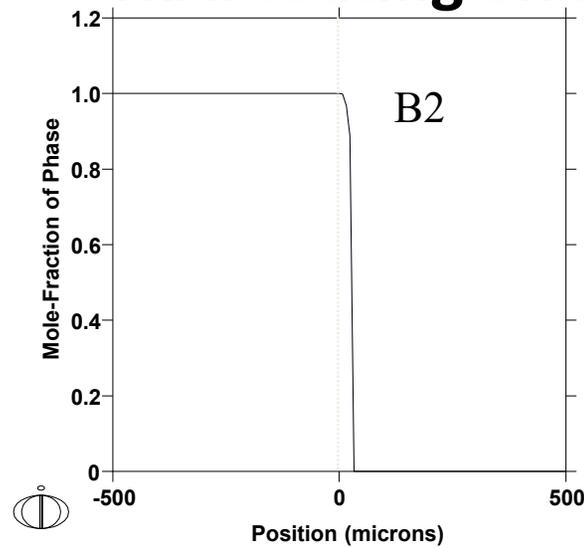
*Temp. 1050°C*  
*Time 96h*



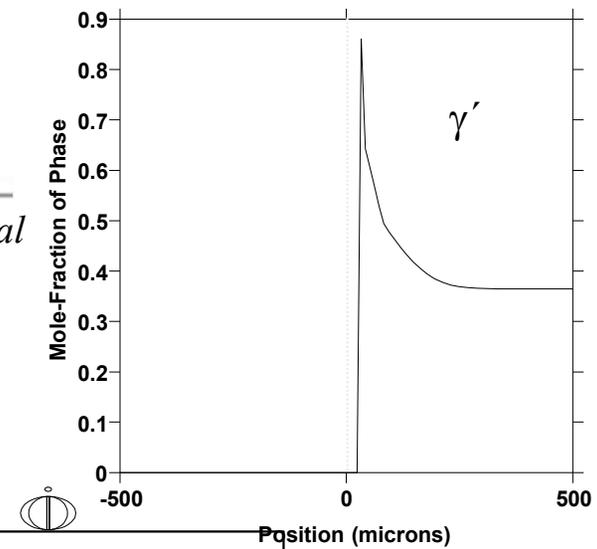
Symbols are experimental data from Perez, Patterson and Sohn, J Phase Equilibria and Diffusion **27**(2006)659

Engström et al. Adv Mater Research 278(2011)198

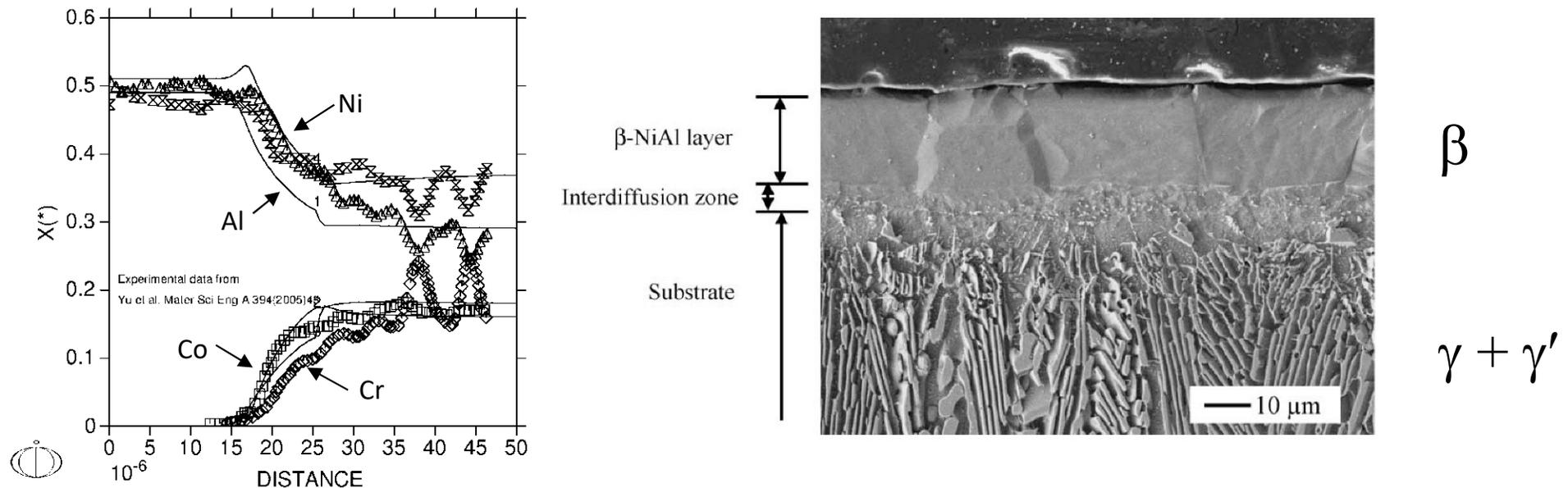
# NiAl coating on superalloy GTD111



Micrograph from Perez et al  
*J Phase Equilibria and  
Diffusion* 27(2006)659



# Simulation of CVD process



Deposition of NiAl on Ni-base alloy by CVD  
Domain is growing during the simulation

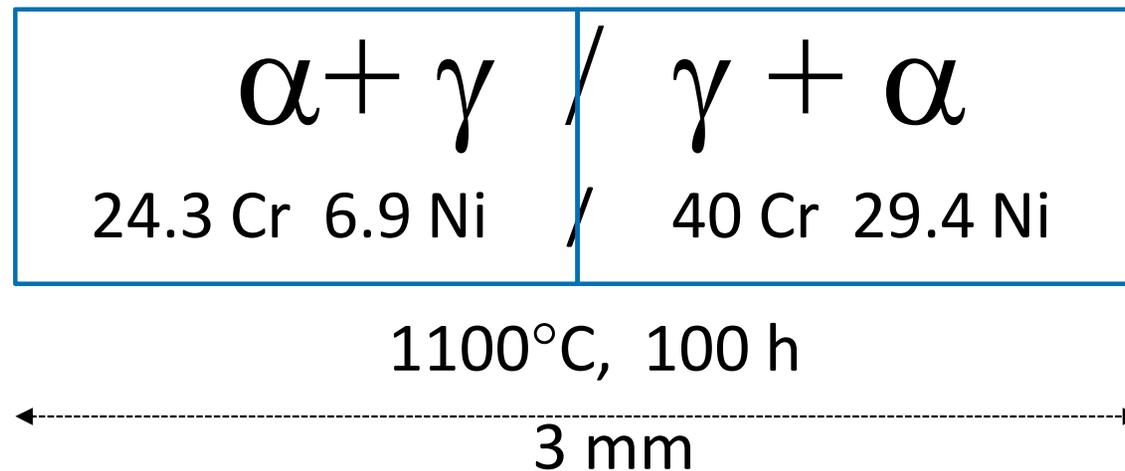
Micrograph and experimental data from Yu et al Mater Sci Eng A 394(2005)43

# Homogenization Model

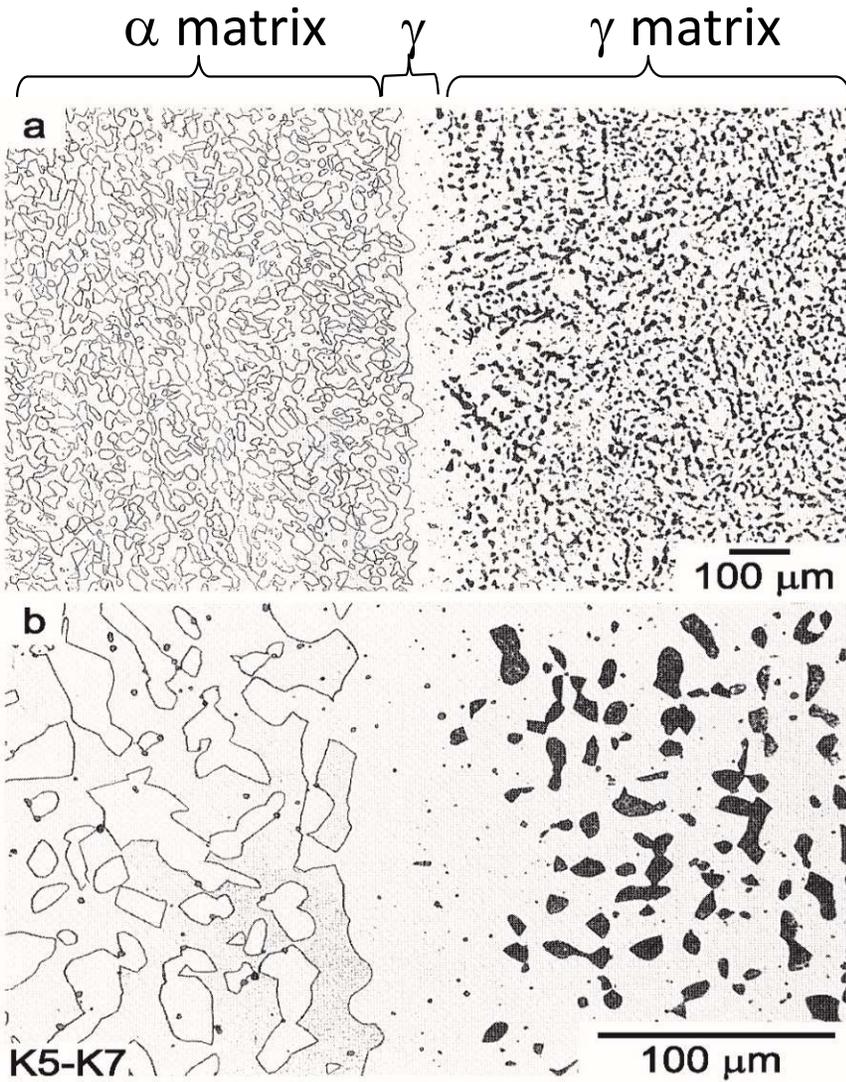
## Example- fcc+bcc/fcc+bcc diffusion couple

# Example: Fe-Cr-Ni diffusion couple

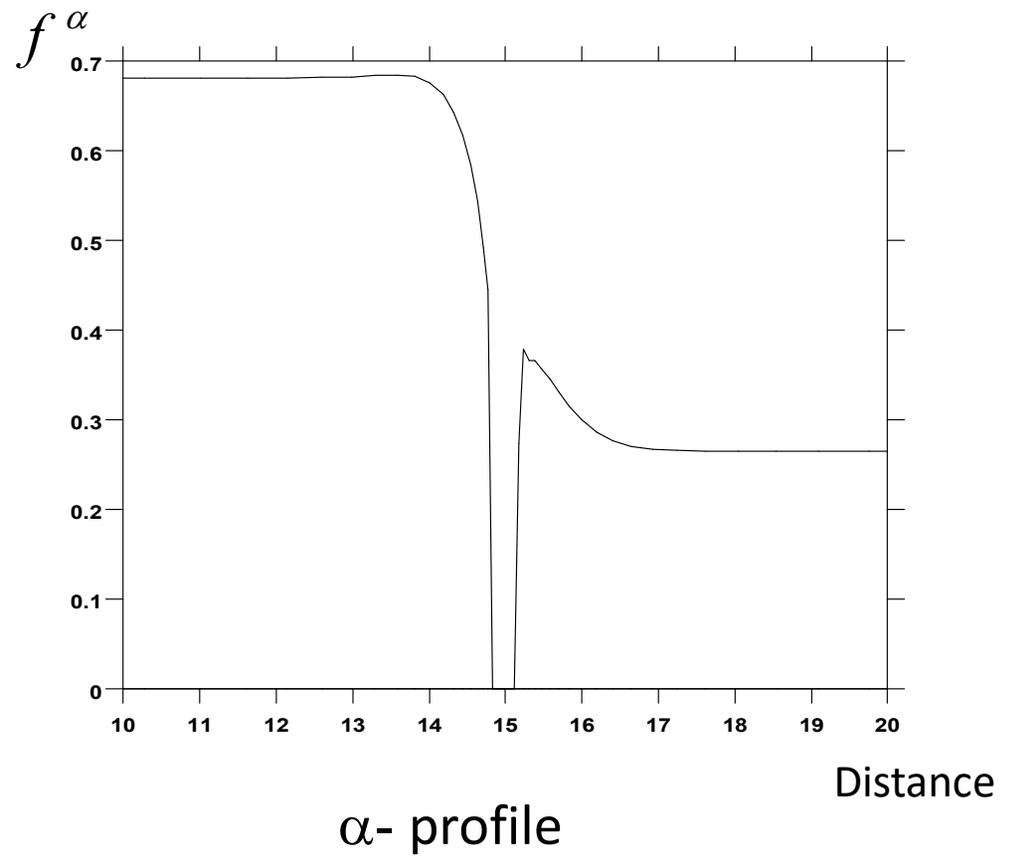
- Homogenization model
- A single region containing both BCC (ferrite) and FCC (austenite)
- Enter the overall composition as the "matrix" composition
- Choice of "matrix" phase does not matter
- Lower Hashin-Shtrikman homogenization function
- Initially a step profile, composition in **wt-%**



# Example: Fe-Cr-Ni diffusion couple



$\alpha + \gamma / \gamma / \gamma + \alpha$

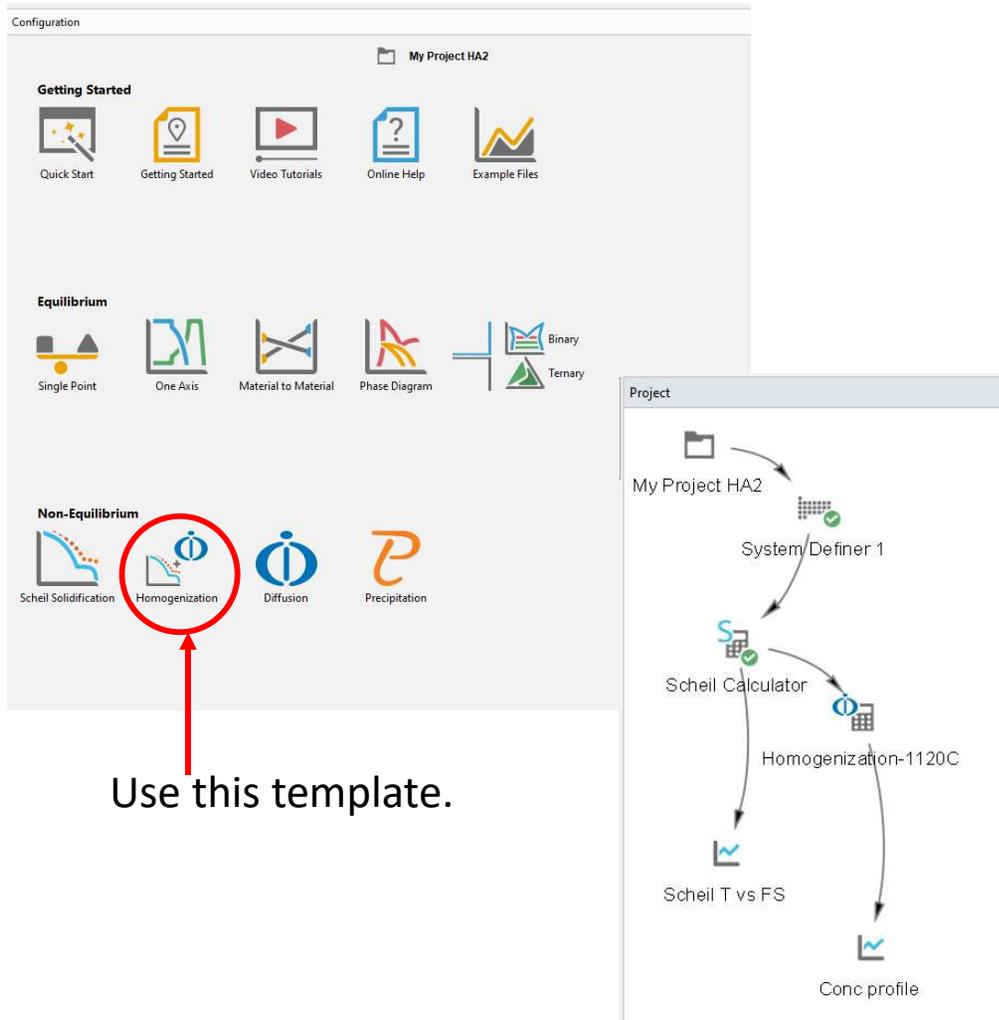


# Q & A

# Home assignment 2

# Home assignment 2: Solidification & Homogenisation

CrNi-steel: Fe(bal.) – 1.9 Ni – 0.95 Cr – 0.65 Mn – 0.4 C (wt-%)



The image shows two parts of the Thermo-Calc software interface. On the left is the 'Configuration' window, which is organized into three sections: 'Getting Started' (with icons for Quick Start, Getting Started, Video Tutorials, Online Help, and Example Files), 'Equilibrium' (with icons for Single Point, One Axis, Material to Material, Phase Diagram, Binary, and Ternary), and 'Non-Equilibrium' (with icons for Scheil Solidification, Homogenization, Diffusion, and Precipitation). The 'Homogenization' icon in the Non-Equilibrium section is circled in red, and a red arrow points from it to the text 'Use this template.' below. On the right is the 'Project' window, which displays a workflow diagram. The workflow starts with 'My Project HA2', leading to 'System Definer 1', then 'Scheil Calculator', and finally 'Homogenization-1120C'. From 'Homogenization-1120C', the workflow branches into two outputs: 'Scheil T vs FS' and 'Conc profile'.

Use this template.

Start with a Classic Scheil simulation, with carbon as a fast diffusing element.

Then use the result of the Scheil as start composition in the homogenisation simulation. Use default settings.

Secondary dendrite arm spacing: 200  $\mu\text{m}$ .  
Temperature 1120  $^{\circ}\text{C}$ .

Time for homogenisation: 72 hours.

Task: Check how the concentration profiles for Ni and Cr change over time.

Compare with exp. data: Fuchs\_1120.exp