Head of the Institute: Prof. Dr.-Ing. H.-J. Christ

InCorr for Windows
Modeling of Corrosion Phenomena

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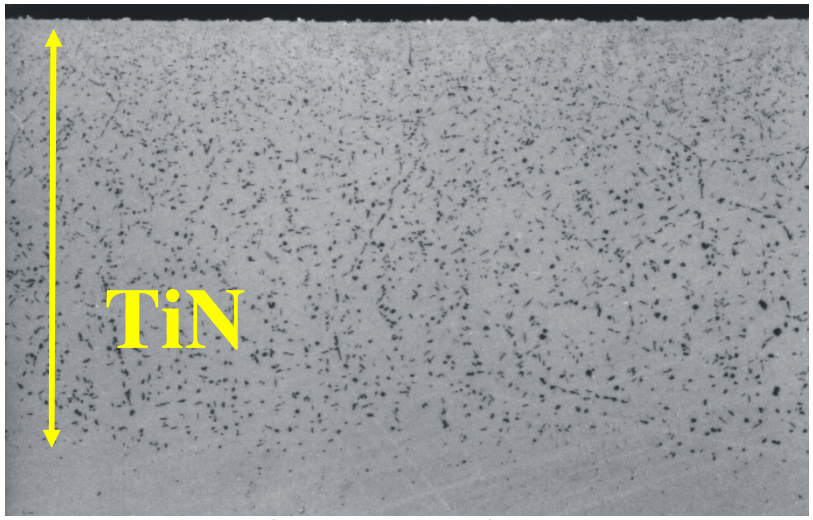
What is InCorr?

- InCorr - a computer-based program for simulation of high-temperature corrosion phenomena
- Use of numerical diffusion calculation in combination with thermodynamic equilibrium concepts
- The application InCorr is parallelized along its functions (function-master, function-slave and function-matlab)

Physical Modeling
and
Computer-Based Simulation

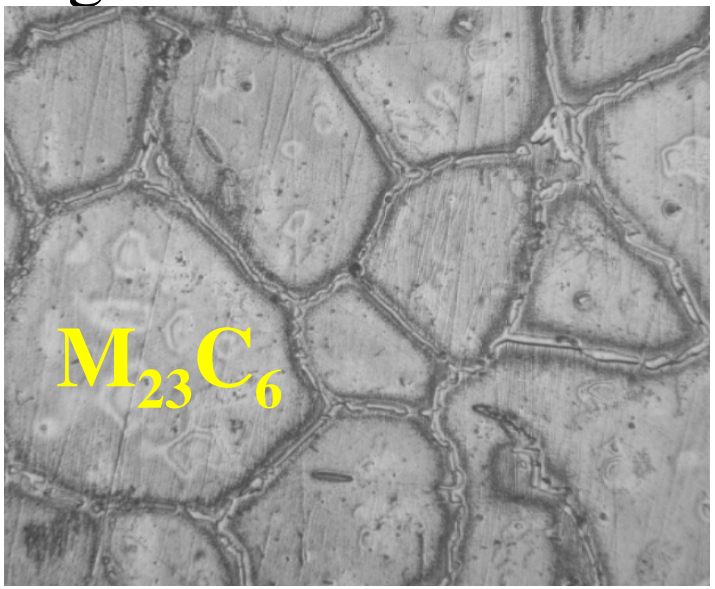
Physical Modeling

homogeneous internal attack

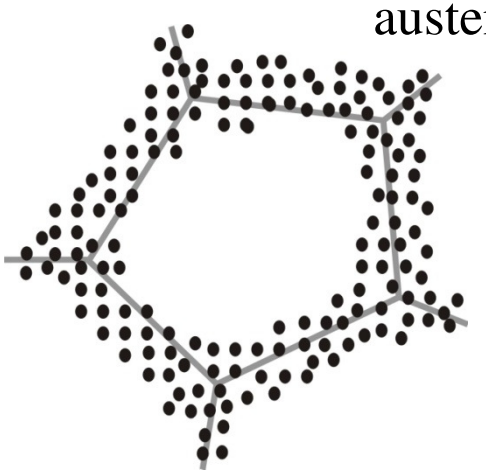


Ni-20Cr-2Ti

intergranular corrosion attack

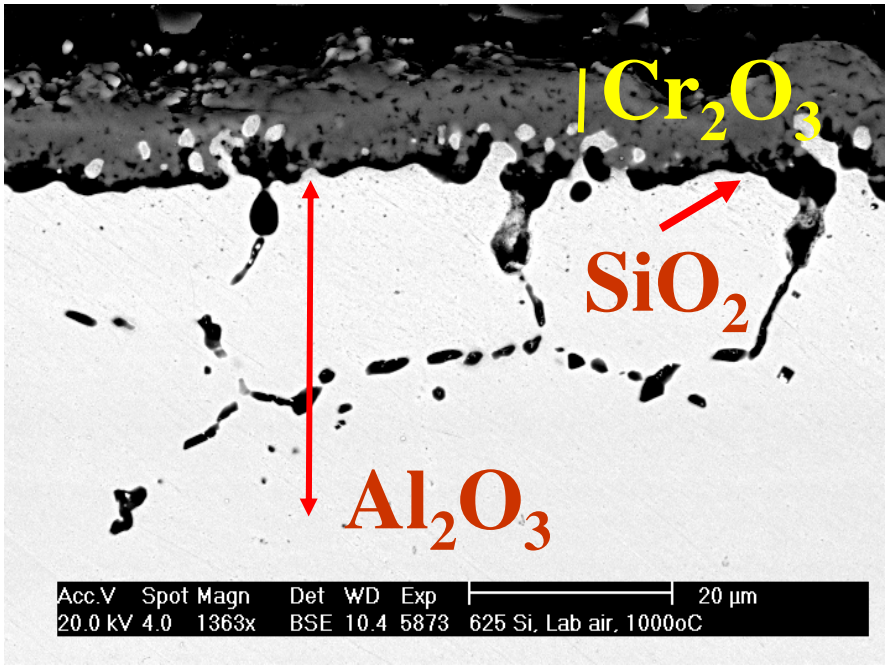


austenitic steel



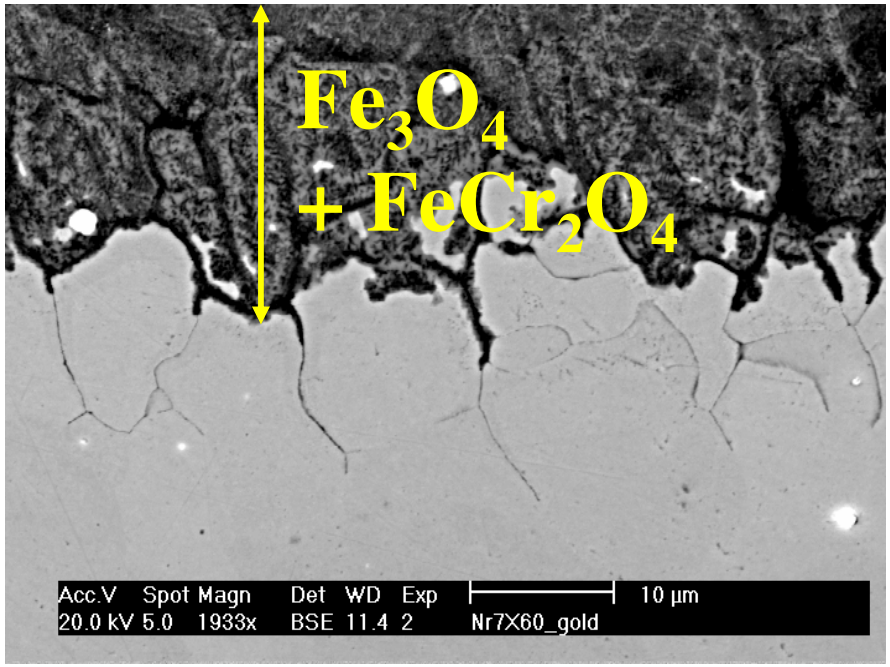
Physical Modeling

outer scale and internal attack



Inconel 625 Si

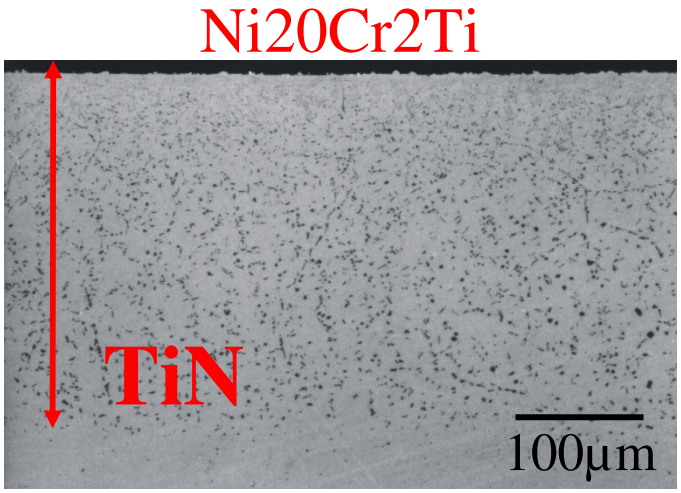
inward-growing scale



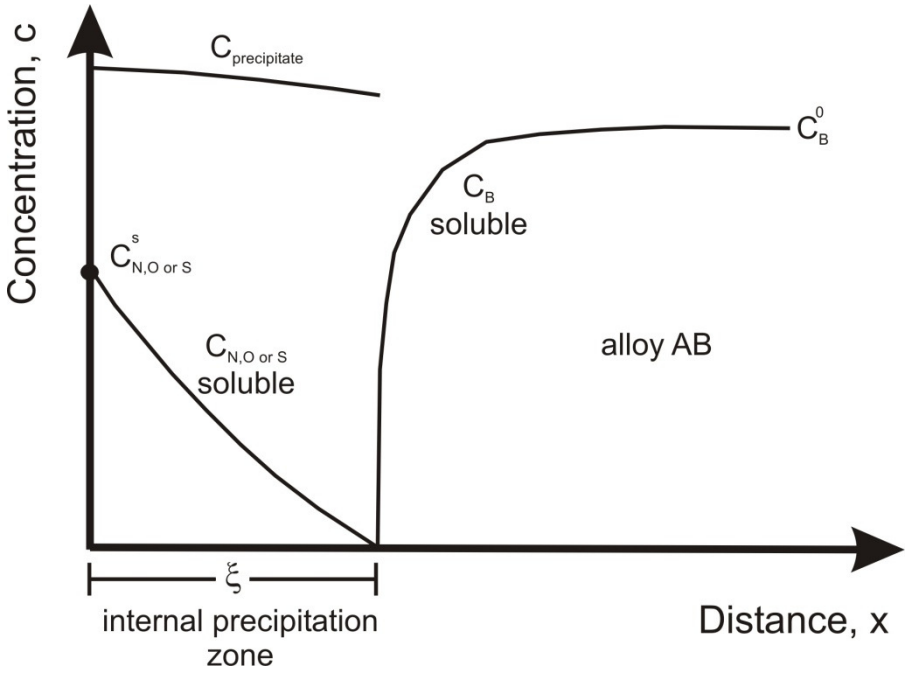
low-Cr steel

C. Wagners Theory of Internal Oxidation

Internal nitridation and oxidation



(100h, 1100°C, N_2 atmosphere)

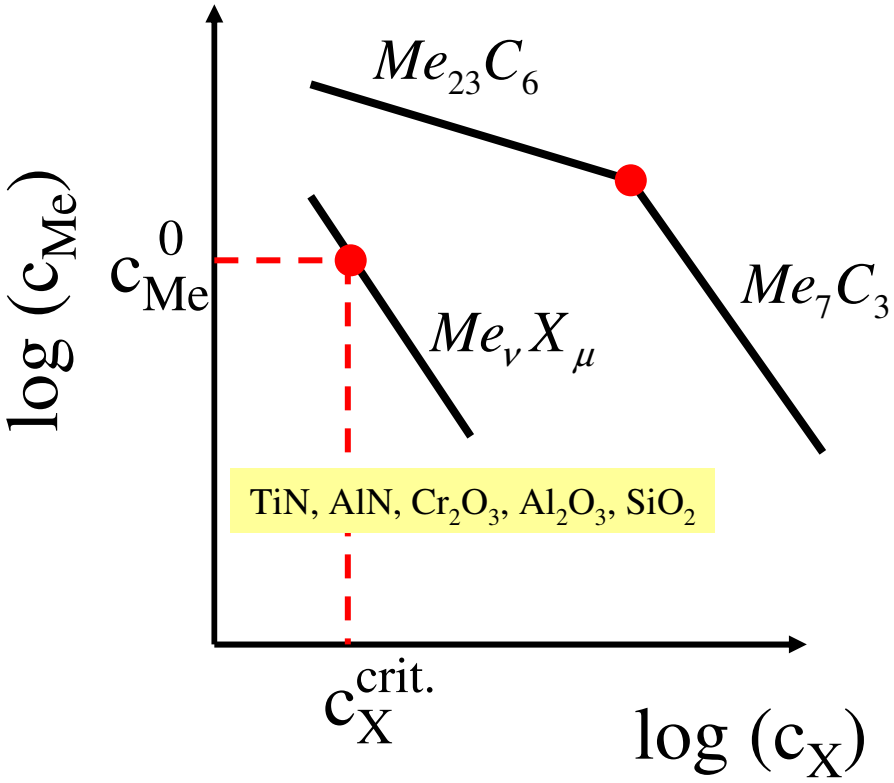


$$c_{N,O,S}(x,t) = c^{(s)}_{N,O,S}\left[\frac{erfc\dfrac{x}{2\sqrt{D_{N,O,S}t}}}{erf\gamma}\right]$$

$$\xi = \sqrt{\frac{2c_O^s D_O t}{\nu c_B^0}}$$

- one kind of precipitate
- very stable precipitate

Calculation using Solubility Product



$$\nu Me + \mu X = Me_\nu X_\mu$$

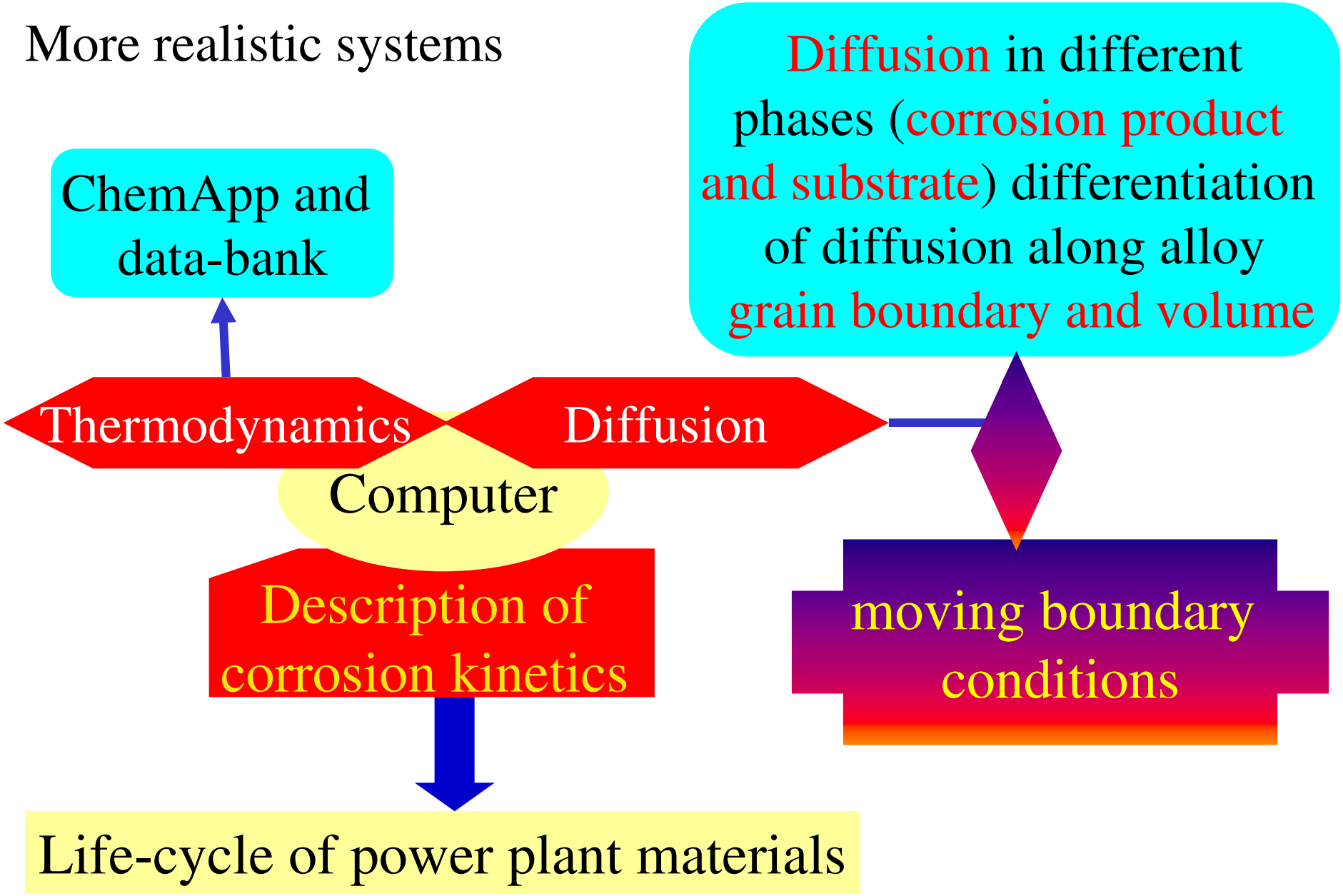
$$SP_{MeX} = [Me]^\nu [X]^\mu$$

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2}$$

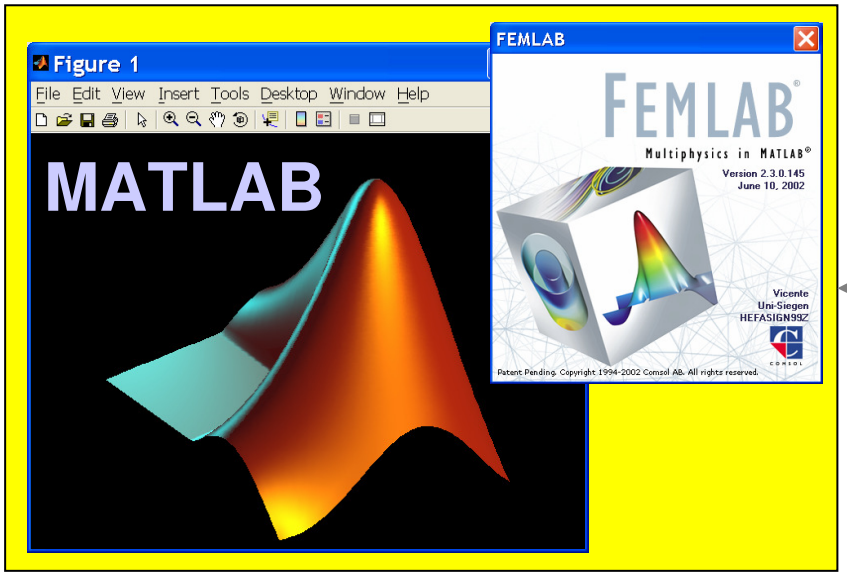
$$\frac{\partial c_X}{\partial t}\left(1+\left(\frac{\nu}{\mu}\right)\left(\frac{SP}{c_X^\nu}\right)\right) = D_X \frac{\partial^2 c_X}{\partial x^2}$$

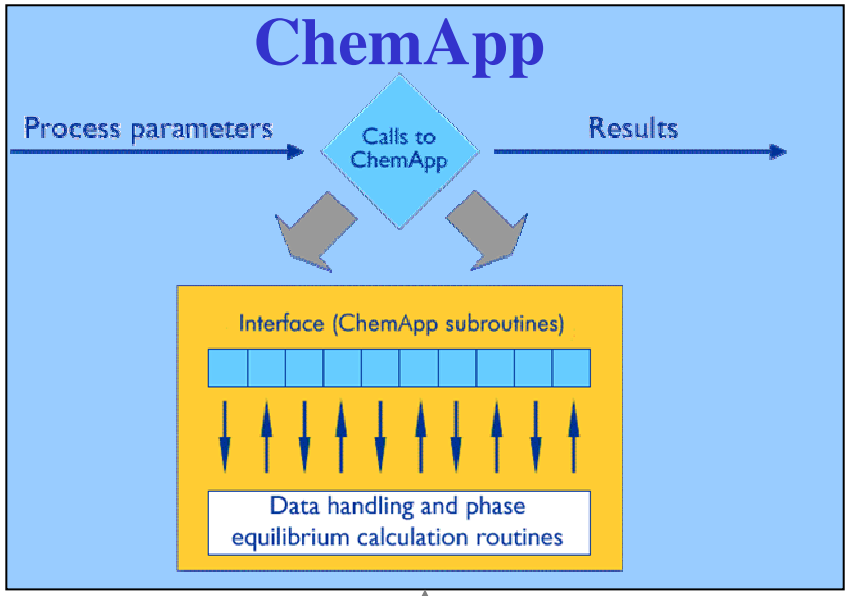
solve numerically

More realistic systems



Modeling





solid state diffusion

representation

high-temperature corrosion

InCor

local thermodynamic equilibrium

G = Minimum

Mathematical Modeling

One-Dimensional

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial c}{\partial x}\right) \xrightarrow{D = f(T)} \frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2}$$

Two-Dimentional

$$\frac{\partial c}{\partial t} = D_x\frac{\partial^2 c}{\partial x^2} + D_y\frac{\partial^2 c}{\partial y^2}$$

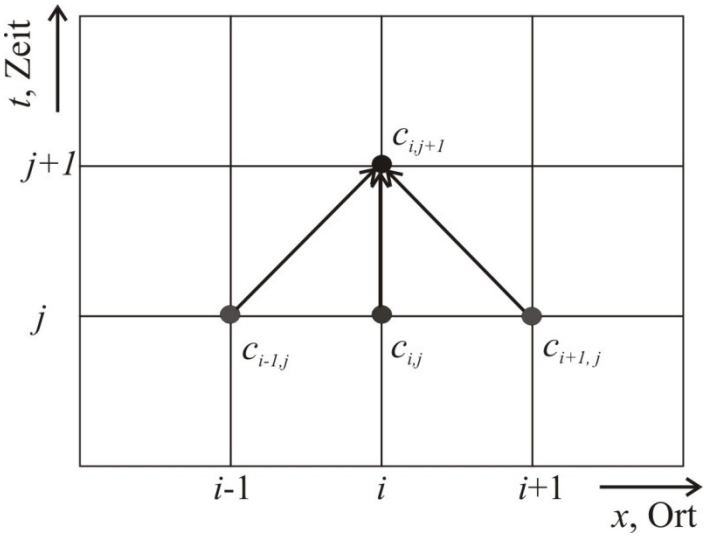
One-Dimensional Problem – explicit finite-difference method

$$\frac{\partial c}{\partial t} \approx \frac{c_{i,j+1} - c_{i,j}}{\Delta t} \qquad \frac{\partial^2 c}{\partial x^2} \approx \frac{c_{i+1,j} - 2c_{i,j} + c_{i-1,j}}{(\Delta x)^2}$$

$$r = \frac{D\Delta t}{(\Delta x)^2} \qquad r \le \frac{1}{2}$$

$$c_{i,j+1} = rc_{i-1,j} + (1-2r)c_{i,j} + rc_{i+1,j}$$

$$\boldsymbol{c}_{j+1} = \boldsymbol{A}\boldsymbol{c}_j + \boldsymbol{b}_j \qquad \boldsymbol{A} = \begin{pmatrix} 1-2r & r & 0 & 0 & 0 & \dots & 0 \\ r & 1-2r & r & 0 & 0 & \dots & 0 \\ 0 & r & 1-2r & r & 0 & \dots & 0 \\ 0 & 0 & r & 1-2r & r & \dots & 0 \\ 0 & 0 & 0 & r & . & \dots & 0 \\ . & . & . & . & . & . & r \\ 0 & 0 & 0 & 0 & 0 & r & 1-2r \end{pmatrix} \qquad \boldsymbol{b}_j = \begin{pmatrix} rc^s \\ 0 \\ 0 \\ . \\ . \\ . \\ 0 \end{pmatrix}$$



One-Dimensional problem – implicit finite-difference method

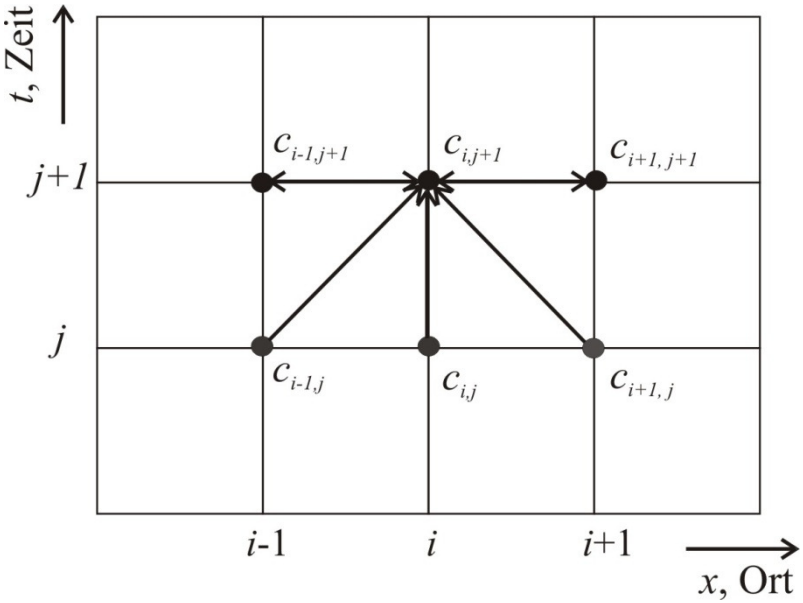
$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2}$$

$$\begin{cases} \dfrac{\partial c}{\partial t} \approx \dfrac{c_{i,j+1} - c_{i,j}}{\Delta t} \\ \dfrac{\partial^2 c}{\partial x^2} \approx \dfrac{1}{2(\Delta x)^2}\left(c_{i+1,j} - 2c_{i,j} + c_{i-1,j} + c_{i+1,j+1} - 2c_{i,j+1} + c_{i+1,j+1} \right) \end{cases}$$

$$\boldsymbol{c}_{j+1} = (2\boldsymbol{I} + \boldsymbol{N})^{-1}(2\boldsymbol{I} - \boldsymbol{N})\boldsymbol{c}_j + (2\boldsymbol{I} + \boldsymbol{N})^{-1}\boldsymbol{b}_j$$

$$\boldsymbol{N} = r\boldsymbol{M}_x$$

$$\boldsymbol{M}_x = \begin{pmatrix} 2 & -1 & 0 & 0 & 0 & \dots & 0 \\ -1 & 2 & -1 & 0 & 0 & \dots & 0 \\ 0 & -1 & 2 & -1 & 0 & \dots & 0 \\ 0 & 0 & -1 & 2 & -1 & \dots & 0 \\ 0 & 0 & 0 & -1 & . & \dots & 0 \\ . & . & . & . & . & . & -1 \\ 0 & 0 & 0 & 0 & 0 & -1 & 2 \end{pmatrix}$$



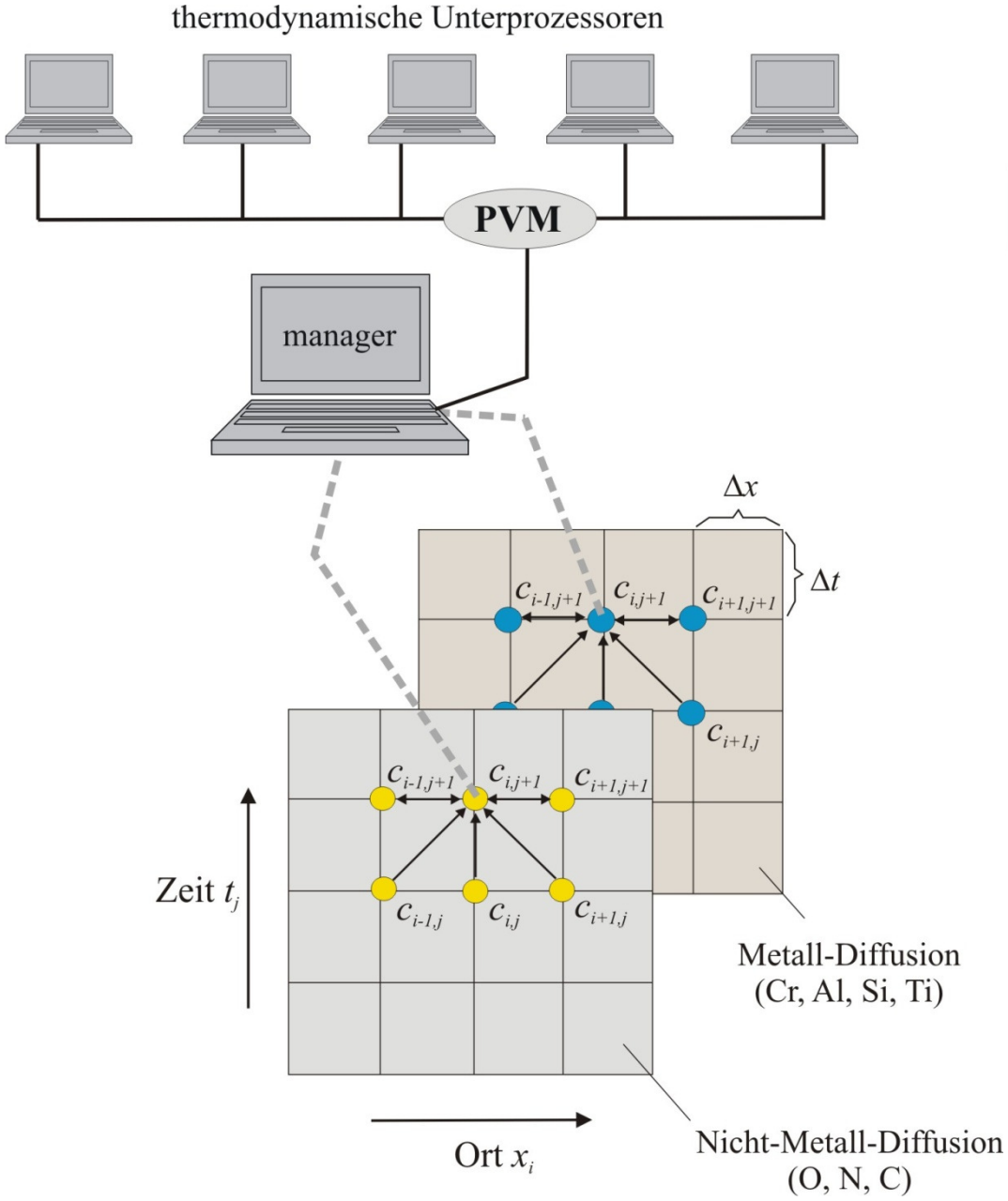
Two-Dimensional Problem – implicit finite-difference method

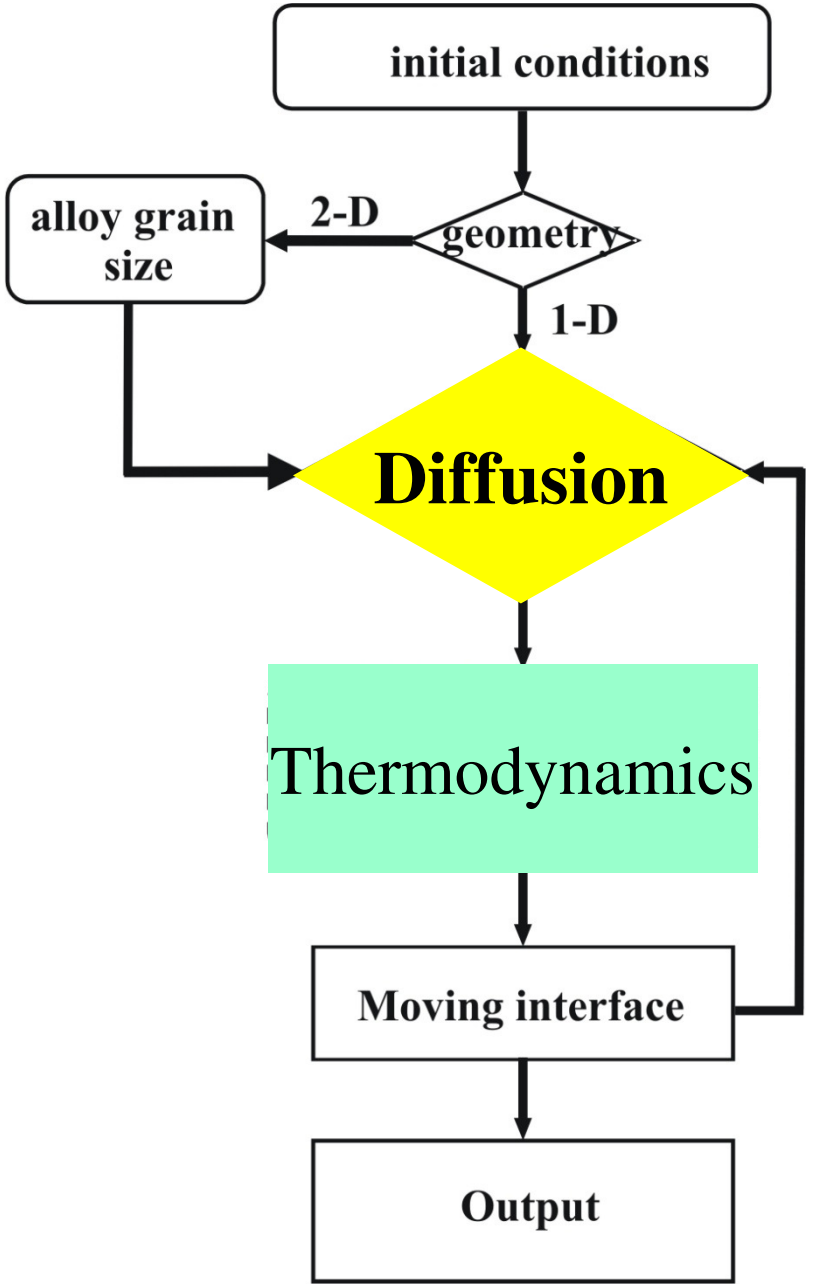
$$\frac{\partial c}{\partial t} = D_x \frac{\partial^2 c}{\partial x^2} + D_y \frac{\partial^2 c}{\partial y^2}$$

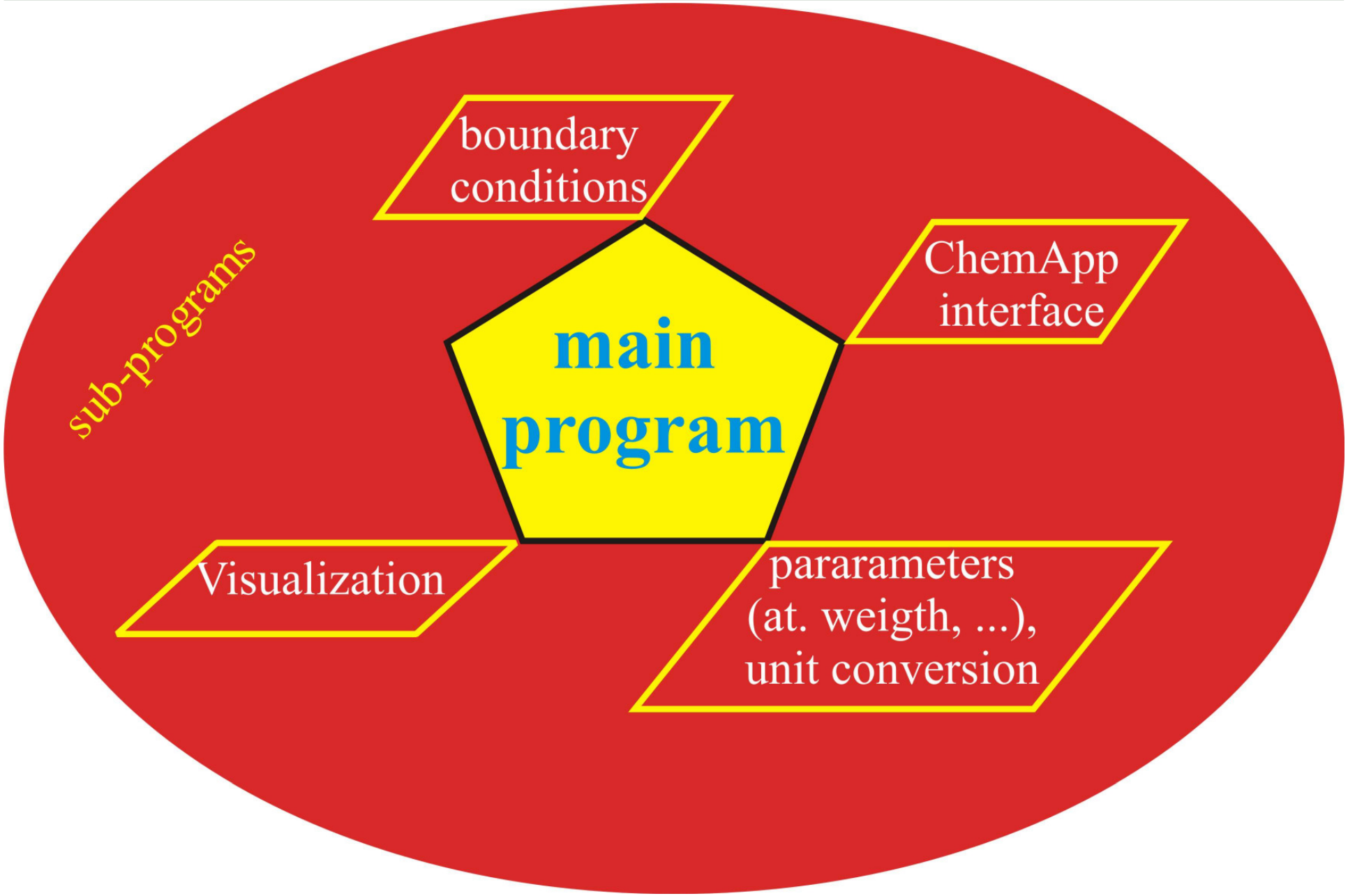
$$r_x = \frac{D_x \Delta t}{(\Delta x)^2} \qquad r_y = \frac{D_y \Delta t}{(\Delta y)^2}$$

$$r_x \cdot \left(c_{ix+1,iy}^{j+1} + c_{ix,iy-1}^{j+1}\right) - 2 \cdot \left(1 + r_x + r_y\right) \cdot c_{ix,iy}^{j+1} + r_y \cdot \left(c_{ix,iy+1}^{j+1} + c_{ix,iy-1}^{j+1}\right) =$$
$$- r_y \cdot \left(c_{ix,iy-1}^{j} + c_{ix,iy+1}^{j}\right) - 2 \cdot \left(1 - r_x - r_y\right) \cdot c_{ix,iy}^{j} - r_x \cdot \left(c_{ix-1,iy}^{j} + c_{ix+1,iy}^{j}\right)$$

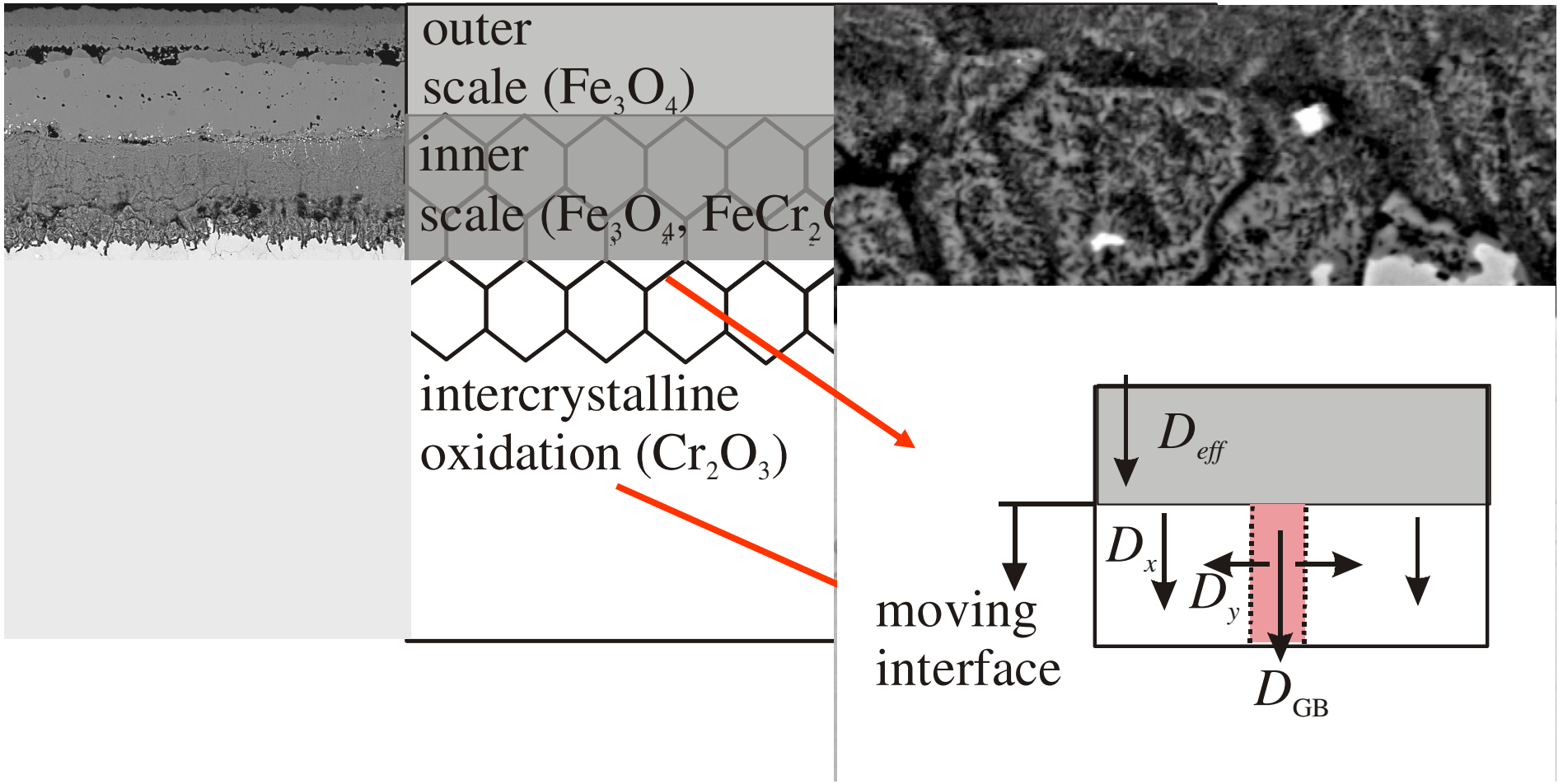
$$\frac{c(x, y, t+\Delta t) - c(x, y, t)}{\Delta t} = \frac{D_x(x, y)}{2(\Delta x(x, y))^2}[c(x - \Delta x, y, t) - 2c(x, y, t) + c(x + \Delta x, y, t)]$$
$$+ \frac{D_x(x, y)}{2(\Delta x(x, y))^2}[c(x - \Delta x, y, t + \Delta t) - 2c(x, y, t + \Delta t) + c(x + \Delta x, y, t + \Delta t)]$$
$$+ \frac{D_y(x, y)}{2(\Delta y(x, y))^2}[c(x, y - \Delta y, t) - 2c(x, y, t) + c(x, y + \Delta y, t)]$$
$$+ \frac{D_y(x, y)}{2(\Delta y(x, y))^2}[c(x, y - \Delta y, t + \Delta t) - 2c(x, y, t + \Delta t) + c(x, y + \Delta y, t + \Delta t)]$$


thermodynamische Unterprozessoren
PVM
manager
Δx
Δt
$c_{i-1,j+1}$
$c_{i,j+1}$
$c_{i+1,j+1}$
$c_{i+1,j}$
$c_{i-1,j}$
$c_{i,j}$
Zeit t_j
Ort x_i
Metall-Diffusion
(Cr, Al, Si, Ti)
Nicht-Metall-Diffusion
(O, N, C)


initial conditions
alloy grain size
2-D
geometry
1-D
Diffusion
Thermodynamics
Moving interface
Output

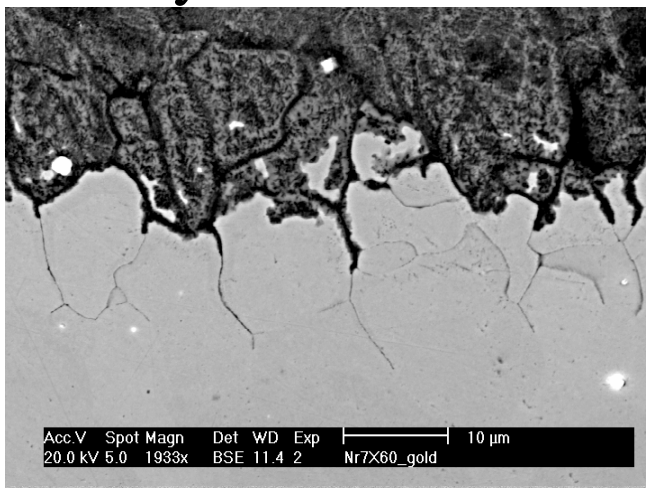

sub-programs
boundary conditions
ChemApp interface
main program
Visualization
pararameters (at. weigth, ...), unit conversion

Computer Simulation of Oxidation Processes



InCorr

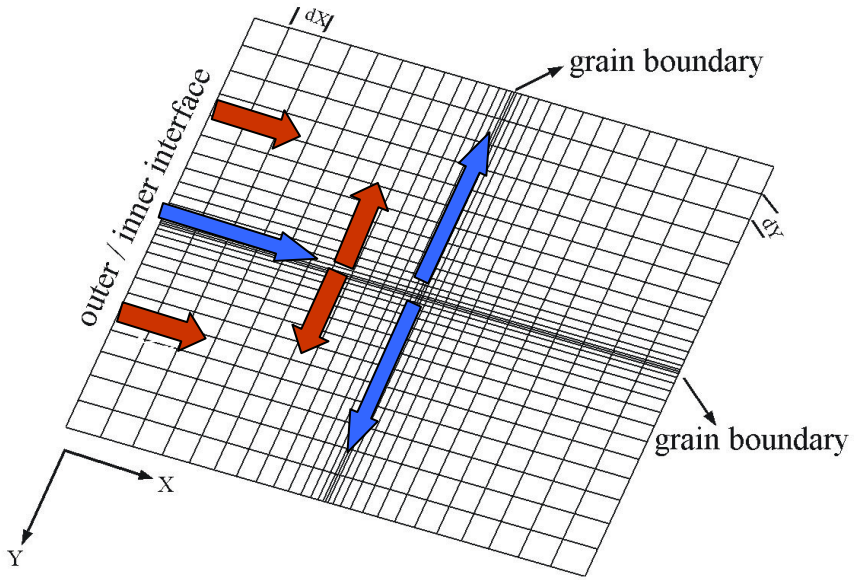
Intercrystalline Oxidation

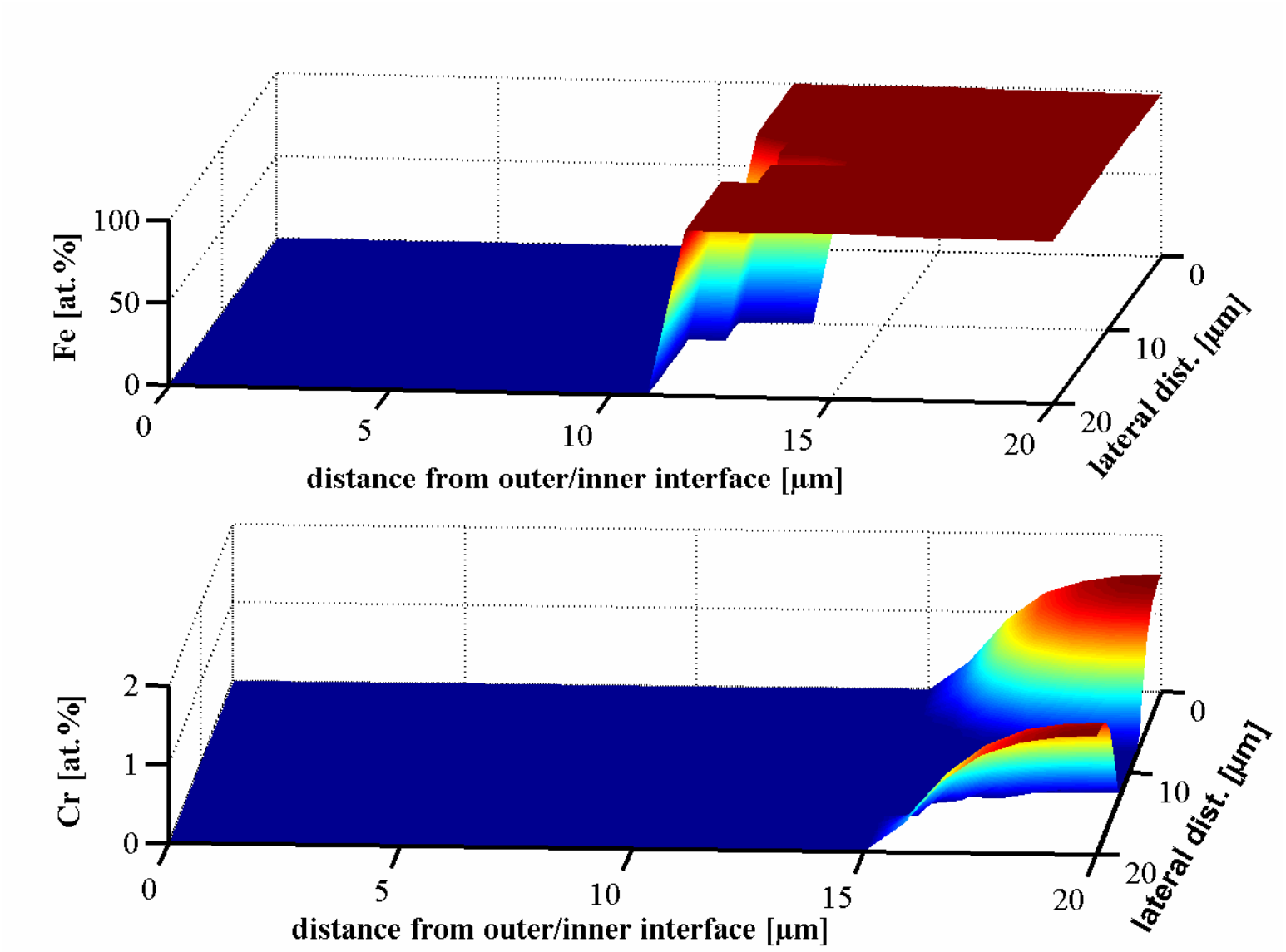


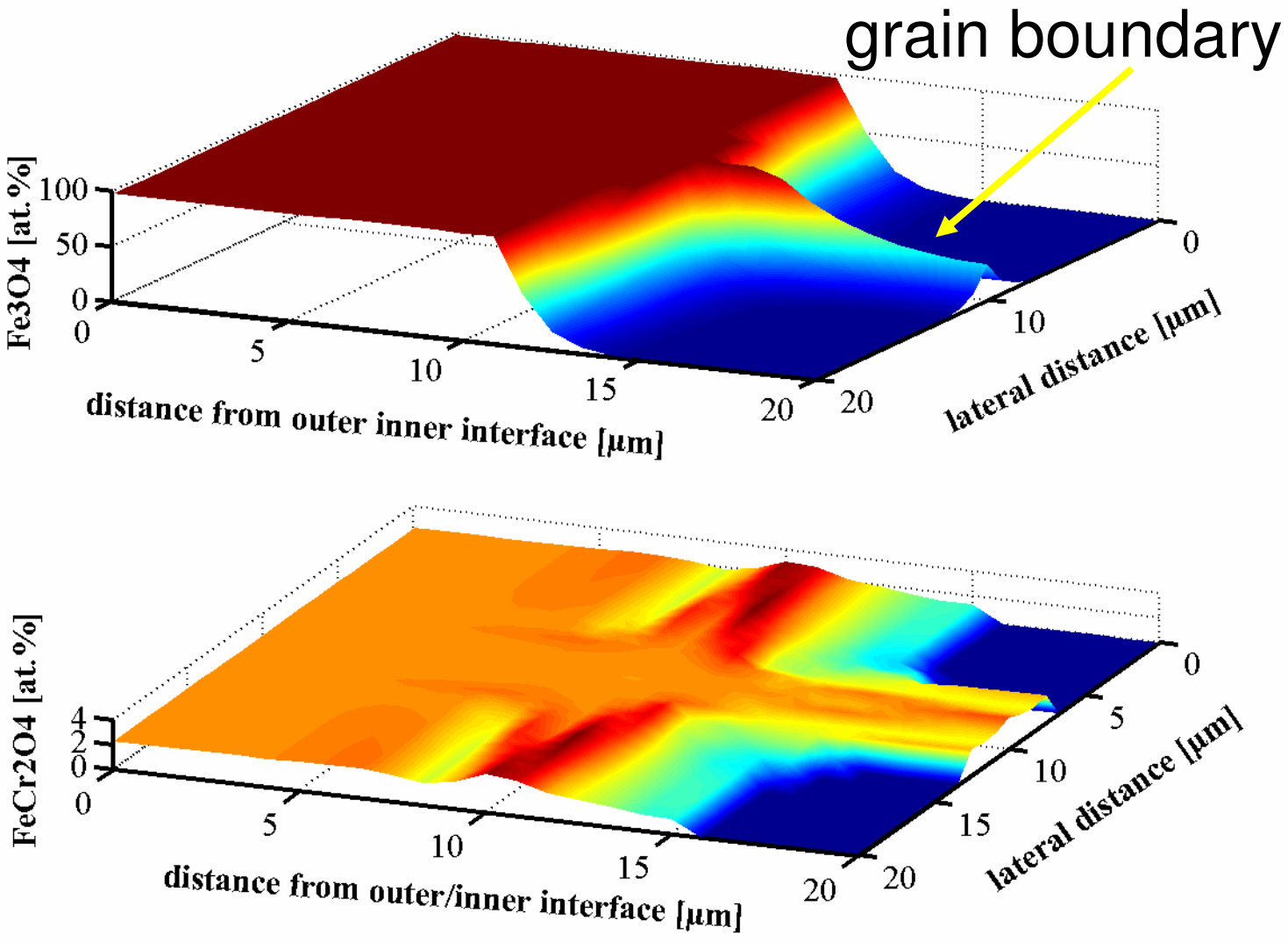
$$D = \begin{cases} D_K & \text{when } (x,y) \text{ is considered in bulk} \\ D_{KG} & \text{when}(x,y) \text{ is considered at grain boundary} \\ D_{eff}. & \text{when } (x,y) \text{ is considered in oxide scale} \end{cases}$$

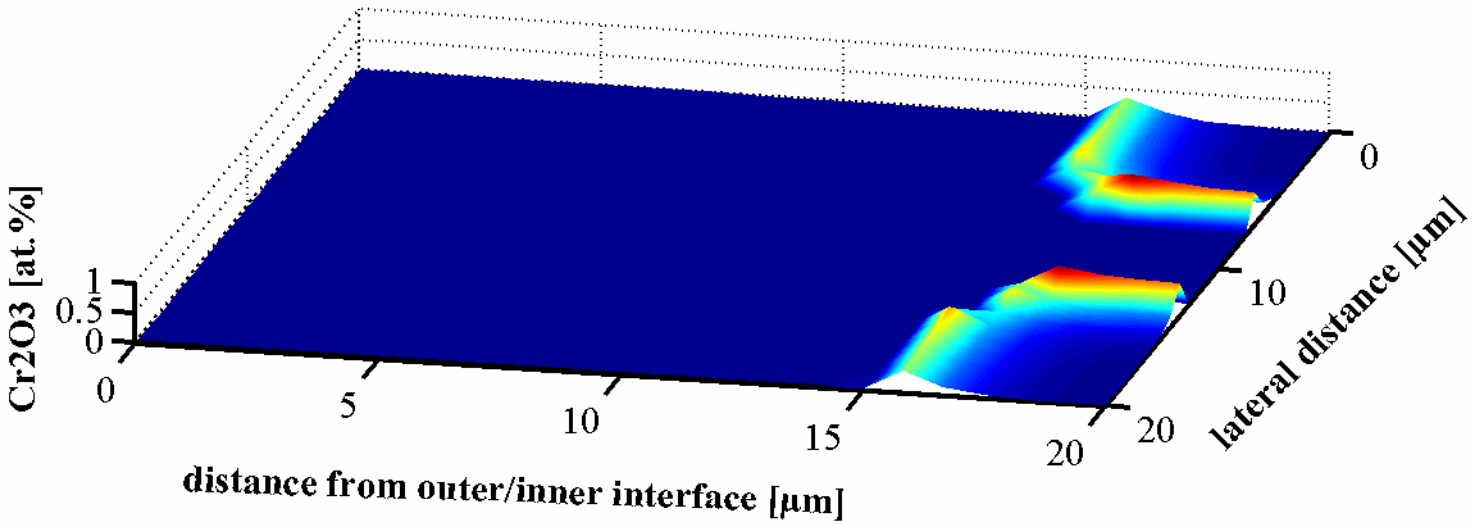
$$R_x = \operatorname{diag} \frac{D_x(x,y)}{2(\Delta x(x,y))^2}$$

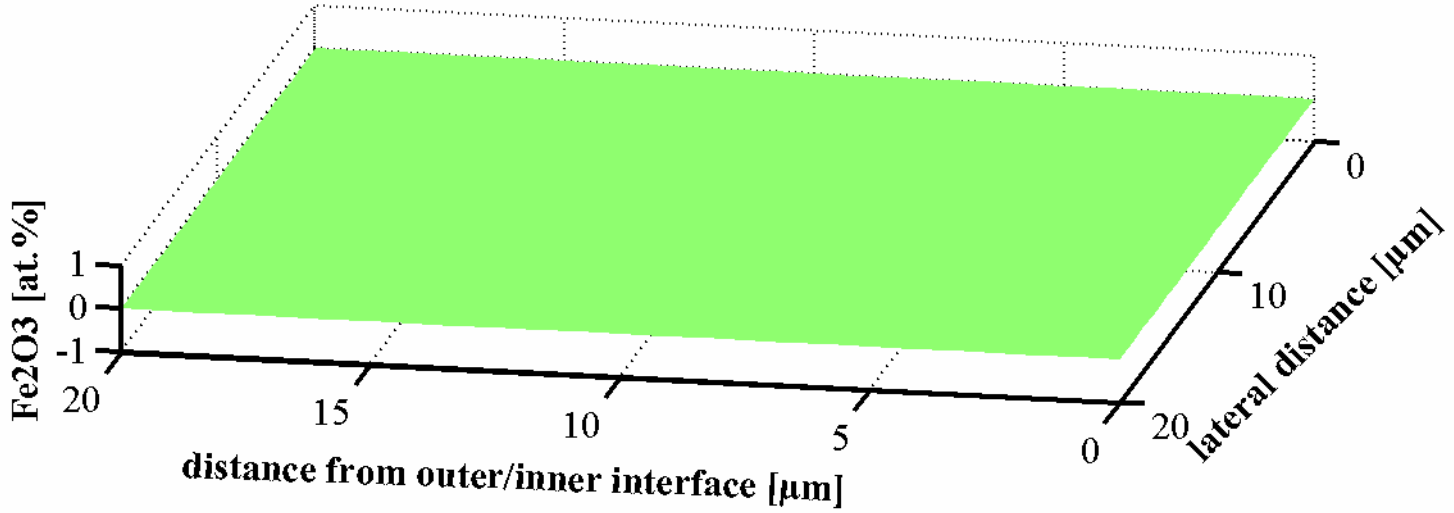
$$R_y = \operatorname{diag} \frac{D_y(x,y)}{2(\Delta y(x,y))^2}$$

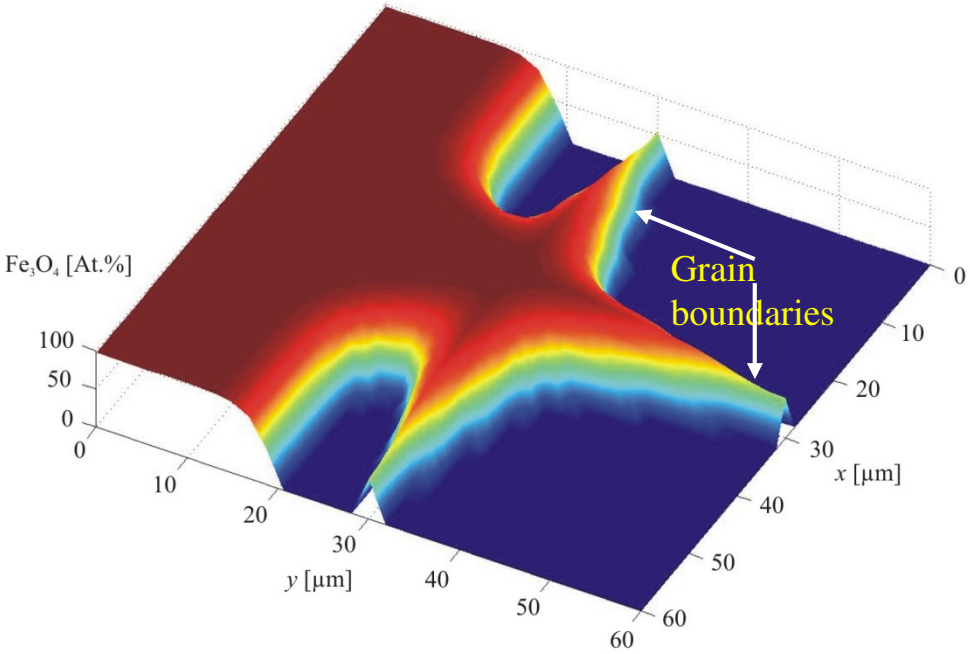


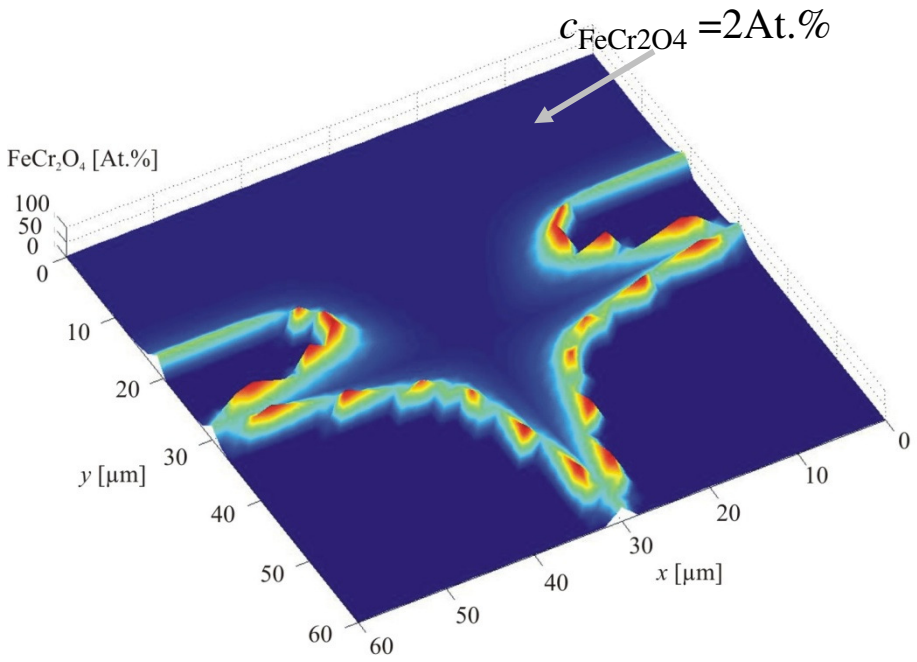

Fe [at.%]
100
50
0
0
5
10
15
20
distance from outer/inner interface [µm]
0
10
20
lateral dist. [µm]
Cr [at.%]
2
1
0
0
5
10
15
20
distance from outer/inner interface [µm]
0
10
20
lateral dist. [µm]


grain boundary
Fe3O4 [at.%]
100
50
0
0
5
10
15
20
distance from outer inner interface [µm]
0
10
20
lateral distance [µm]
FeCr2O4 [at.%]
4
2
0
0
5
10
15
20
distance from outer/inner interface [µm]
0
5
10
15
20
lateral distance [µm]


Cr2O3 [at.%]
1
0.5
0
0
5
10
15
20
distance from outer/inner interface [µm]
0
10
20
lateral distance [µm]

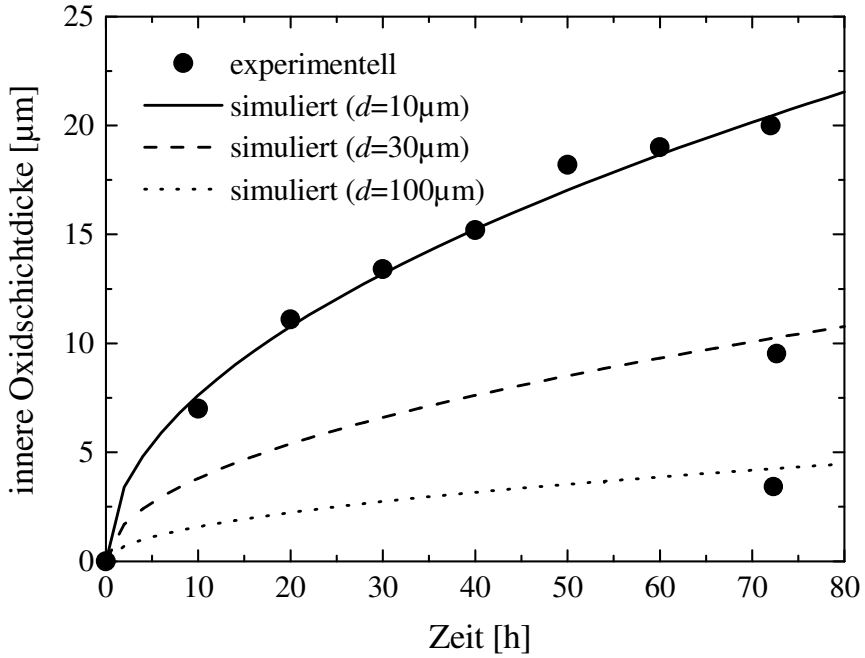

Fe2O3 [at.%]
1
0
-1
20
15
10
5
0
distance from outer/inner interface [µm]
0
10
20
lateral distance [µm]

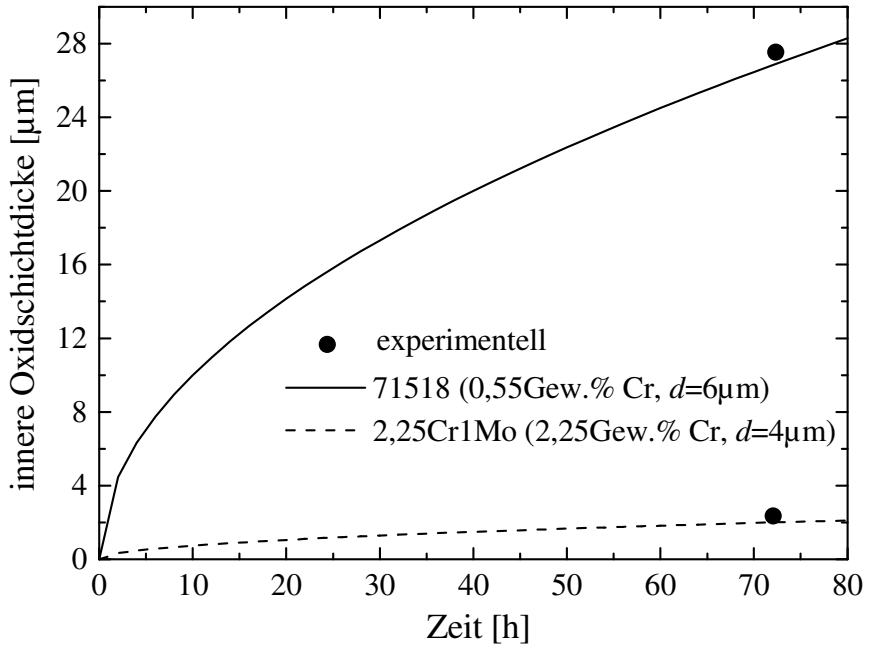




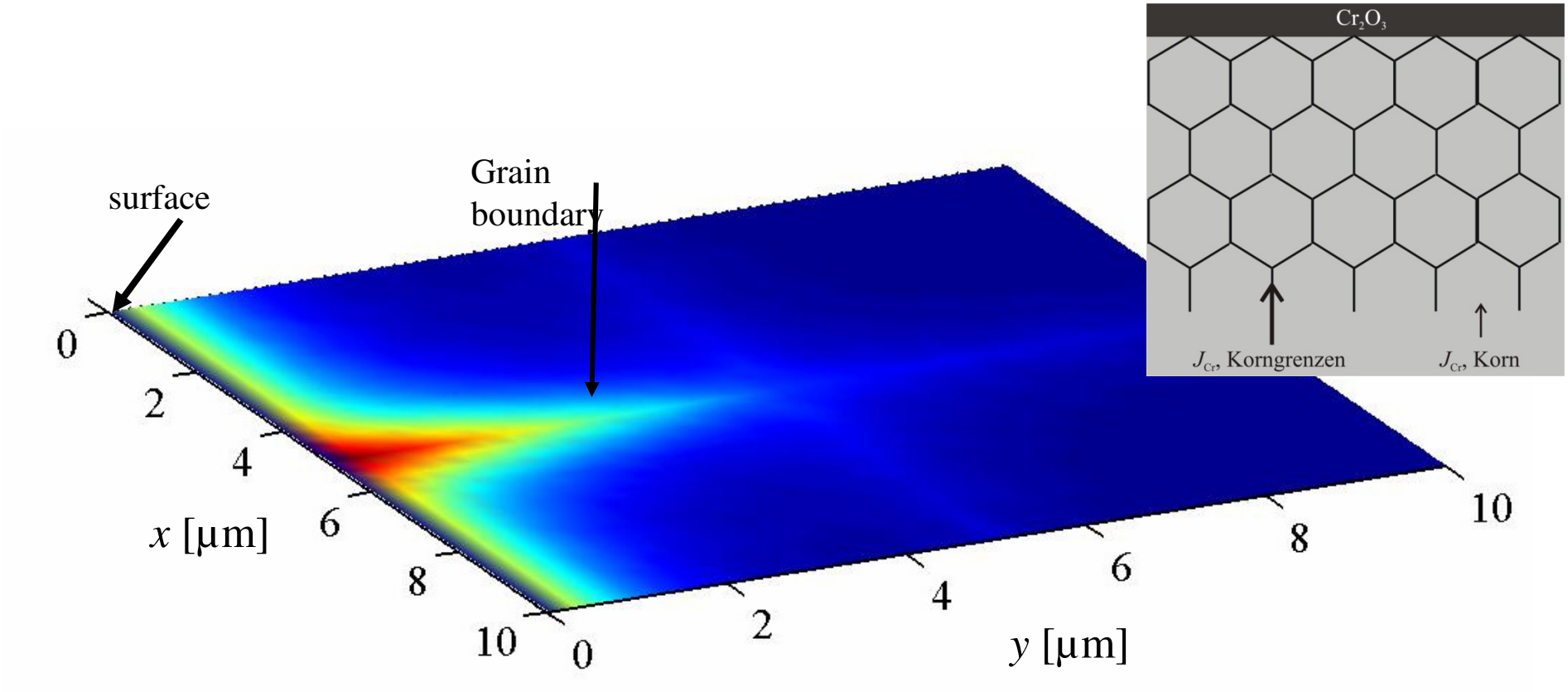
Duration = 270 hrs
T = 550°C
d = 30 µm
Lab air

Comparison of simulated and experimentally observed inner oxide thickness

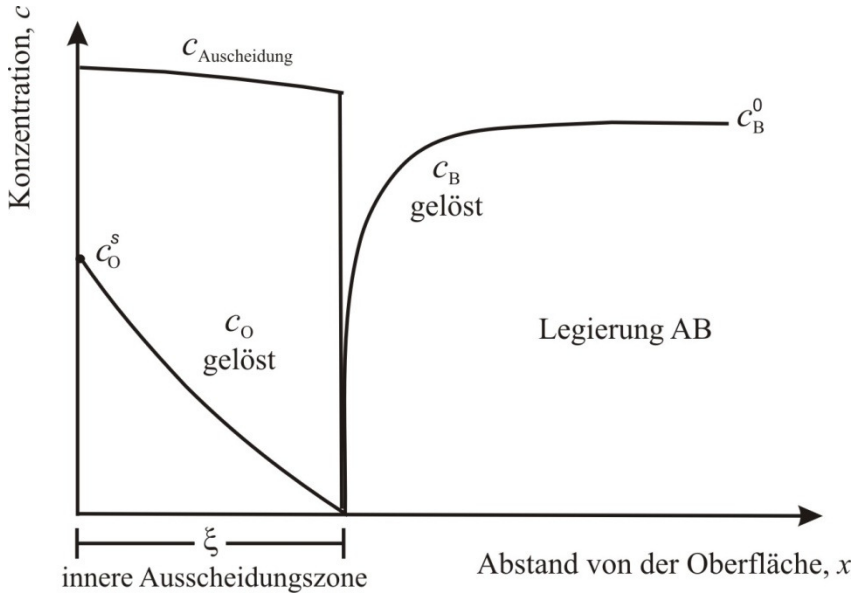


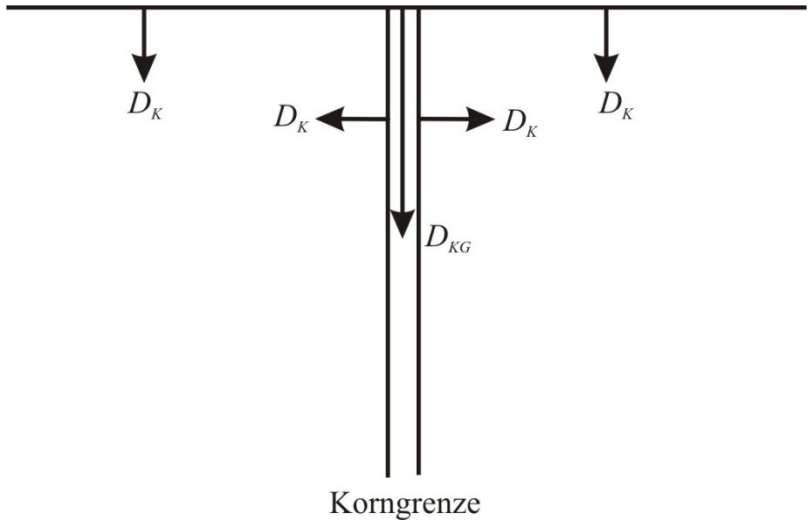


Simulation of Cr-enrichment along grain boundaries of substrate on a fine austenitic stainless steel TP347 (d = 5 µ m) at T = 750oC

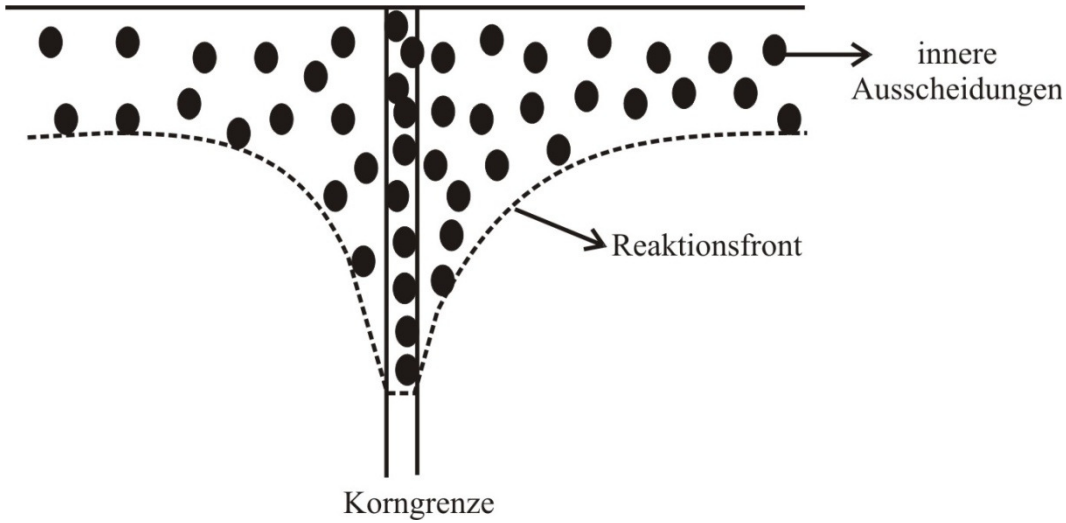


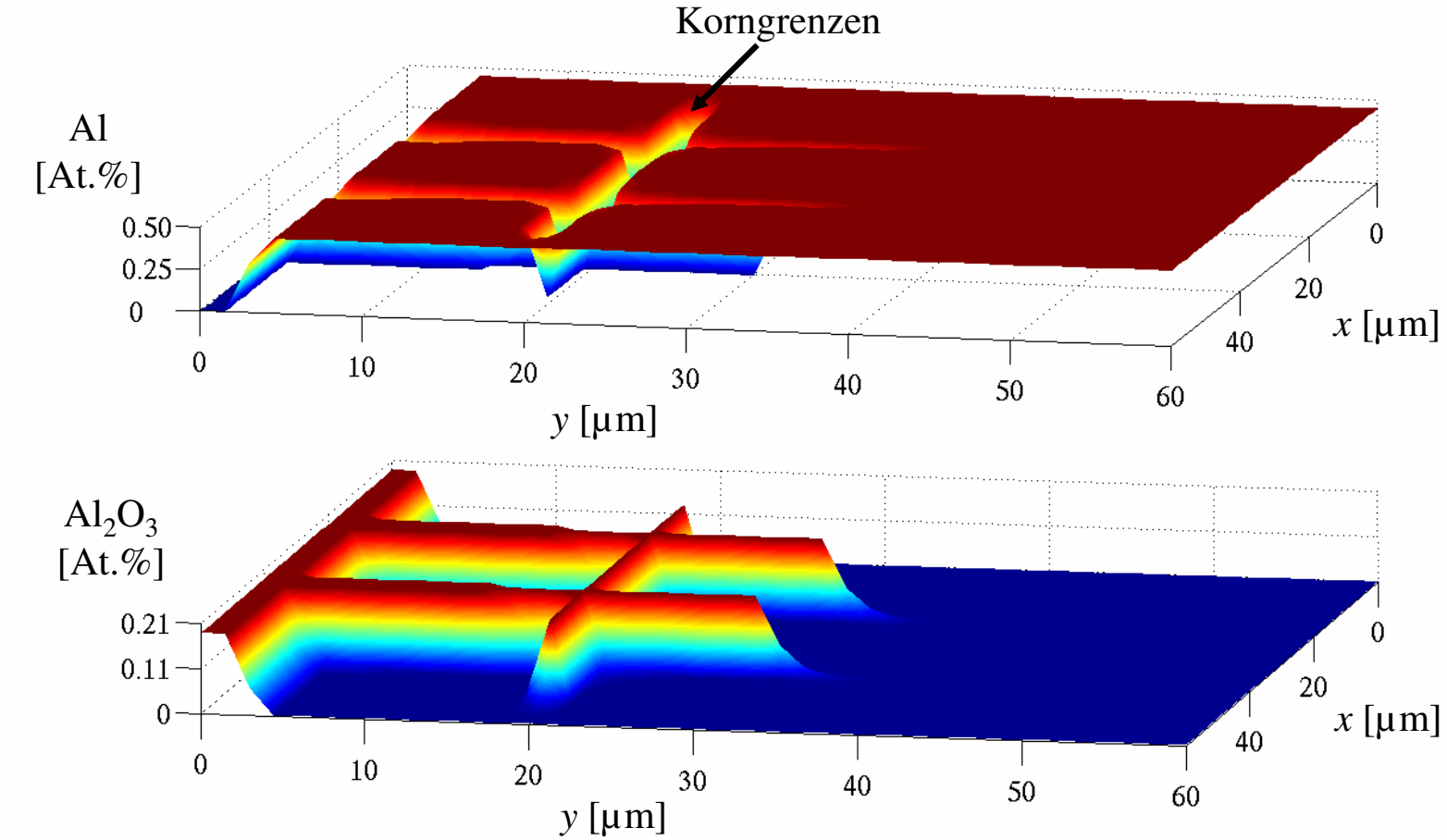
Classical case



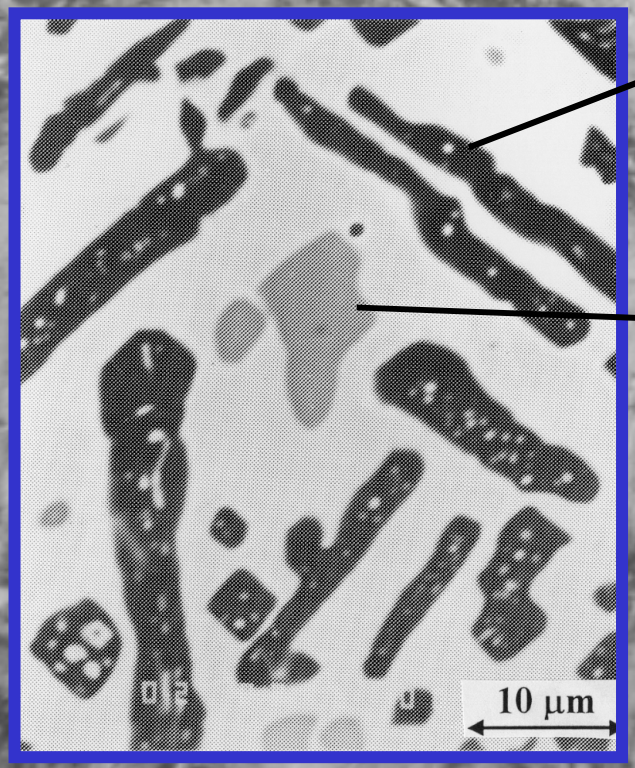


Planar reactions front



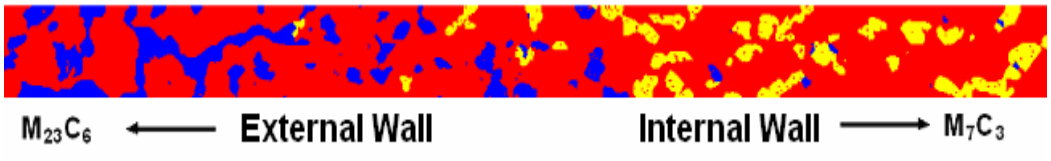

Korngrenzen
Al
[At.%]
0.50
0.25
0
0
10
20
30
40
50
60
y [µm]
0
20
40
x [µm]
Al2O3
[At.%]
0.21
0.11
0
0
10
20
30
40
50
60
y [µm]
0
20
40
x [µm]

Carburization of Austenitic Steels

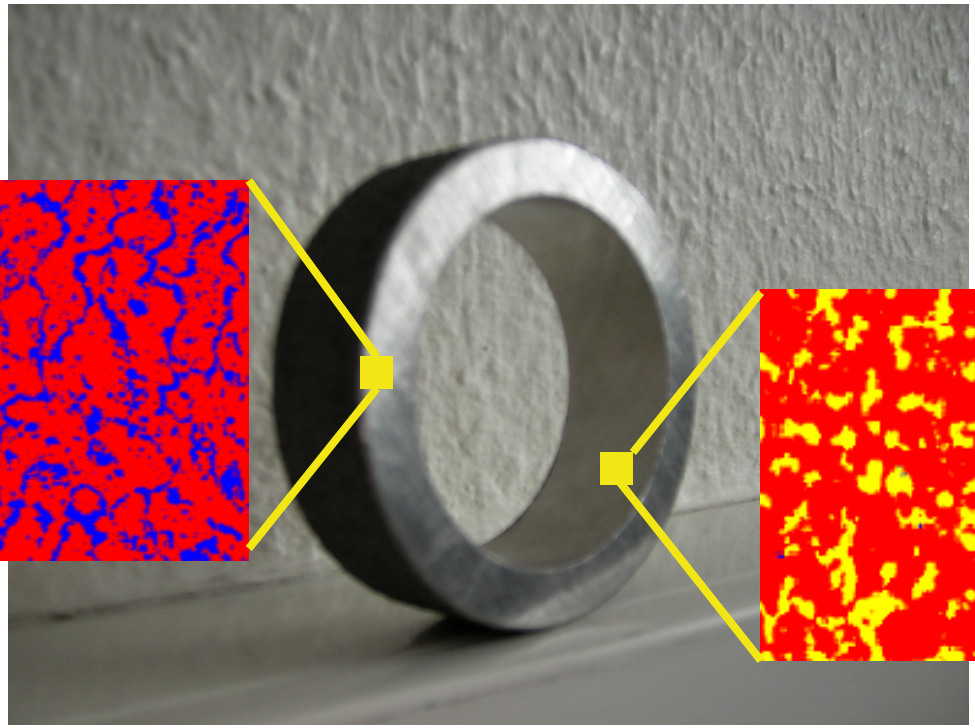


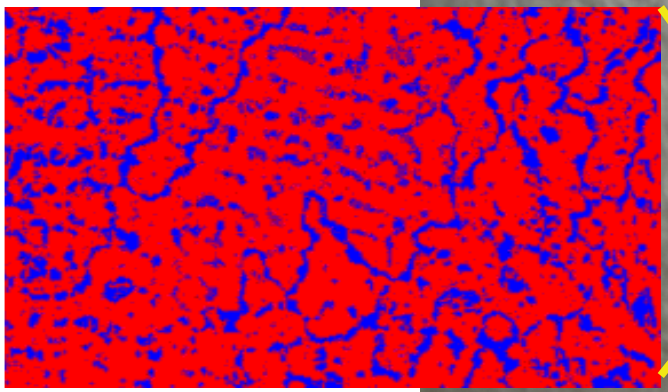
HP steel, pyrolyse furnace

EBSD-Characterization

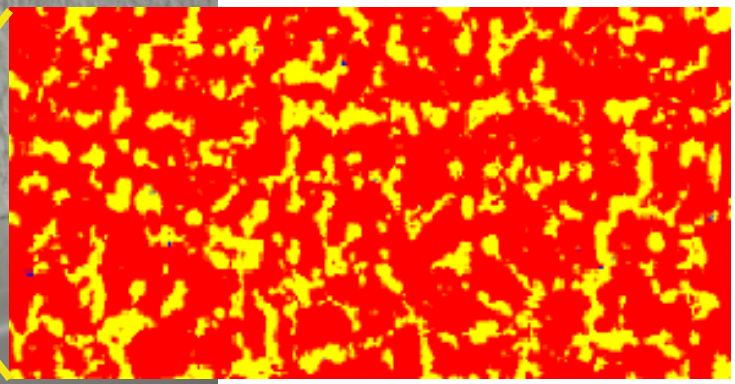


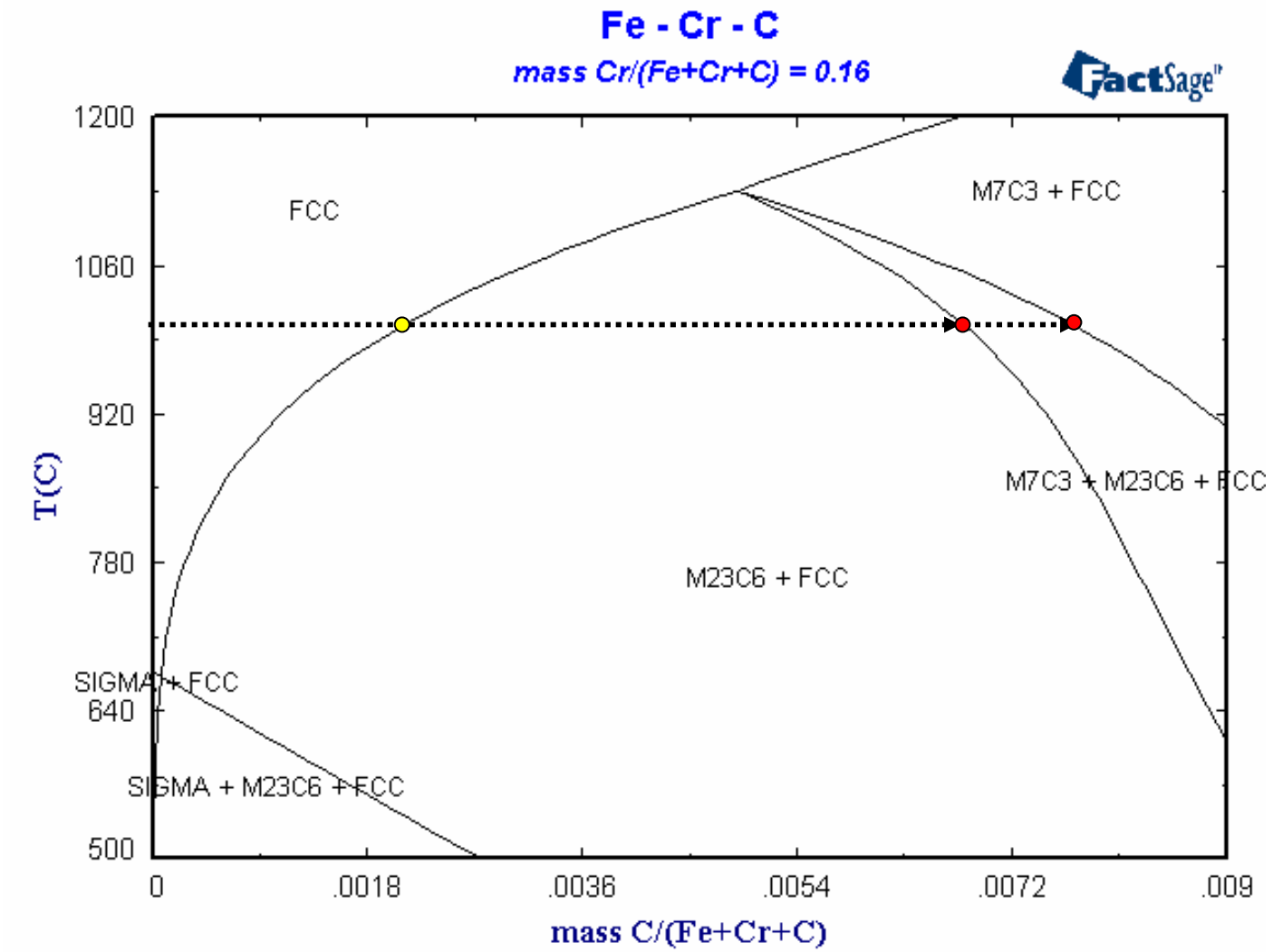
$M_{23}C_6$





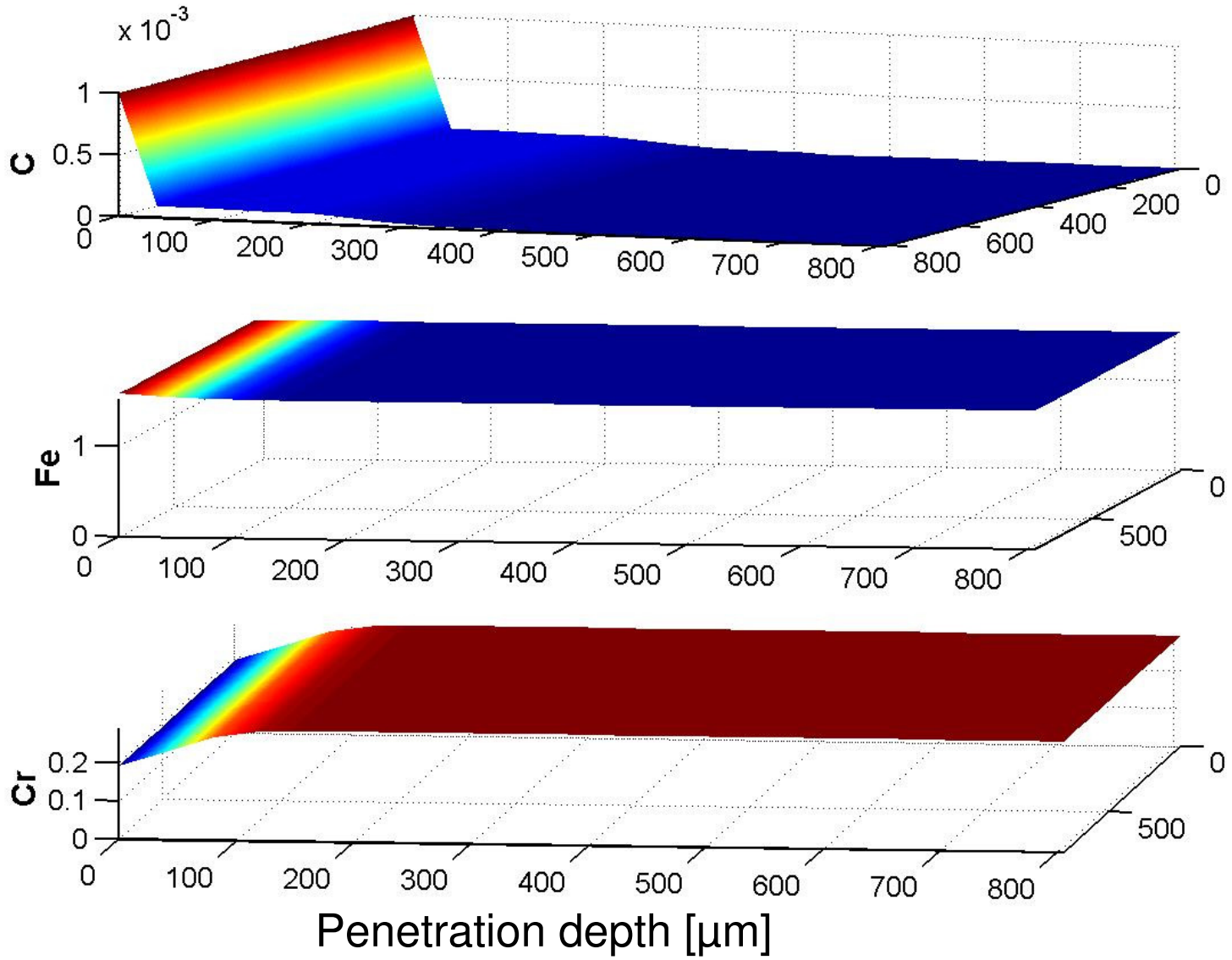
M_7C_3




Fe - Cr - C
mass Cr/(Fe+Cr+C) = 0.16
FactSage
1200
1060
920
780
640
500
T(C)
FCC
M7C3 + FCC
M7C3 + M23C6 + FCC
M23C6 + FCC
SIGMA + FCC
SIGMA + M23C6 + FCC
0
.0018
.0036
.0054
.0072
.009
mass C/(Fe+Cr+C)

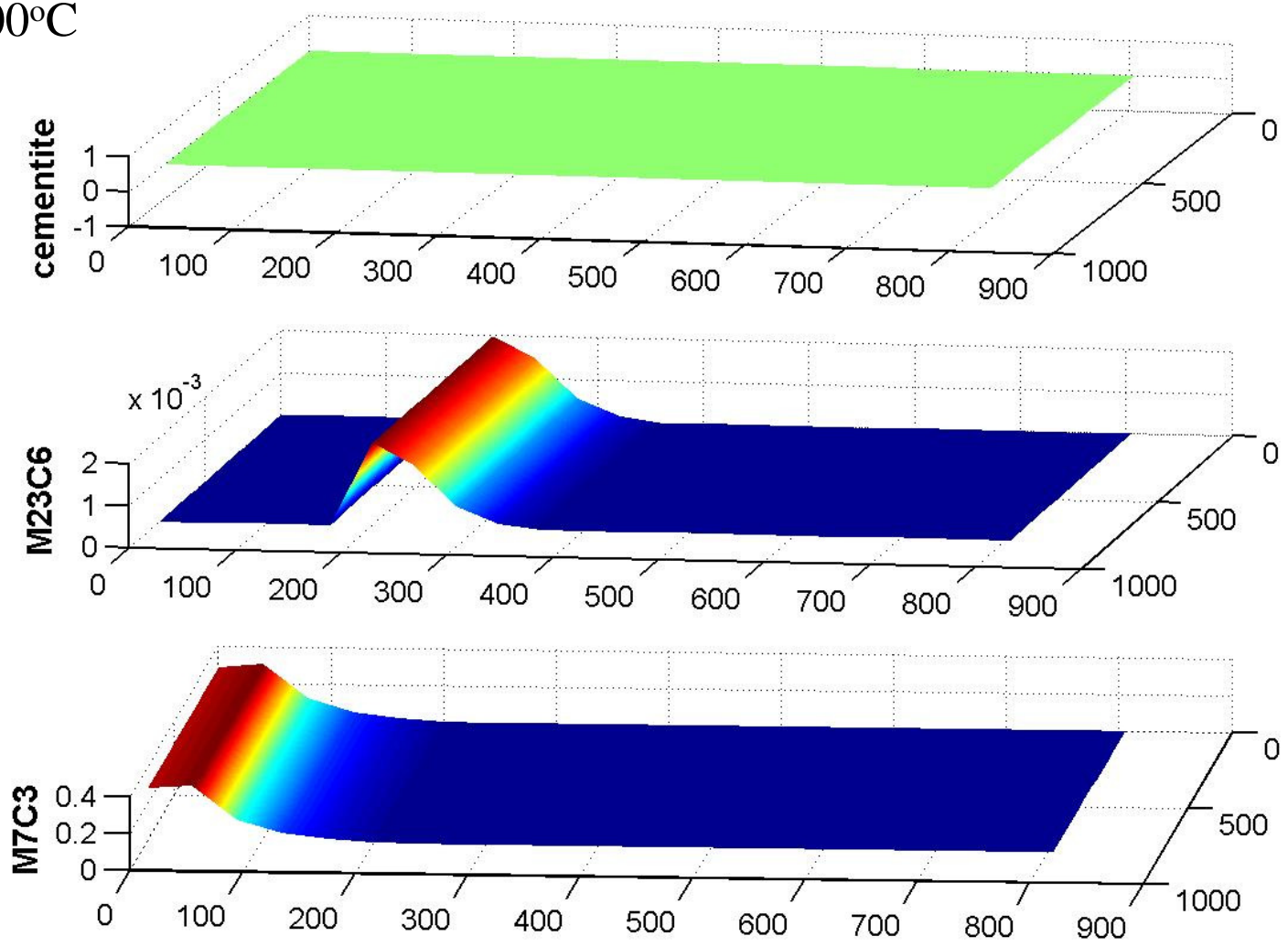
time = 100h
T = 1000°C

Calculation with InCorr



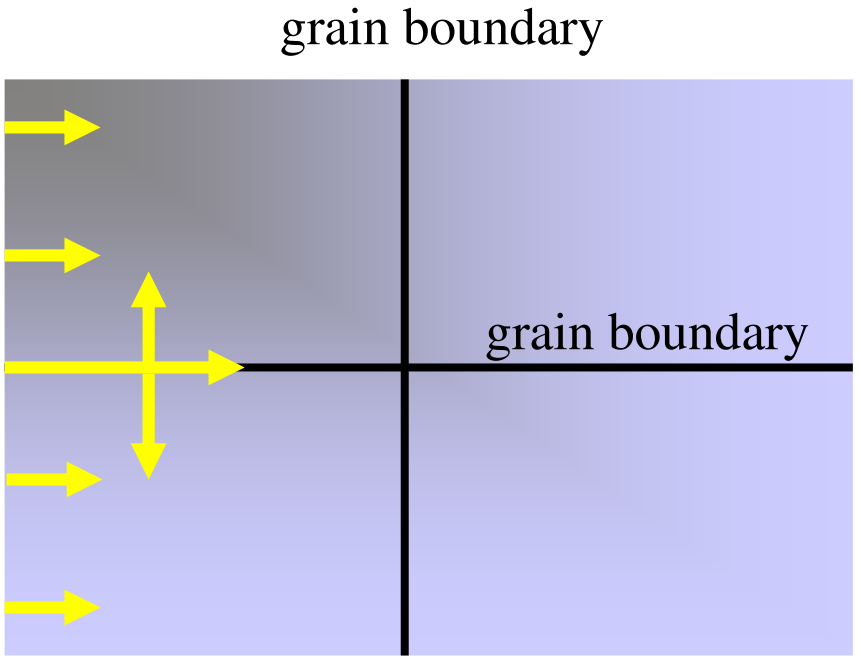
time = 100h
T = 1000°C

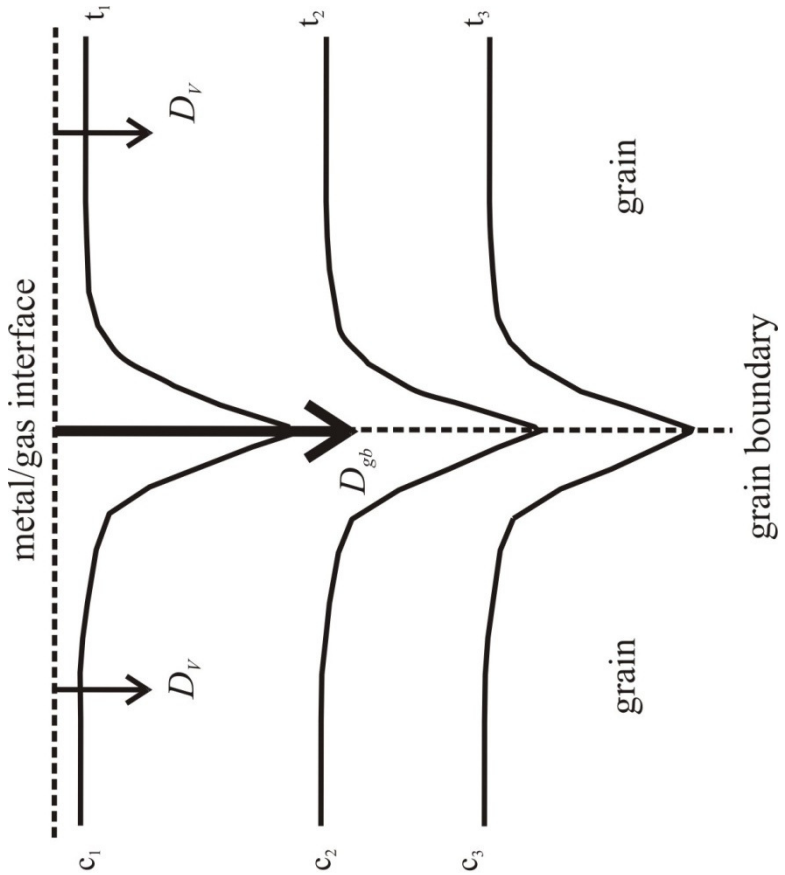
Calculation with InCorr



Penetration depth [µm]

Themodynamics + Kinetics (InCorr)

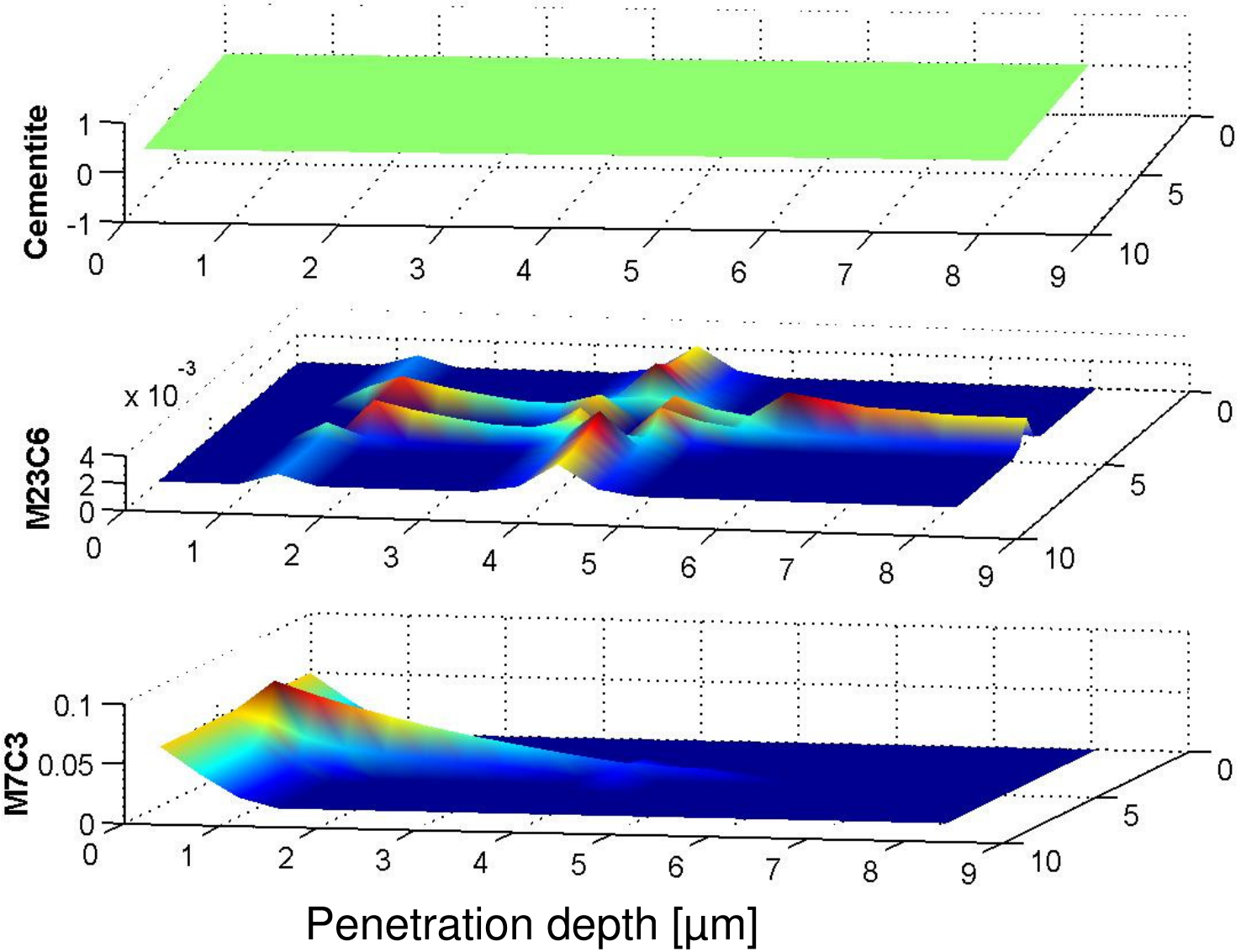




iso-concentration curves

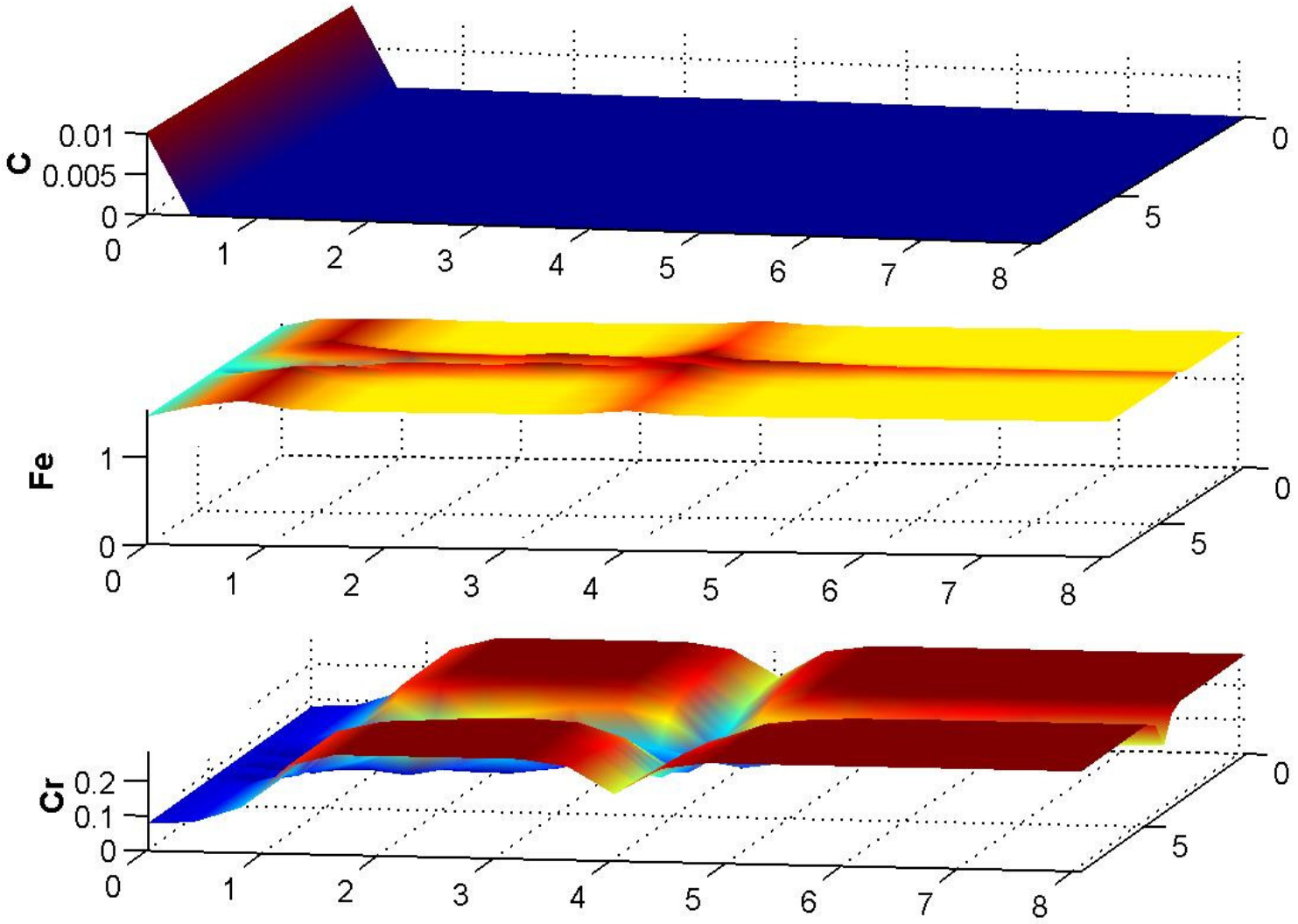
time = 10h
T = 800°C

Calculation with InCorr



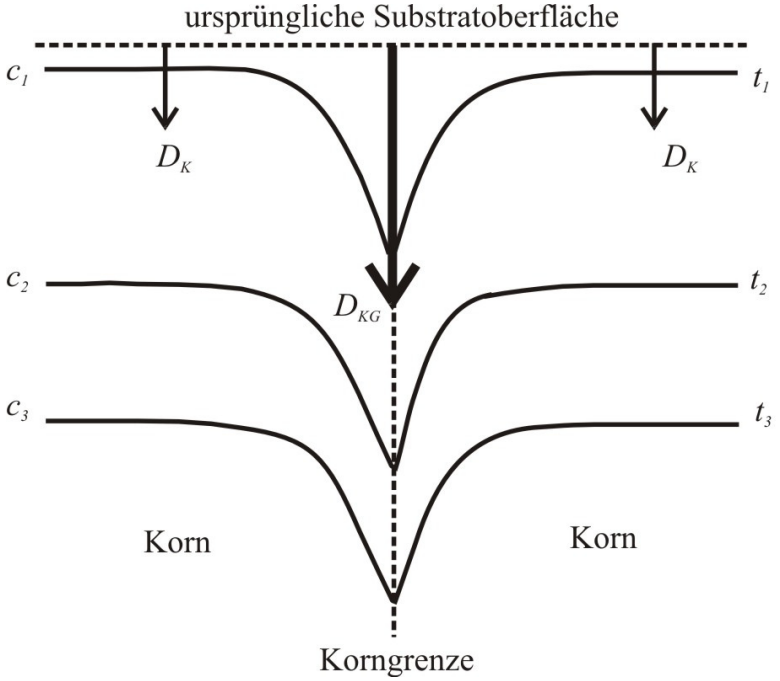
time = 10h
T = 800°C

Calculation with InCorr

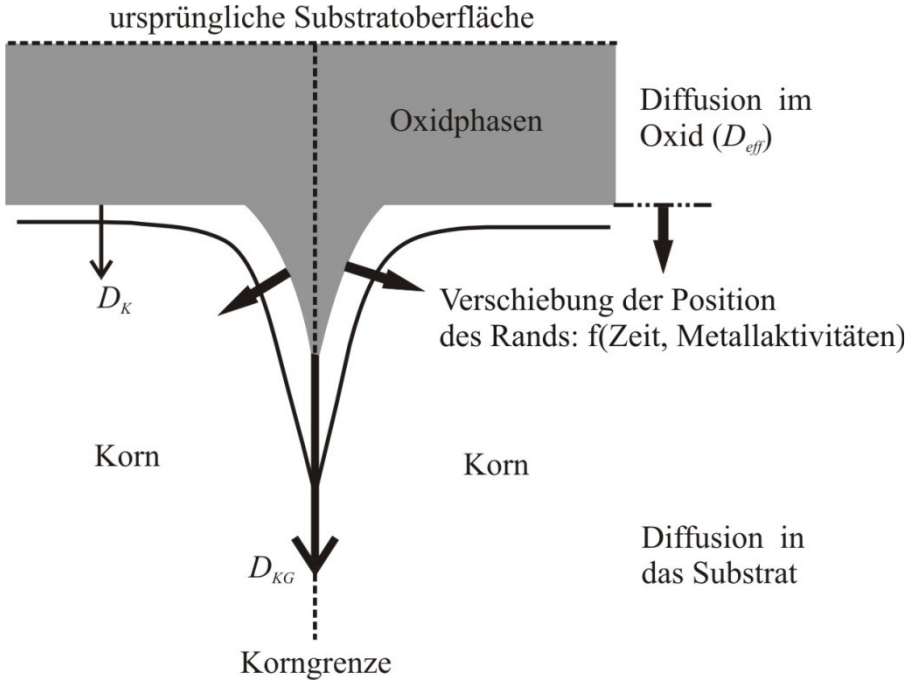


Penetration depth [µm]

Inner layer growth

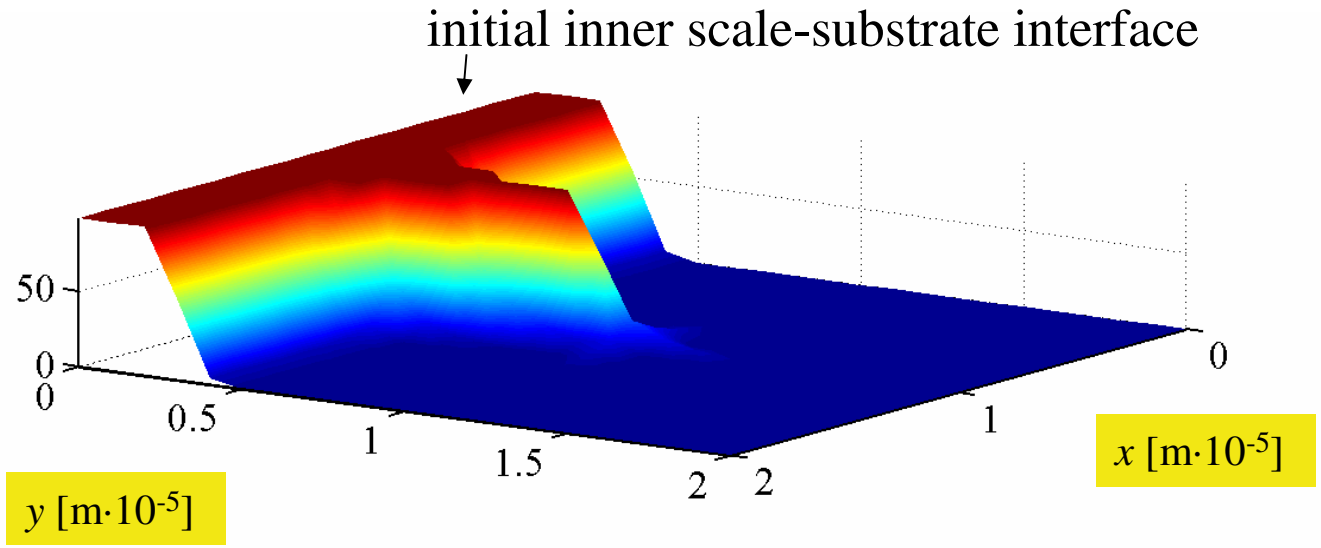


Diffusion in das Substrat

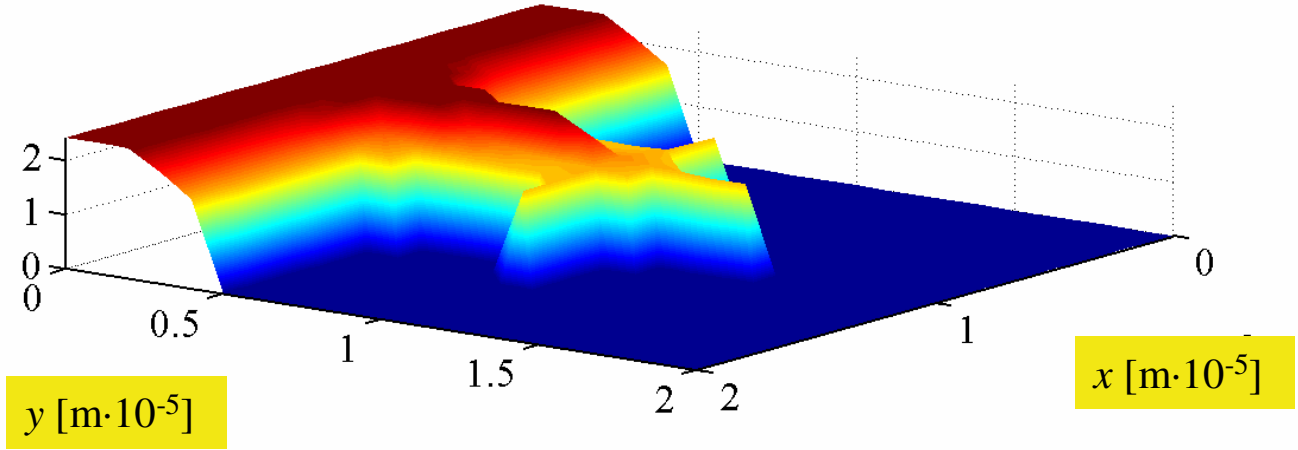


$$D_{eff} = \frac{\xi^2}{t\left[\ln\left(p(O_2)Fe_3O_4\right) - \ln\left(p(O_2)FeCr_2O_4\right)\right]}$$

Fe_3O_4



$FeCr_2O_4$



InCorr

Recent work and future aspects

- Converting from Linux to Windows environment.
- Matlab, ChemApp can work in windows
- Now PVM is also available in windows
- Addition of outward scale growth
- Simulating the effect of shotpeening effect in InCorr
- Effect of water vapour on oxidation

Conclusions

oxidation and internal nitridation of steels

carburization of steels

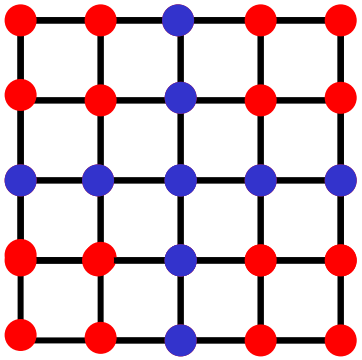
The developed software **InCorr** is capable to account for:
local thermodynamic equilibrium,
solid state diffusion and alloy microstructure

It can be calculated: concentration profiles of C, Cr, Fe, etc.
mass gain as a function of time

The high performance of the developed software ***InCorr*** is sustained by a solid theoretical background.

Now InCorr is available in Windows platform.So it is easy to carry Incorr with you.

Moving Interface Condition and Diffusion Matrix



$$D_{i,j} = \begin{pmatrix} D11 & D12 & D13 & D14 & D15 \\ D21 & D22 & D23 & D24 & D25 \\ D31 & D32 & D33 & D34 & D35 \\ D41 & D42 & D43 & D44 & D45 \\ D51 & D52 & D53 & D54 & D55 \end{pmatrix}$$

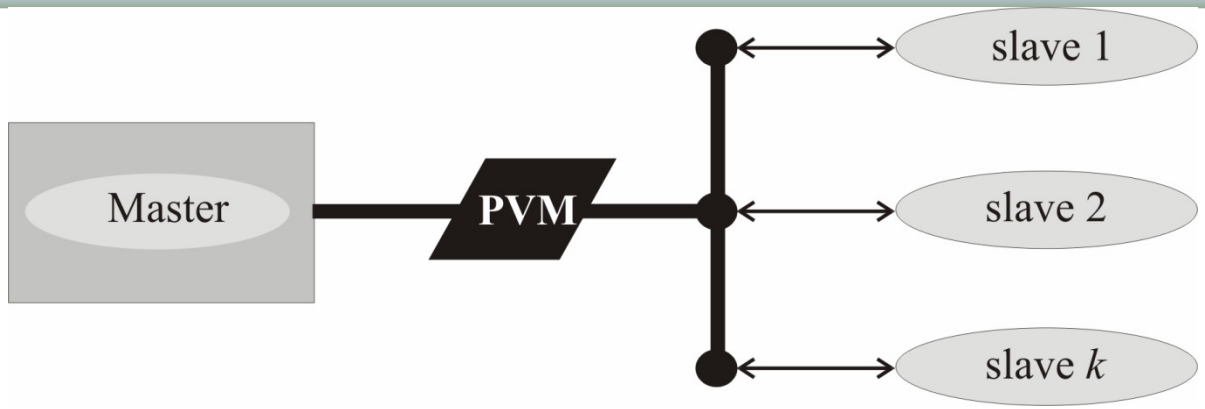
time = 100 h
dimension = 1 mm^2

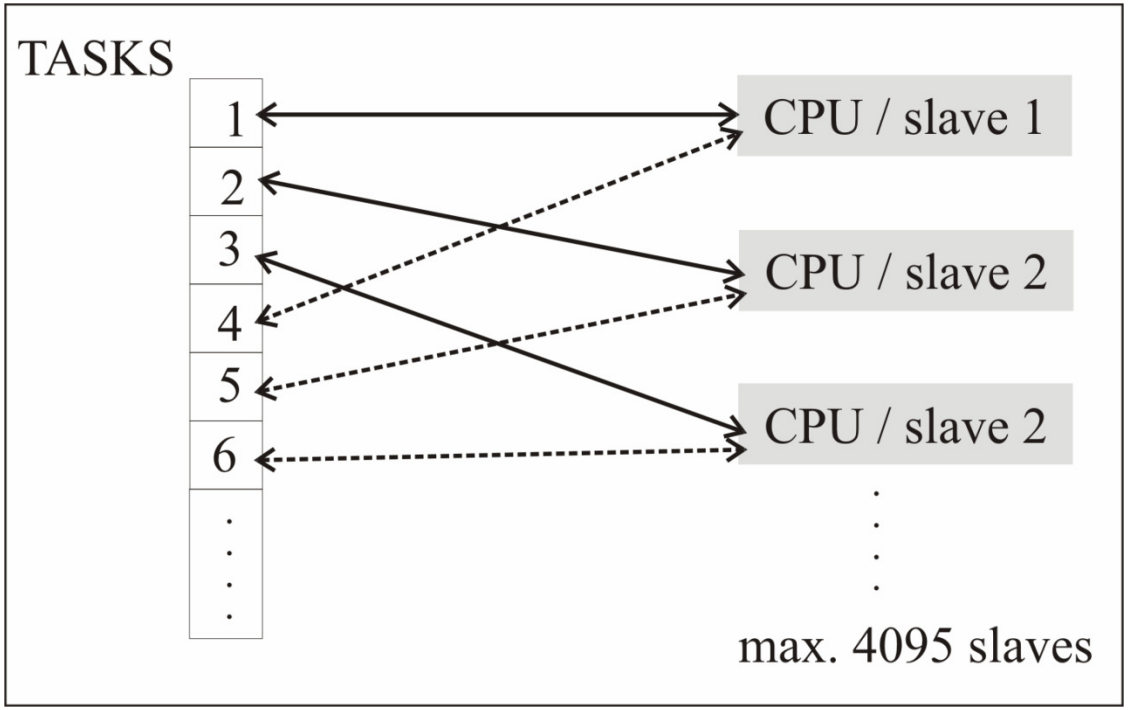
$\Delta x = \Delta y = 0.1\ \mu m$
nx = ny = 10 000
$\Delta t = 1$ s
nt = 360 000

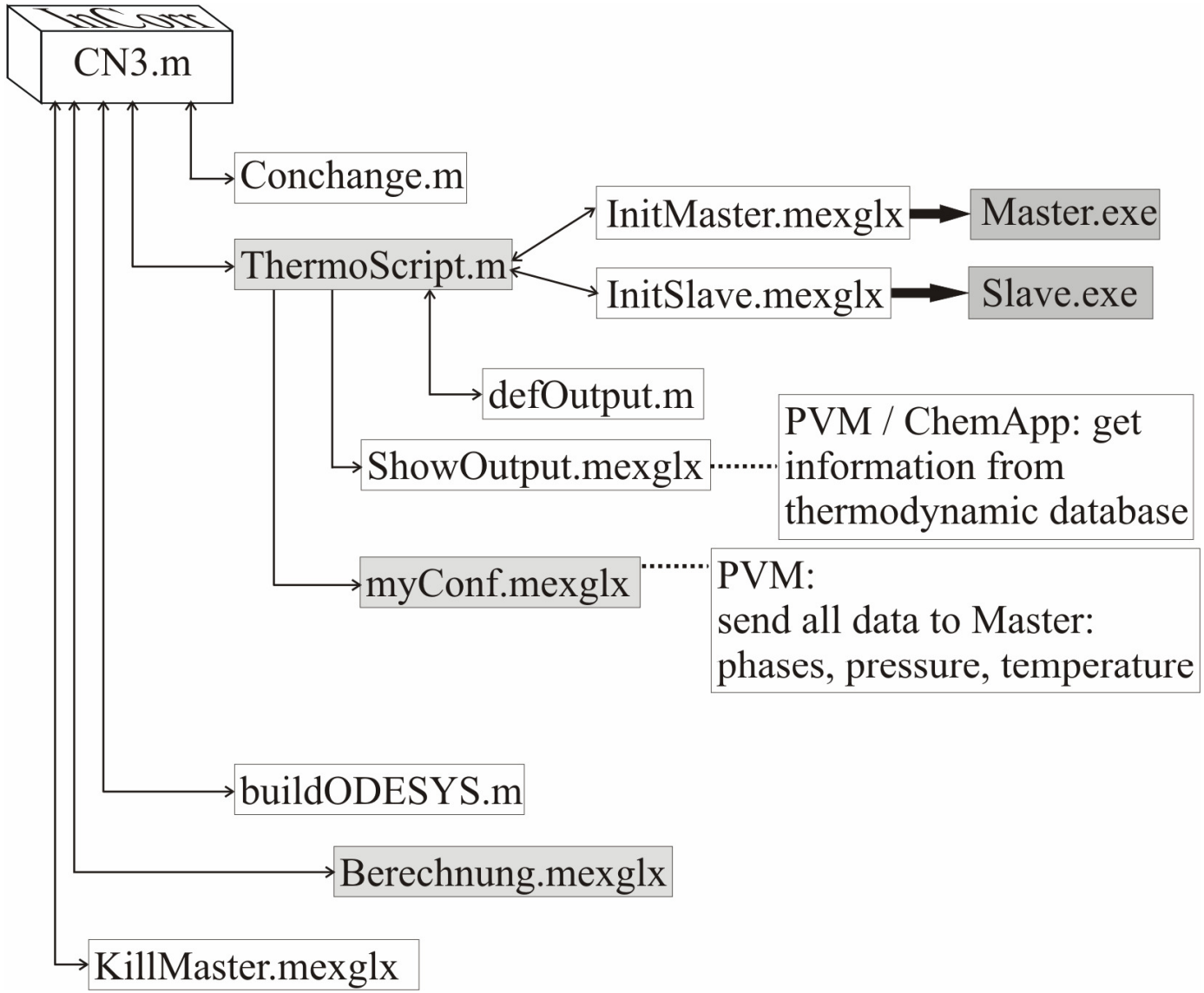
$D_{i,j} =$

- Dx = Dy if (i,j) is not a gb and $c_{Fe} > 0$
- D_{gb} if (i,j) is a gb and $c_{Fe} > 0$
- D_{oxide} if in (i,j) $c_{Fe} = 0$

this must be checked 360 000 times at every (i,j)


Master
PVM
slave 1
slave 2
slave k


TASKS
1
2
3
4
5
6
CPU / slave 1
CPU / slave 2
CPU / slave 2
max. 4095 slaves


CN3.m
Conchange.m
ThermoScript.m
InitMaster.mexglx
Master.exe
InitSlave.mexglx
Slave.exe
defOutput.m
ShowOutput.mexglx
PVM / ChemApp: get information from thermodynamic database
myConf.mexglx
PVM:
send all data to Master:
phases, pressure, temperature
buildODESYS.m
Berechnung.mexglx
KillMaster.mexglx