

Phase Diagrams with FACTSage

Speaking different Languages for Thermochemical Properties

Michael Auinger



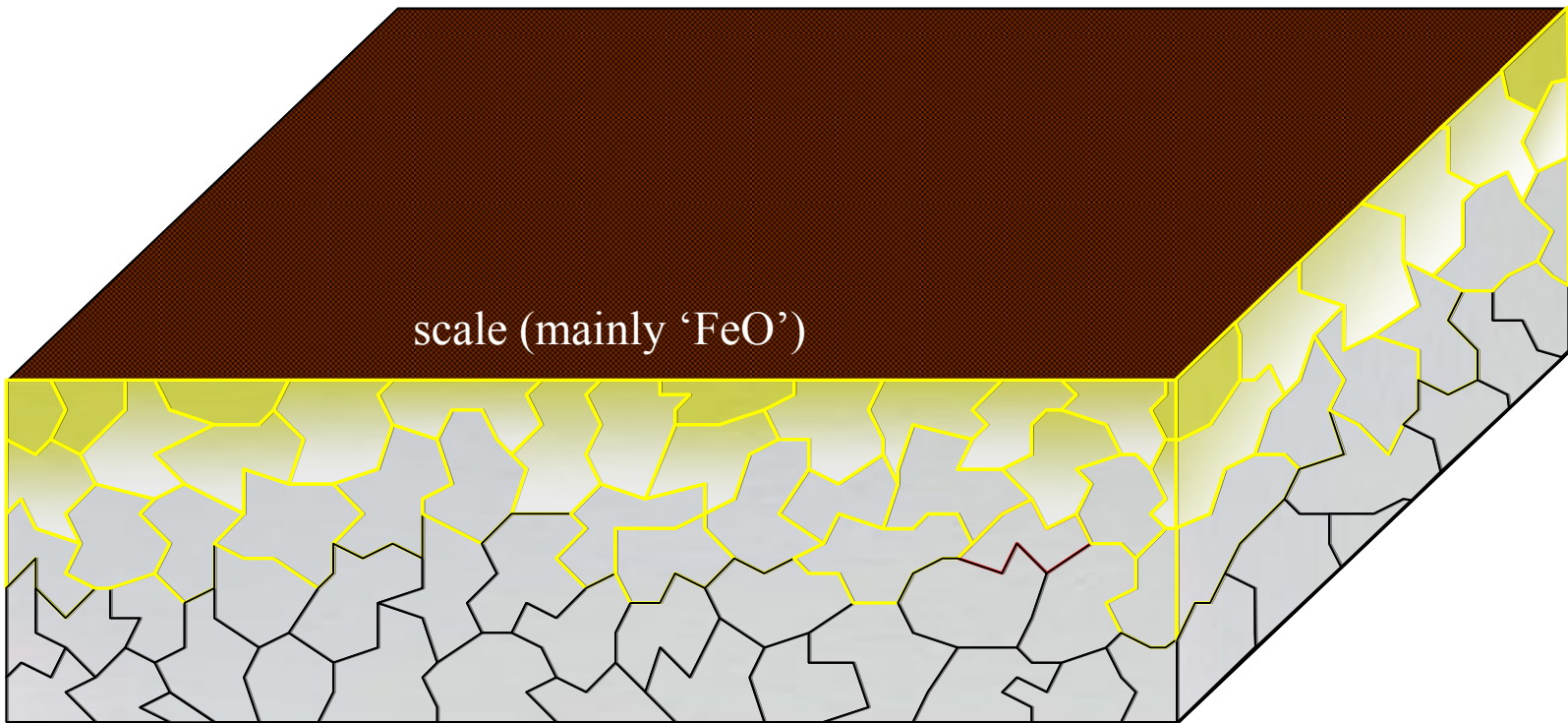
GTT-Technologies Annual Workshop and User's Meeting
Herzogenrath-Kohlscheid (Aachen, Germany)

5th July, 2013



- Motivation
- Thermochemical Properties in Oxides
 - Ellingham-Richardson Diagrams
 - Stability Diagrams
- Thermochemistry of Oxides and Nitrides
 - Nitrides in the System Iron - Chromium - Carbon
 - Nitrogen and Oxygen in Iron - Silicon
- Summary

Oxidation Processes in Steels



Grain Boundary Oxidation

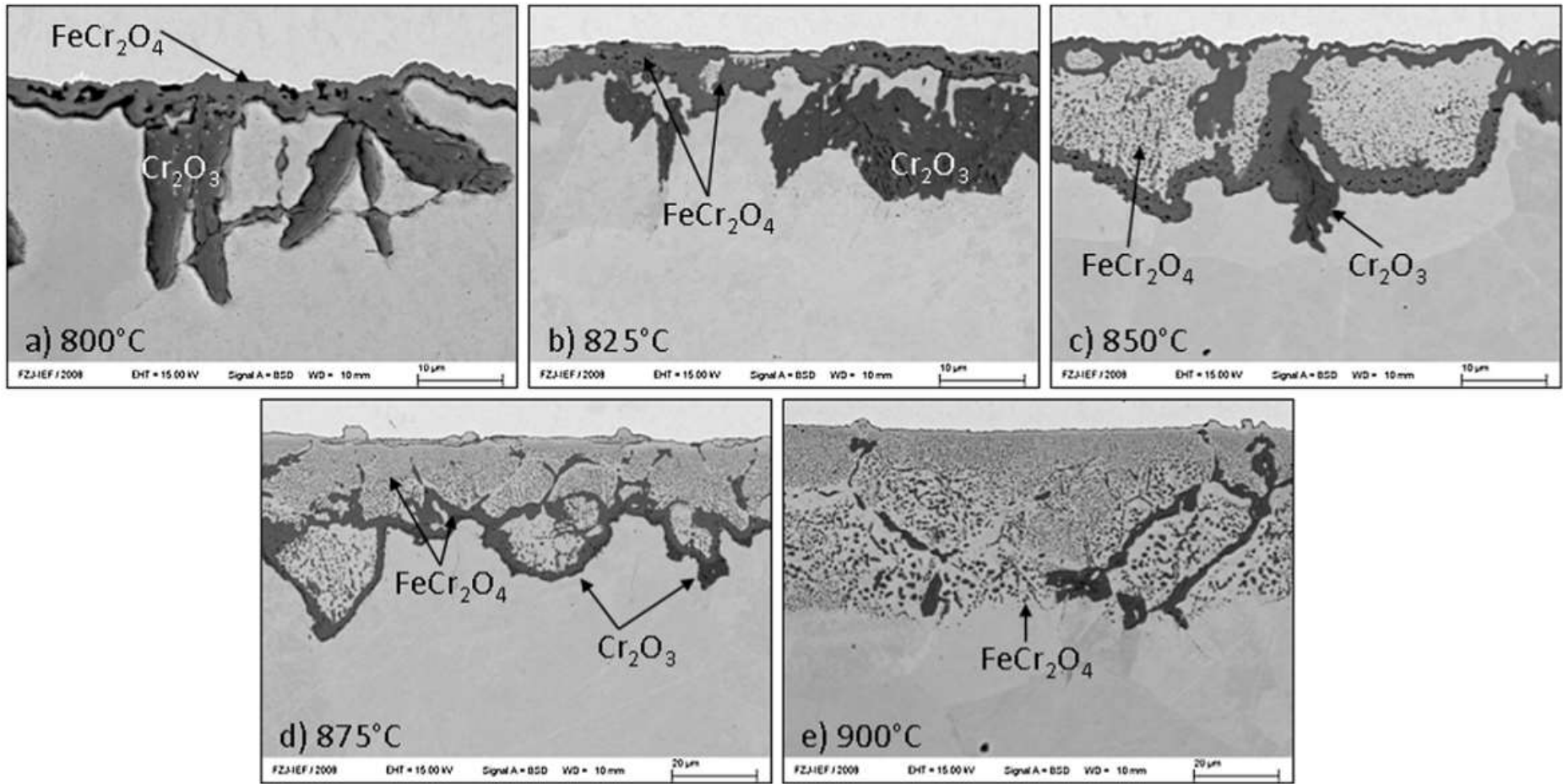
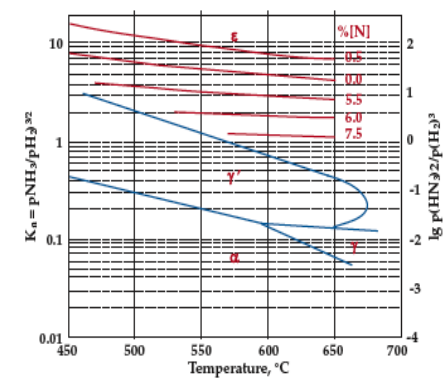
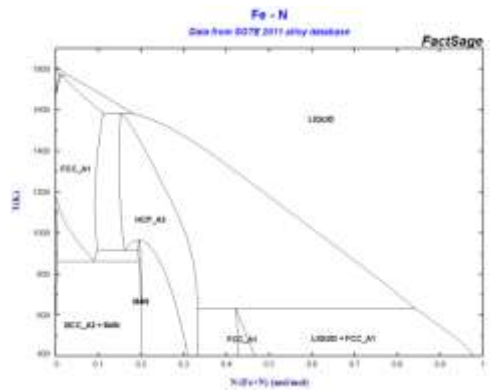
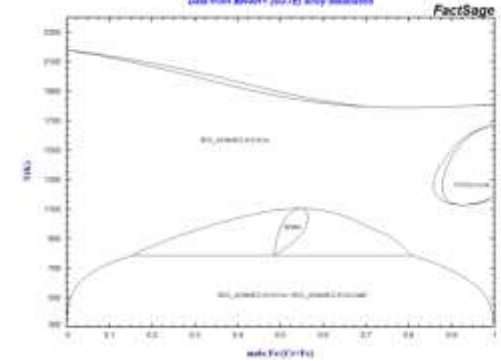
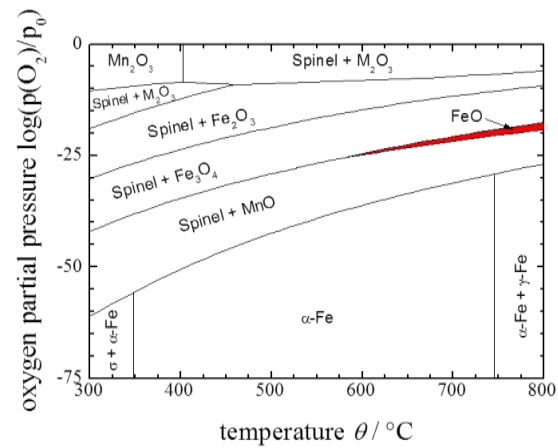
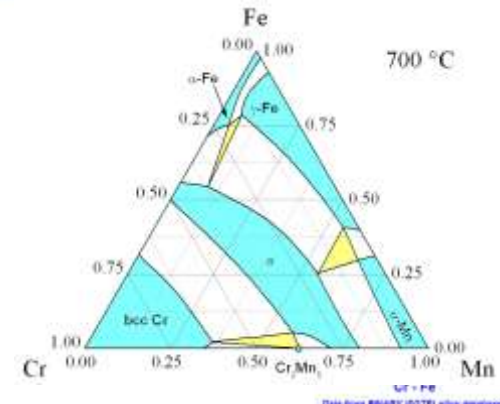
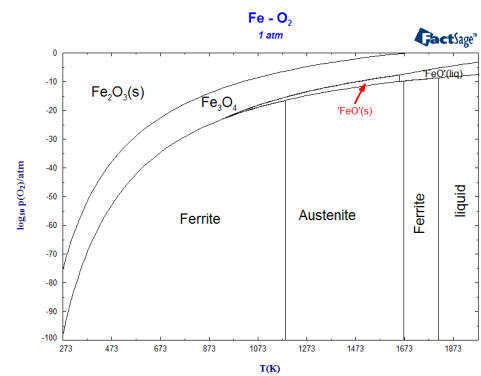
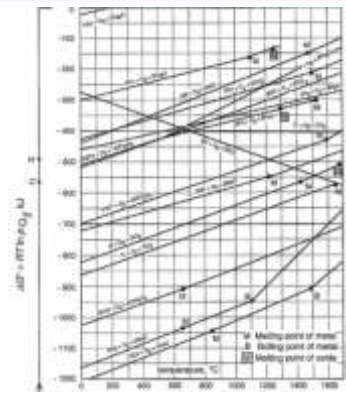
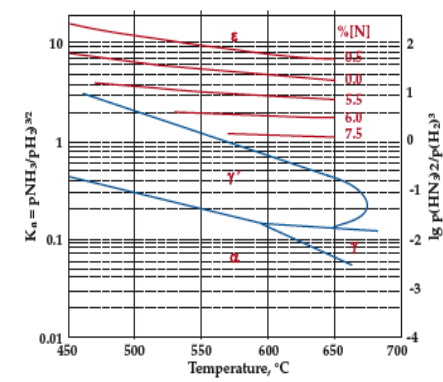
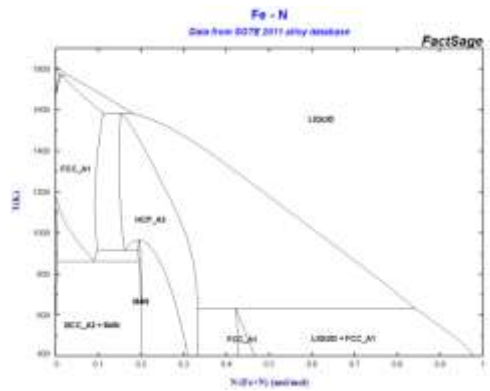
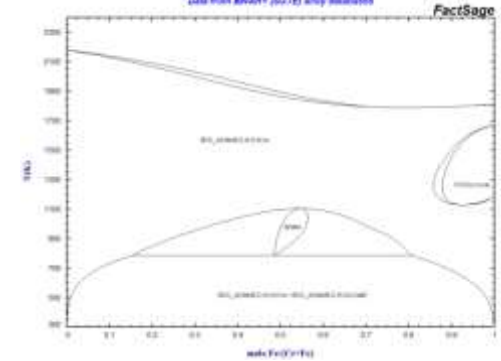
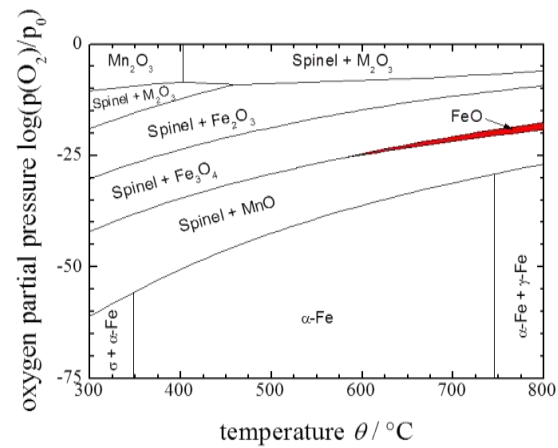
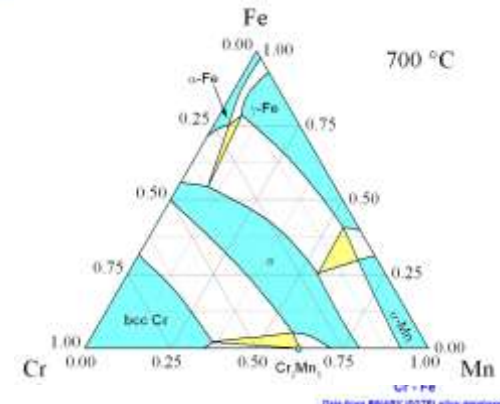
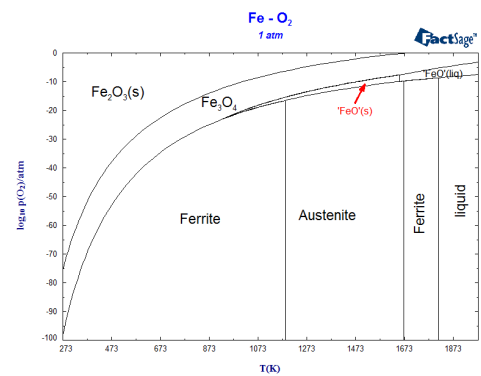
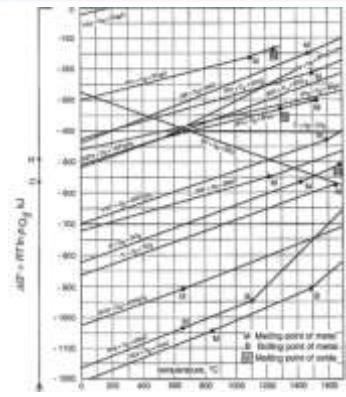


Figure 18. Cross-section SEM micrographs of Fe-10Cr after isothermal oxidation for 72 h at temperatures between 800 and 900 °C in Ar-4% H_2 -2% H_2O

The Problem



The Problem



„আমি তাপগতিবিদ্যা
পছন্দ“

„Мне нравится
термодинамики“

„أنا أحب الديناميكا
الحرارية“



„我喜歡熱力學“

„Μου αρέσει
θερμοδυναμική“

„나는 열역학을
좋아“

„আমি তাপগতিবিদ্যা
পছন্দ“

„Мне нравится
термодинамики“



„أنا أحب الديناميكا
الحرارية“

„我喜歡熱力學“

„Μου αρέσει
θερμοδυναμική“

„나는 열역학을
좋아“

„আমি তাপগতিবিদ্যা
পছন্দ“

„Мне нравится
термодинамики“

„أنا أحب الديناميكا
الحرارية“



„我喜歡熱力學“

„Μου αρέσει
θερμοδυναμική“

„나는 열역학을
좋아“



Part I

Thermochemical Properties of Oxides

Ellingham Diagram

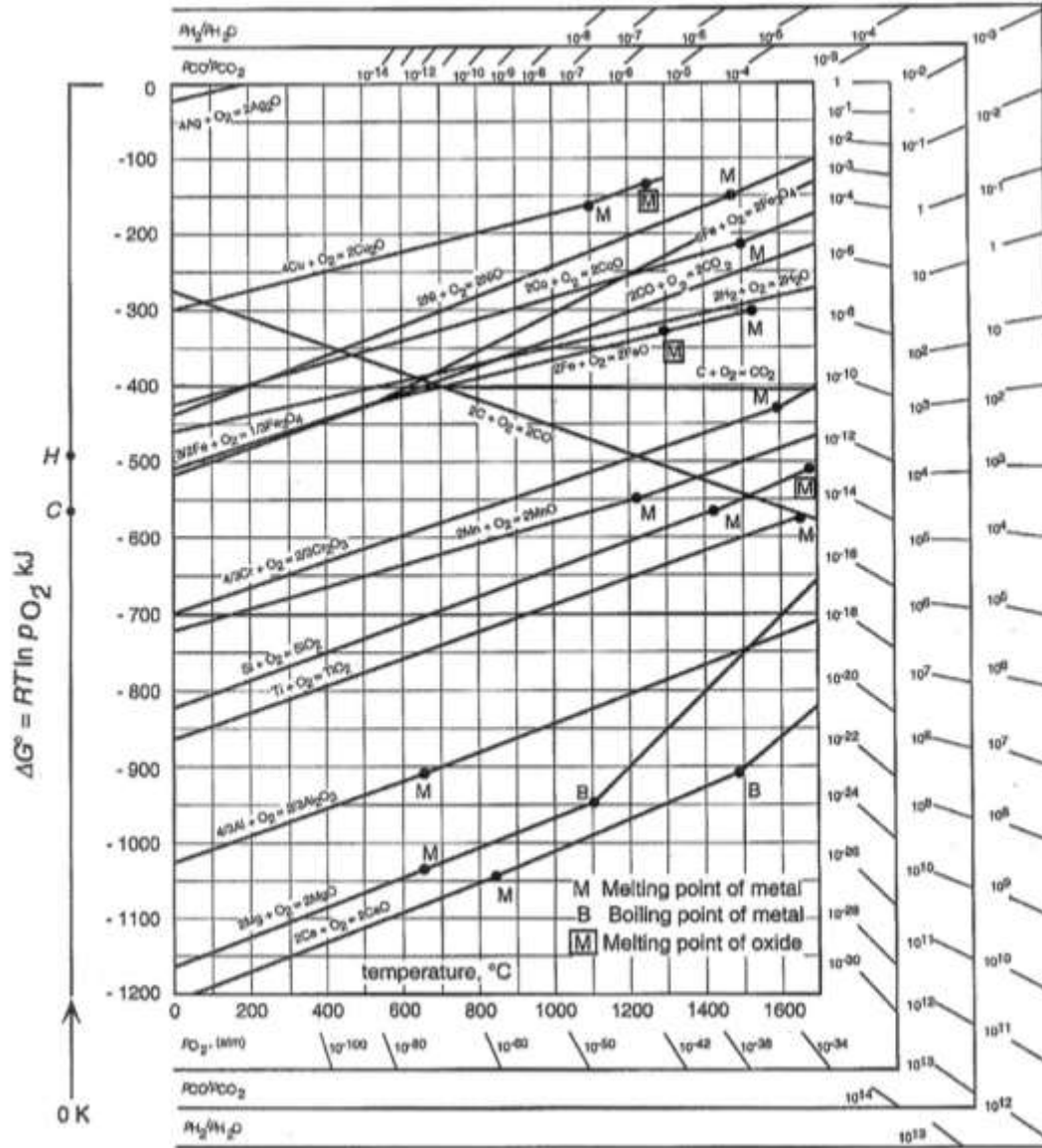
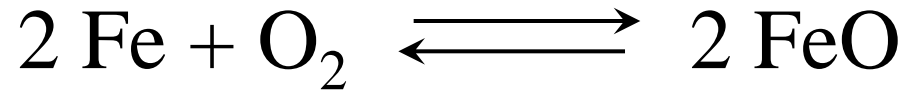


Figure 12.13 The Ellingham diagram for selected oxides.

Ellingham Diagram with FACTSage



$$-2 G_{(T)}^{o, \text{FeO}} + 2 G_{(T)}^{o, \text{Fe}} + G_{(T)}^{o, \text{O}_2} = -R \ln \left(\frac{p_{\text{O}_2}}{p_o} \right) T$$

Menu - Phase Diagram: last system

File Units Parameters Variables Help

T(K) P(atm) Energy(J) Mass(mol) Vol(litre)

Components [2]

Variables: Fe-O2 R(T/K)ln p(O2)/bar (J) vs T(K)

Variables

compositions 0

RTln(a) 1

Y steps: 50

X steps: 50

Next >>

T and P

Temperature

T(K) X-axis

Max: 1973

Min: 273

Pressure or Volume

P(atm) constant

log P

V(litre) 1

log V

Chemical Potentials

#1 R(T/K)ln(p/bar) Y-axis

O2 0

gas -1200000

Cancel OK

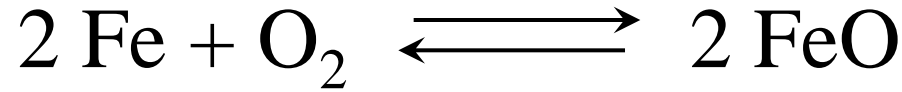
T(K)	RTln(p(O2))			
273	1973	-1200000	0	

RTln p(O2) vs T(K)

Calculate >>

FactSage 6.3

Ellingham Diagram with FACTSage



$$-2 G_{(T)}^{o, \text{FeO}} + 2 G_{(T)}^{o, \text{Fe}} + G_{(T)}^{o, \text{O}_2} = -R \ln \left(\frac{p_{\text{O}_2}}{p_o} \right) T$$

Menu - Phase Diagram: last system

File Units Parameters Variables Help

T(K) P(atm) Energy(J) Mass(mol) Vol(litre)

Components [2]

Variables: Fe-O2 R(T/K)ln p(O2)/bar (J) vs T(K)

Variables

compositions 0

RTln(a) 1

Next >>

T and P

Temperature

T(K) X-axis

Max: 1973

Min: 273

Pressure or Volume

P(atm) constant

log P

V(litre) 1

log V

Chemical Potentials

#1 R(T/K)ln(p/bar) Y-axis

O2 0

gas -1200000

Cancel OK

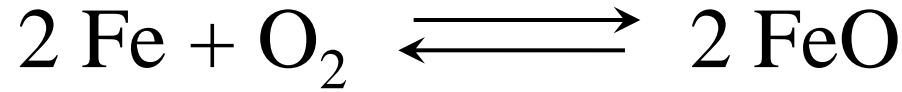
T(K)	RTln(p(O2))			
273	1973	-1200000	0	

RTln p(O2) vs T(K)

Calculate >>

FactSage 6.3

Ellingham Diagram with FACTSage



$$-2 G_{(T)}^{o, \text{FeO}} + 2 G_{(T)}^{o, \text{Fe}} + G_{(T)}^{o, \text{O}_2} = -R \ln \left(\frac{p_{\text{O}_2}}{p_o} \right) T$$

Menu - Phase Diagram: last system

File Units Parameters Variables Help

T(K) P(atm) Energy(J) Mass(mol) Vol(litre)

Components [2]

Variables: Fe-O2 R(T/K)ln p(O2)/bar (J) vs T(K)

Variables

compositions 0

RTln(a) 1

Next >>

T and P

Temperature

T(K) X-axis

Max: 1973

Min: 273

1/TK

Press

log

log

log

Chemical Potentials

#1 R(T/K)ln(p/bar) Y-axis

O2 0

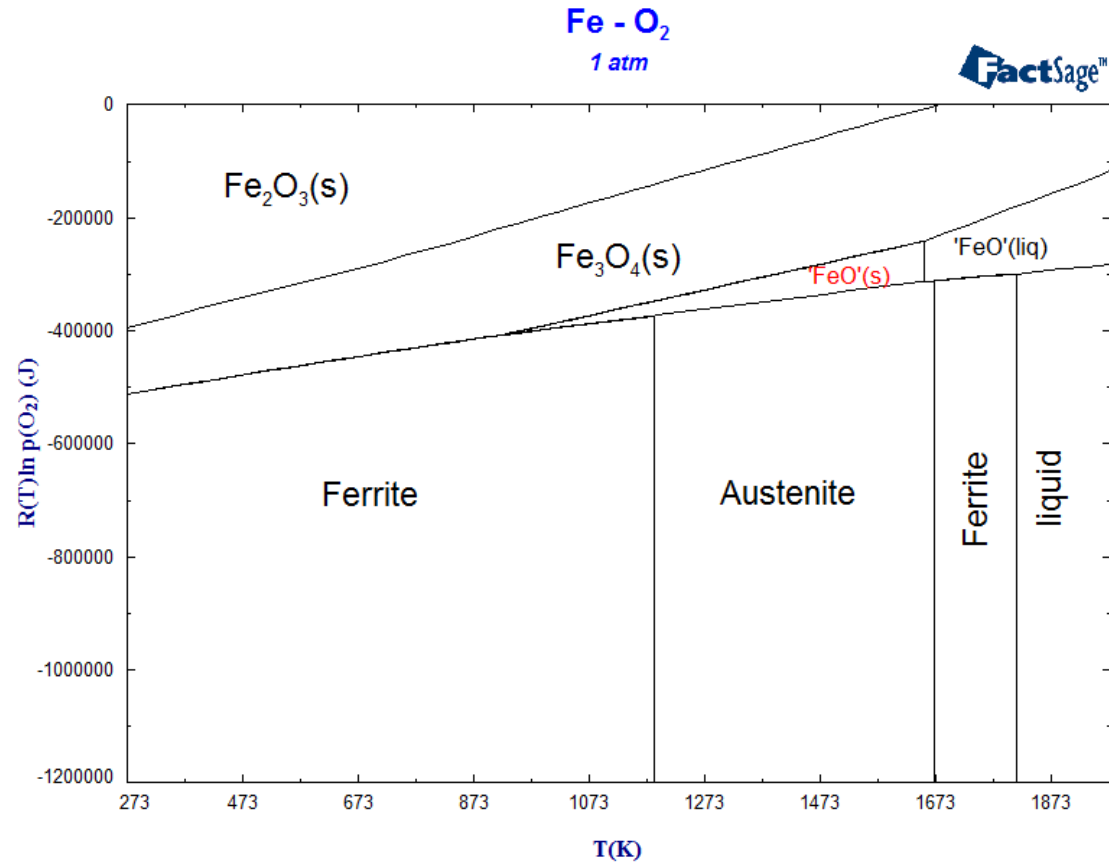
gas -1200000

Cancel

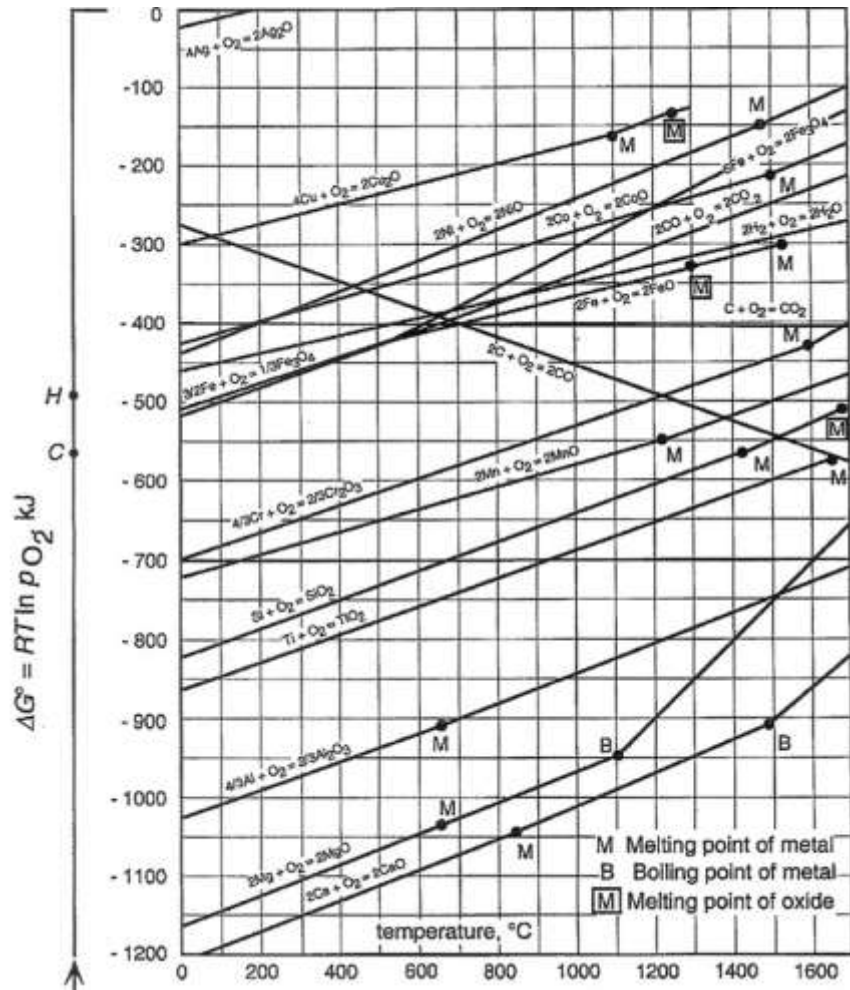
T(K)	RTln(p(O2))
273	1973
	-1200000

RTln p(O2) vs T(K)

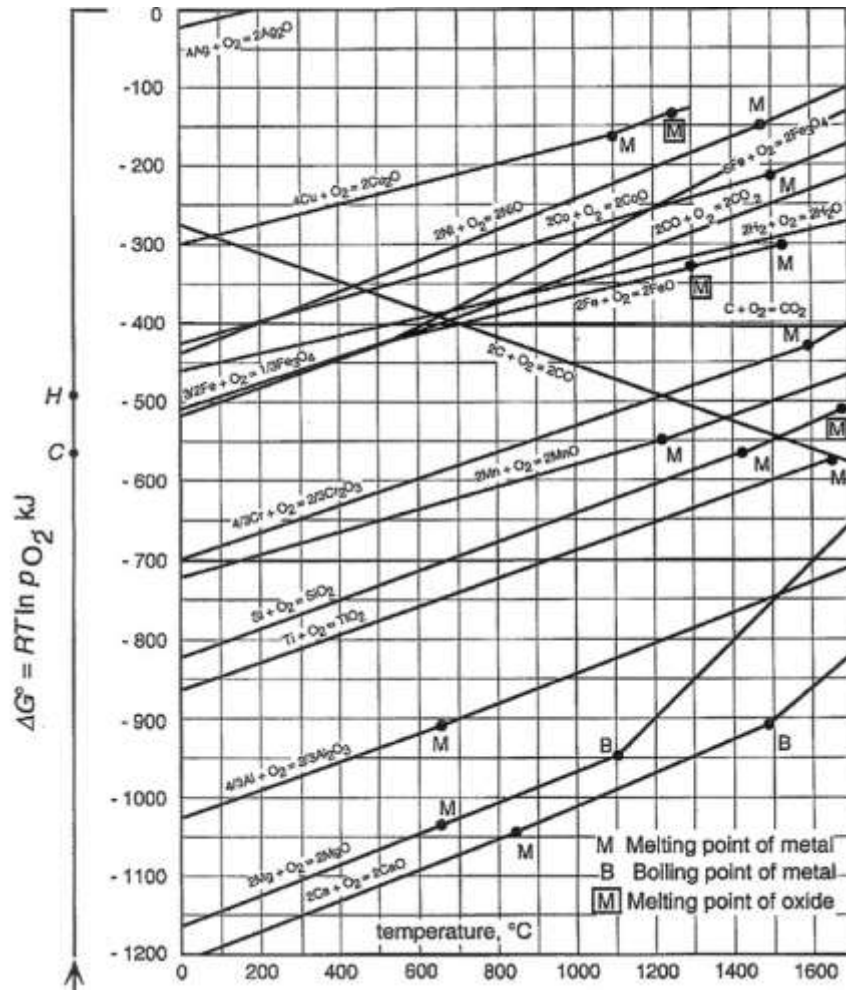
FactSage 6.3



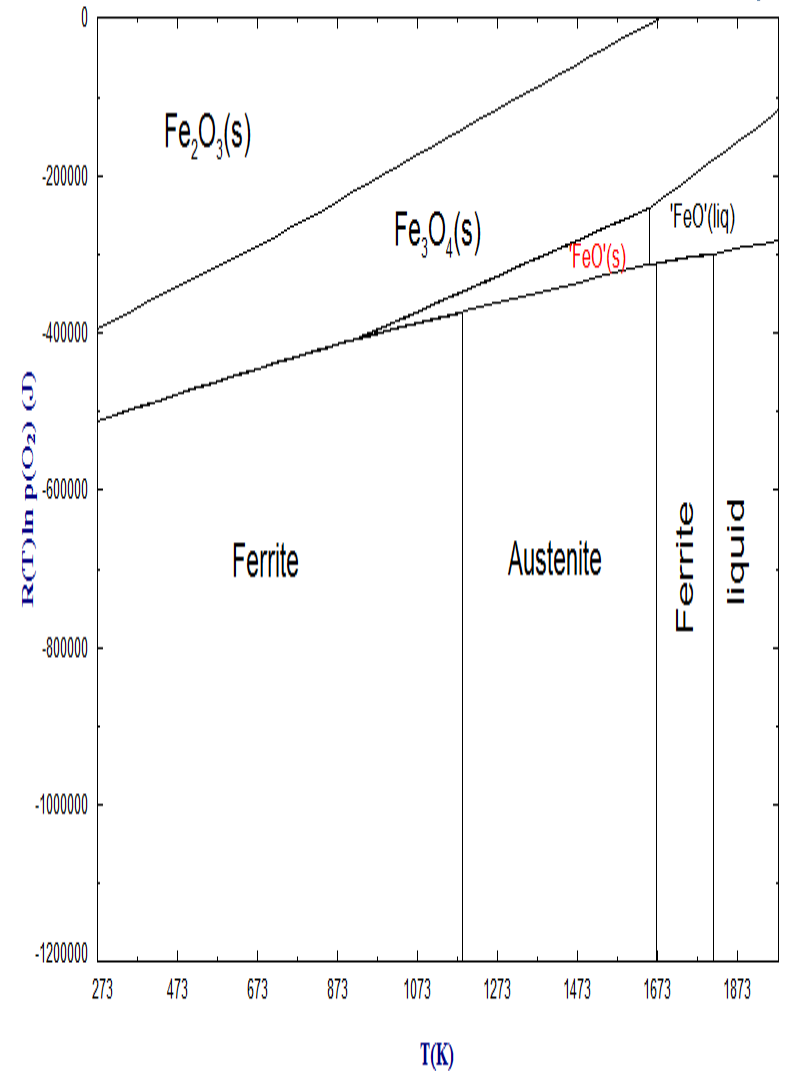
Ellingham Diagrams for Oxide Formation



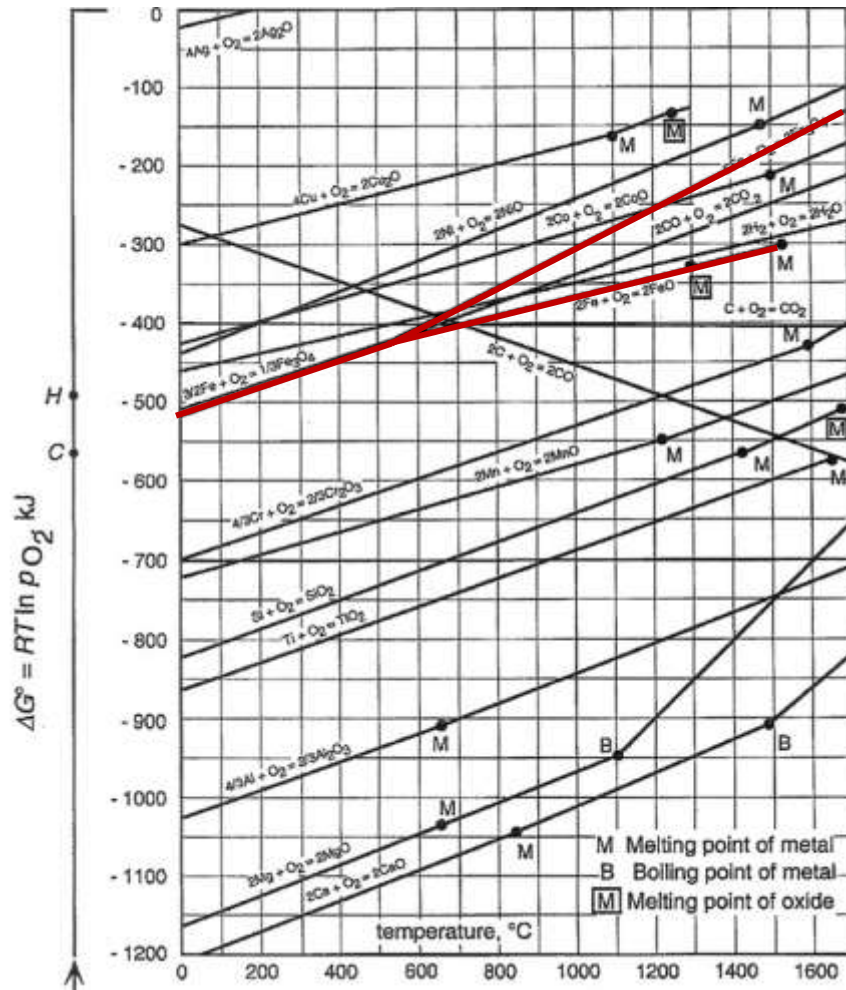
Ellingham Diagrams for Oxide Formation



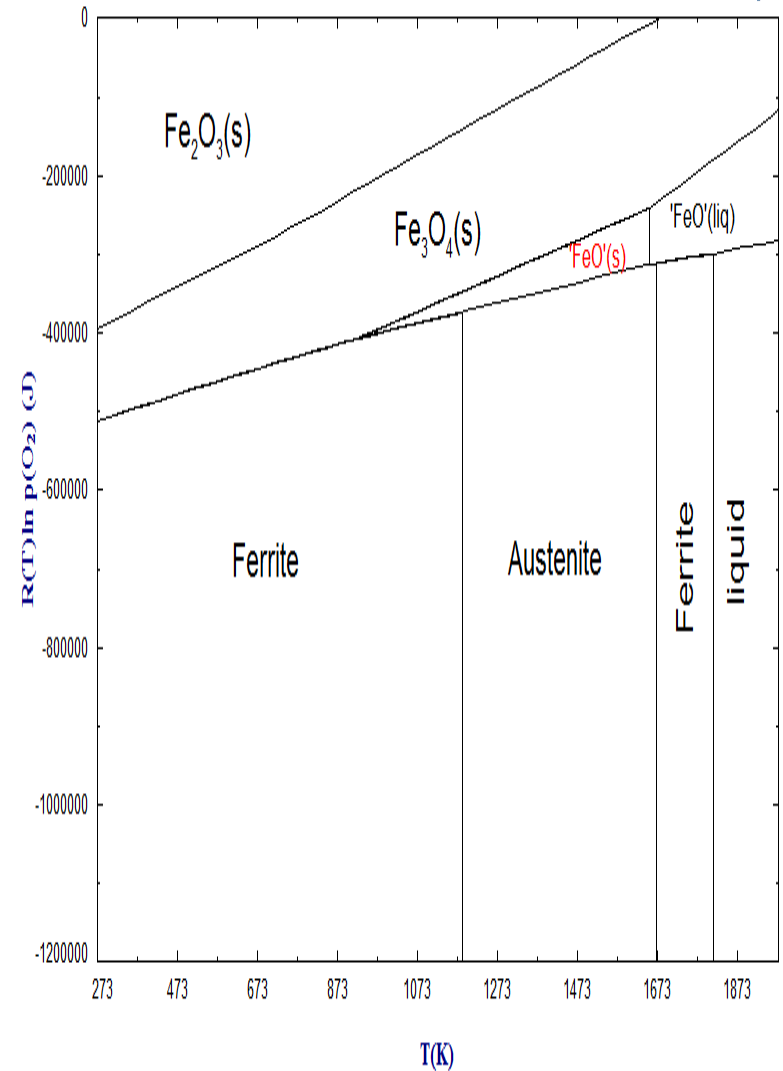
Fe - O₂
1 atm



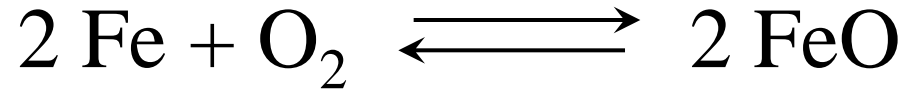
Ellingham Diagrams for Oxide Formation



Fe - O₂
1 atm



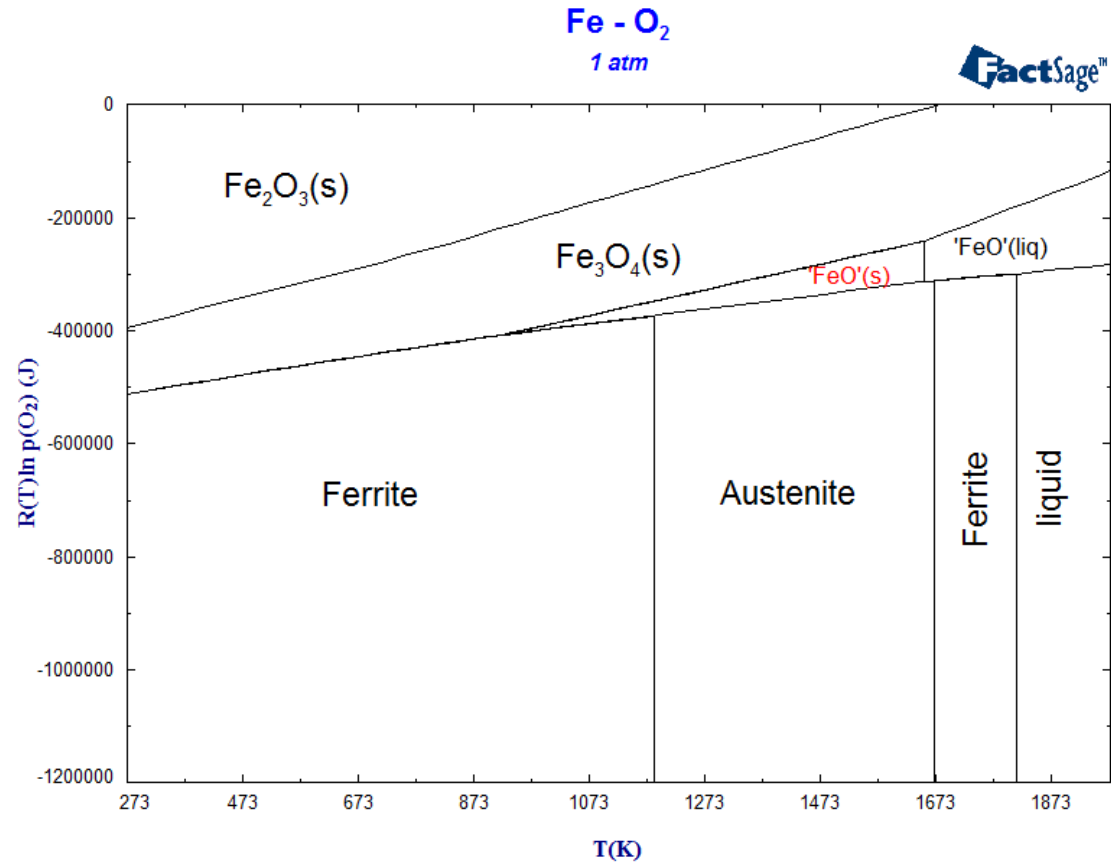
Ellingham Diagram with FACTSage



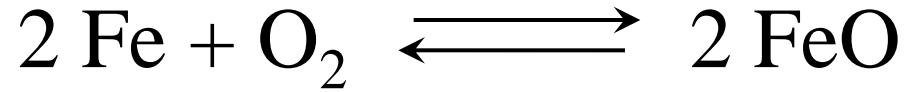
The screenshot shows the FACTSage software interface for generating an Ellingham diagram. The main window is titled "Menu - Phase Diagram: last system". A sub-window titled "Variables: Fe-O2 R(T/K)ln p(O2)/bar (J) vs T(K)" is open, showing the following settings:

- Variables:** A dropdown menu is set to "RTln(a)" and a text box next to it contains the value "1".
- Chemical Potentials:** A table with two columns: "#1 R(T/K)ln(p/bar)" and "Y-axis". The first row is "O2" with a value of "0". The second row is "gas" with a value of "-1200000".
- Temperature:** The X-axis is set to "T(K)" with a range from "Min: 273" to "Max: 1973".

T(K)	RTln(p(O2))
273	1973
1973	-1200000



Stability Diagrams with FACTSage



Menu - Phase Diagram: last system

File Units Parameters Variables Help

T(K) P(atm) Energy(J) Mass(mol) Vol(litre)

Components [2]

Variables: Fe-O2 log10 p(O2)/atm vs T(K)

Variables

compositions 0

log10(a) 1

Next >>

T and P

Temperature

T(K) X-axis

Max: 1973

Min: 273

1/T(K)

Pressure or Volume

P(atm) constant

log P

V(litre) 1

log V

Chemical Potentials

#1 log10(p/atm) Y-axis

O2 0

gas -100

Cancel OK

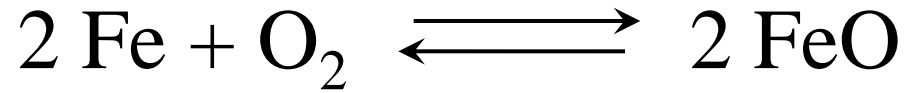
T(K)	log10(p(O2))			
273	1973	-100	0	

log10 p(O2)/atm vs T(K)

Calculate >>

FactSage 6.3

Stability Diagrams with FACTSage



Menu - Phase Diagram: last system

File Units Parameters Variables Help

T(K) P(atm) Energy(J) Mass(mol) Vol(litre)

Components [2]

Variables: Fe-O2 log10 p(O2)/atm vs T(K)

Variables: **log10(a)** 1

Chemical Potentials

#1	log10(p/atm)
O2	0
gas	-100

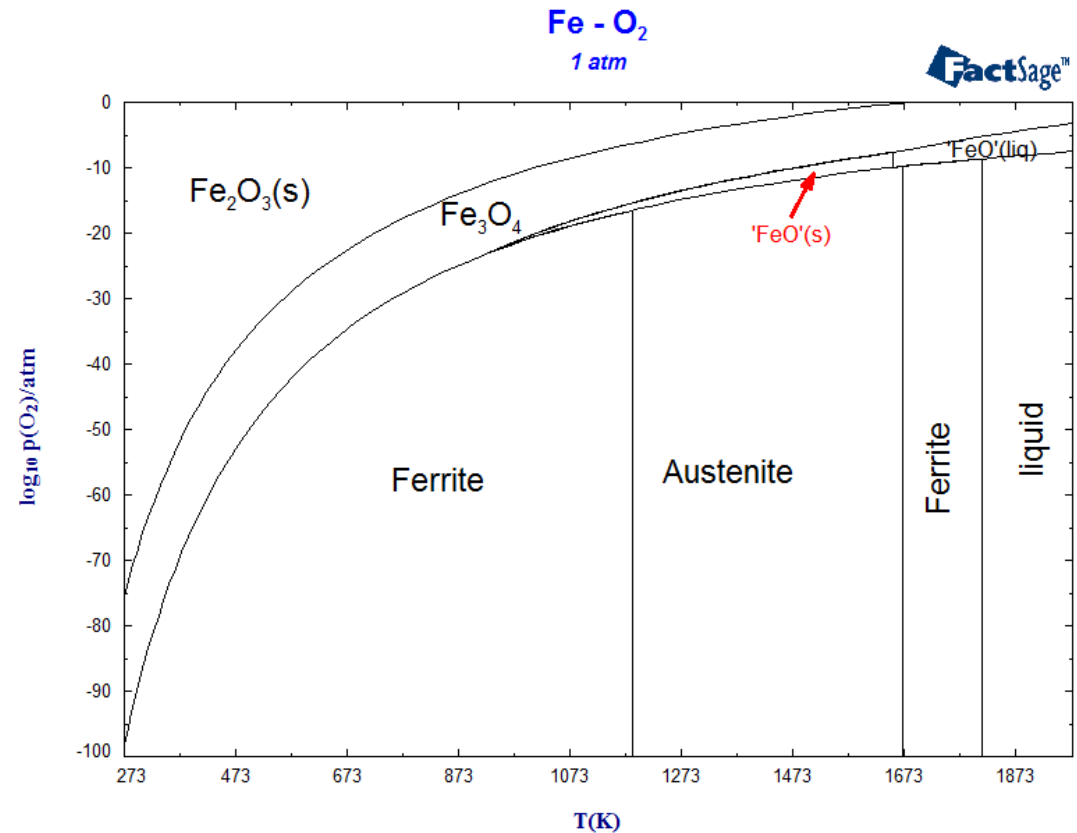
Next >>

Cancel

T(K)	log10(p(O2))
273	1973
1973	-100

log10 p(O2)/atm vs T(K)

FactSage 6.3

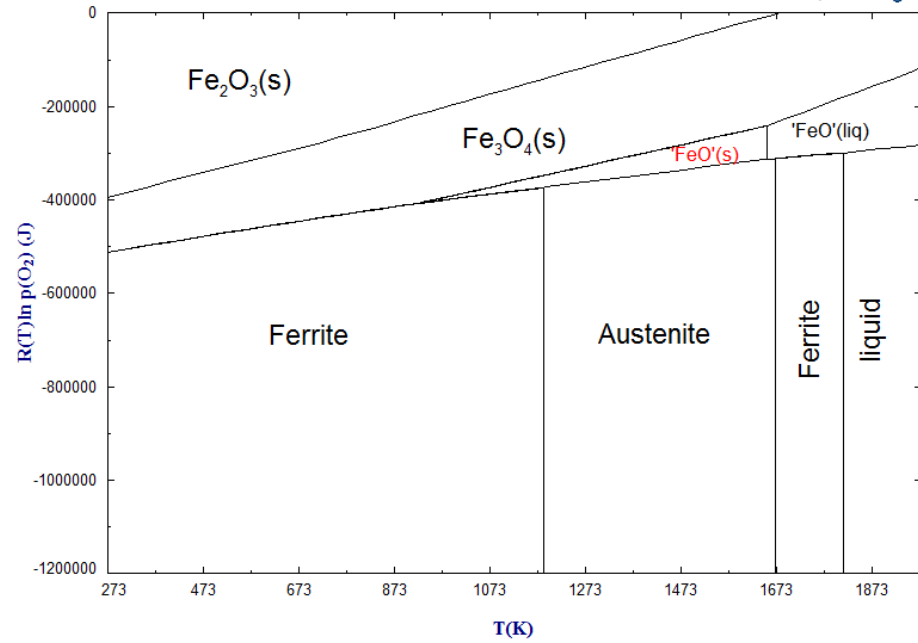


Comparison



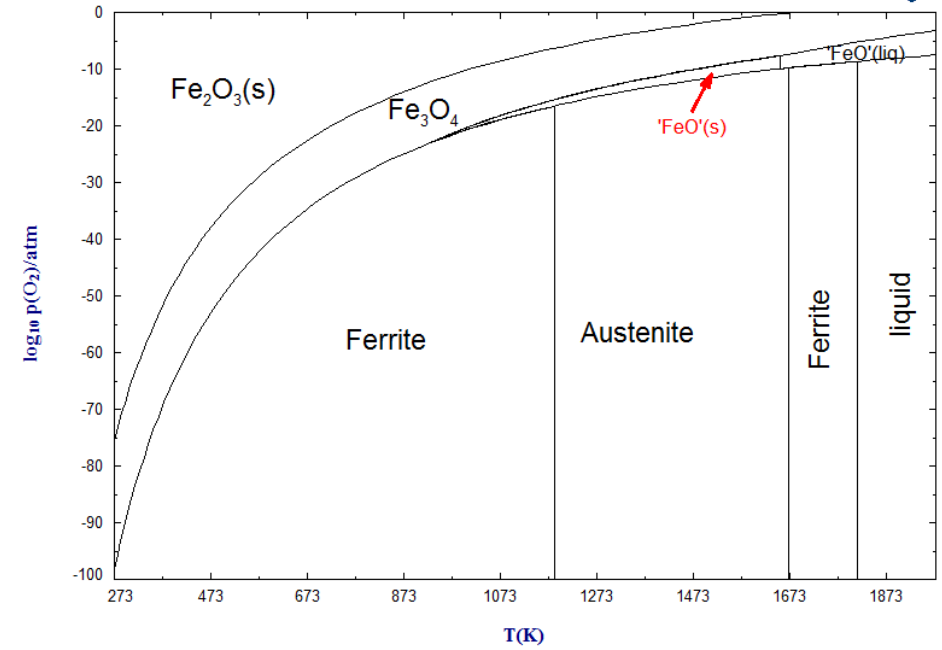
Fe - O₂
1 atm

FactSage™



Fe - O₂
1 atm

FactSage™



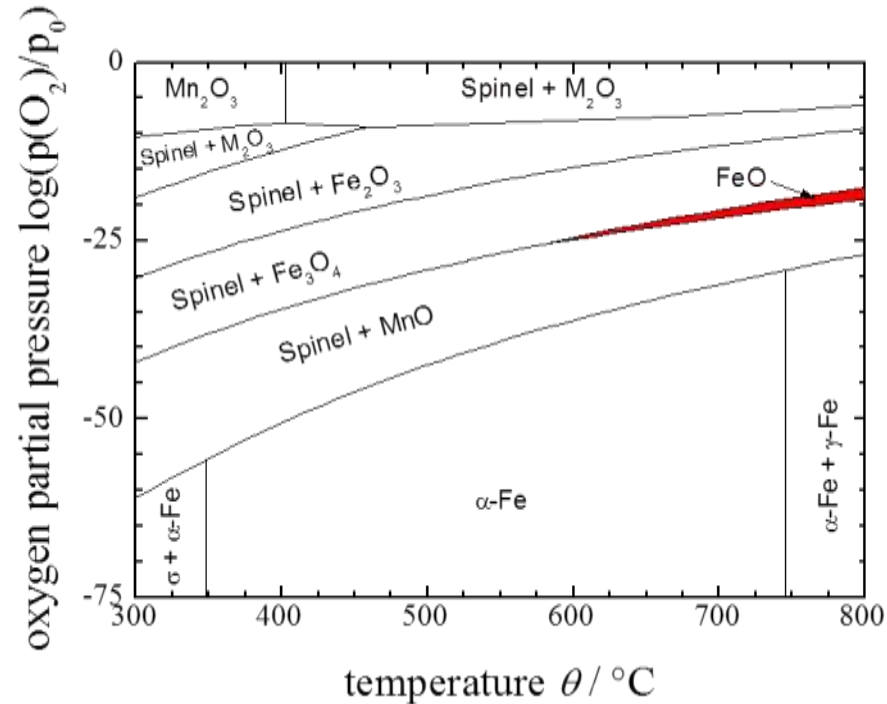
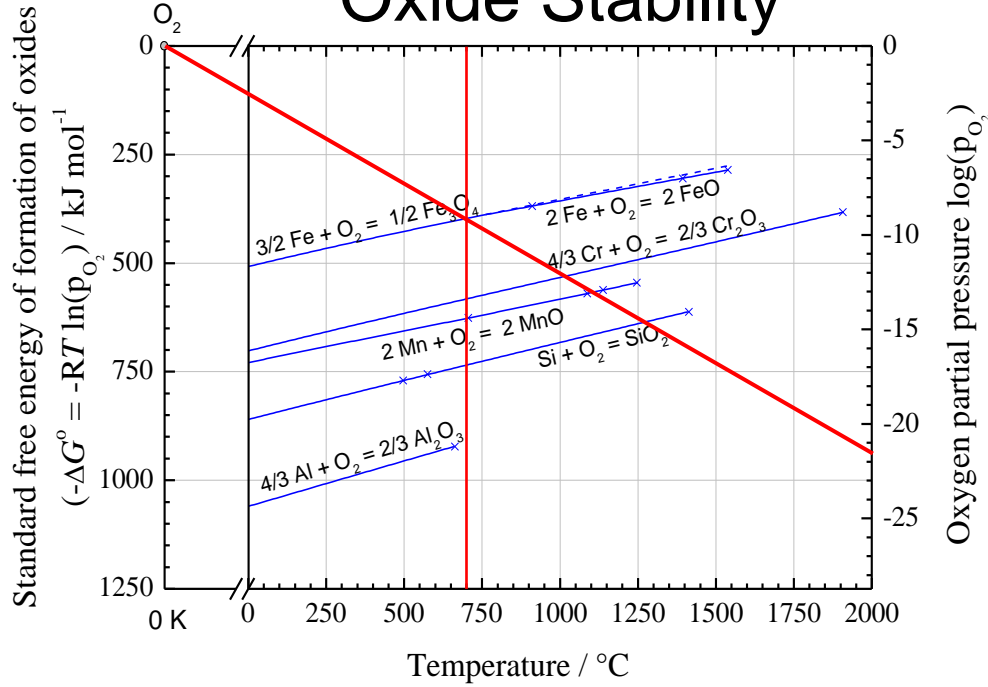
$$-2 G_{(T)}^{o, FeO} + 2 G_{(T)}^{o, Fe} + G_{(T)}^{o, O_2} = -R \ln \left(\frac{p_{O_2}}{p_o} \right) T$$

$$-\frac{2 G_{(T)}^{o, FeO} - 2 G_{(T)}^{o, Fe} - G_{(T)}^{o, O_2}}{RT} = \ln \left(\frac{p_{O_2}}{p_o} \right)$$

Properties of Oxygen



Oxide Stability



Iron – Manganese – Chromium alloy

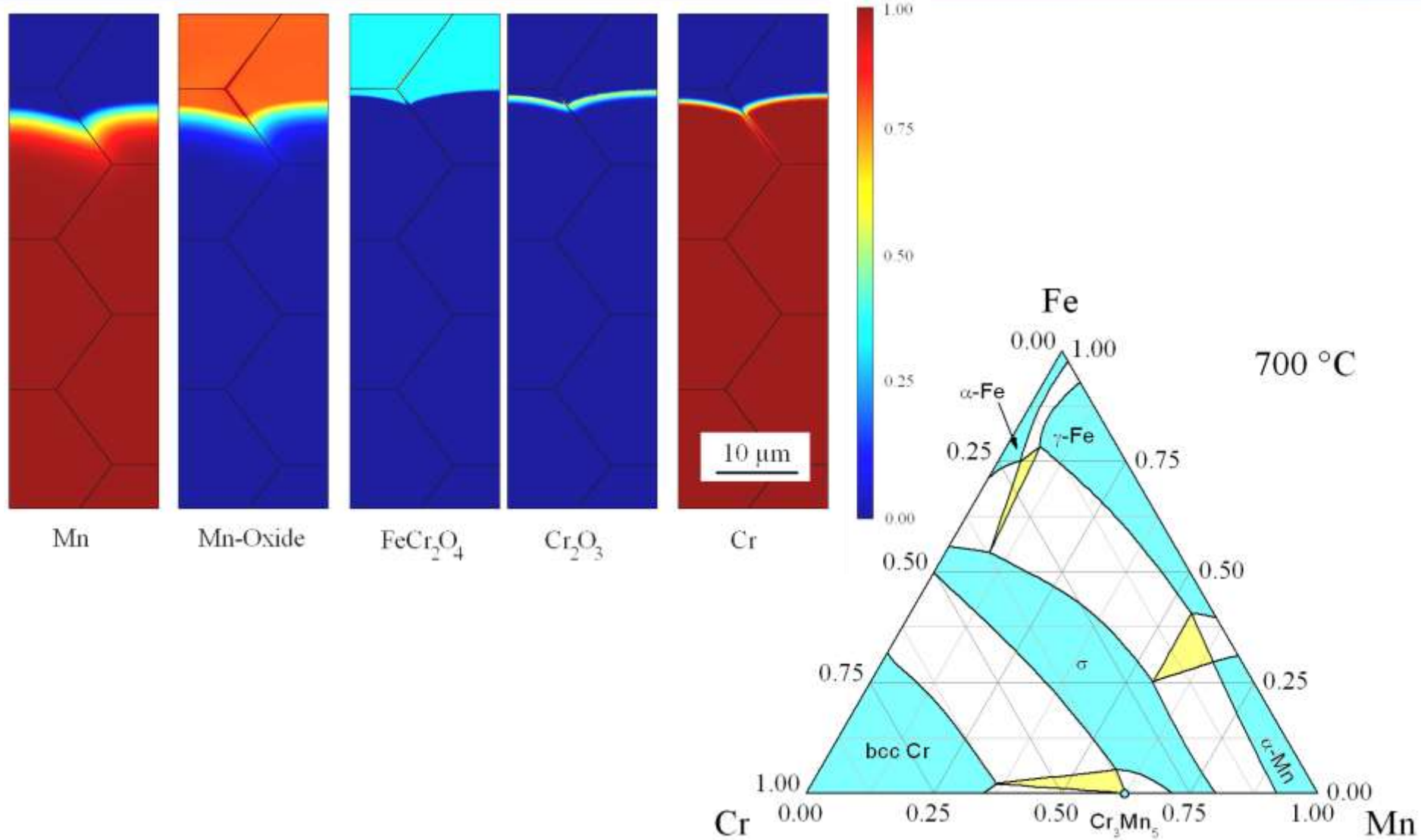


Figure: Spatial phase distribution in an Fe, 2 wt-% Mn, 0.8 wt-% Cr alloy after oxidation at $p(\text{O}_2) = 3 \cdot 10^{-22}$ bar and 700 °C for 120 min and ternary phase diagram.

Part II

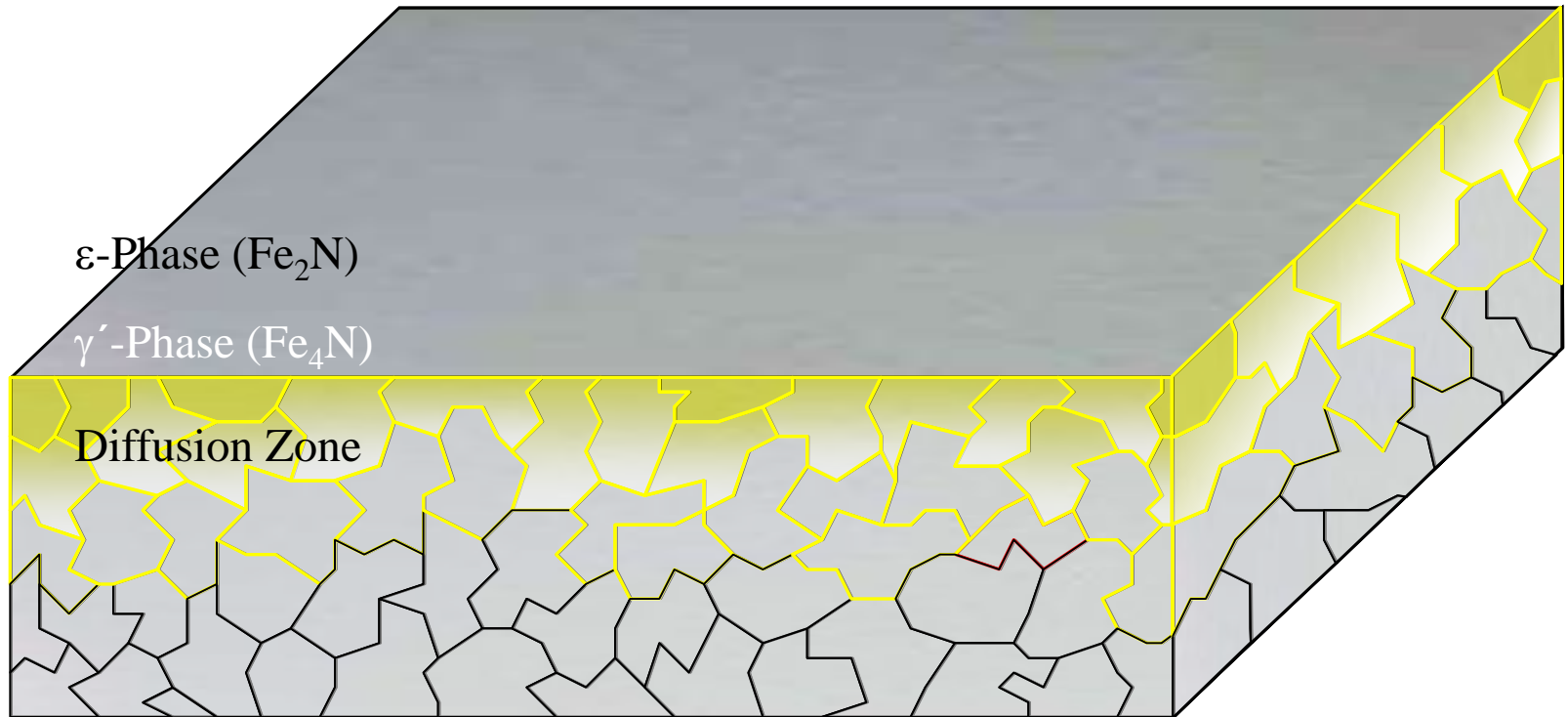
Gaseous Nitriding in the system Fe – Cr – C

Nitriding of Fe, 1 wt-% Cr, 0.10 wt-% C and

Conditions: 48 h at 500 °C

$p(\text{NH}_3) : p(\text{H}_2) = 100$ ($K_N = 1\,000$)

Gaseous Nitriding Process



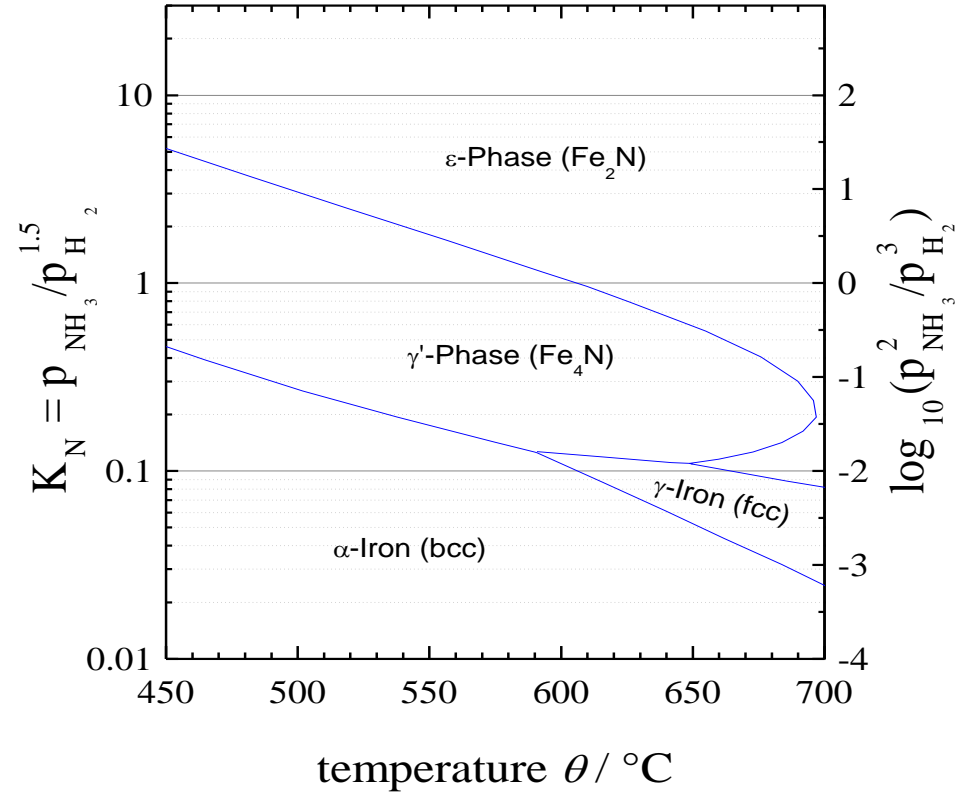
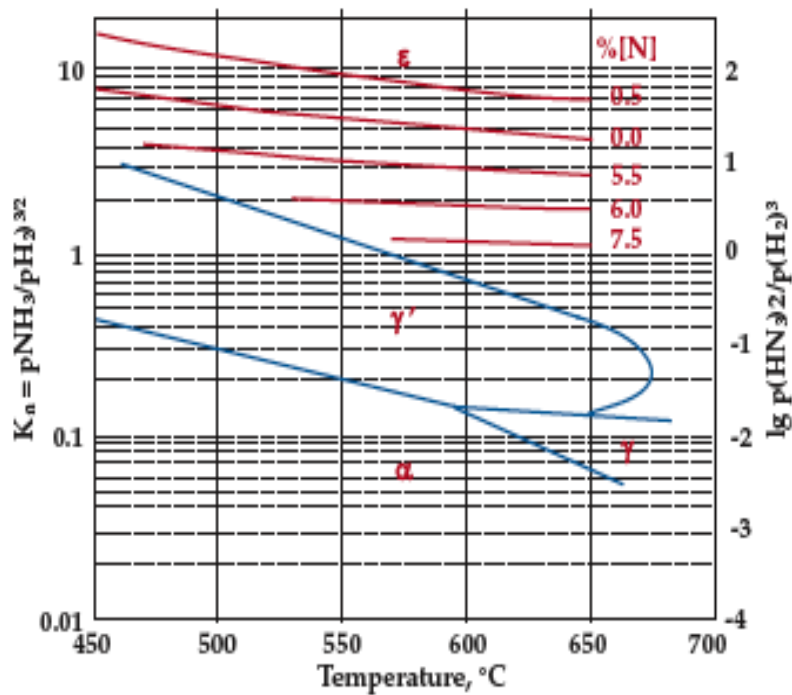


Figure: Lehrer-Diagramm of iron nitrides according to literature (left) and calculated with the programme FactSage (right).

Iron – Chromium – Carbon alloy

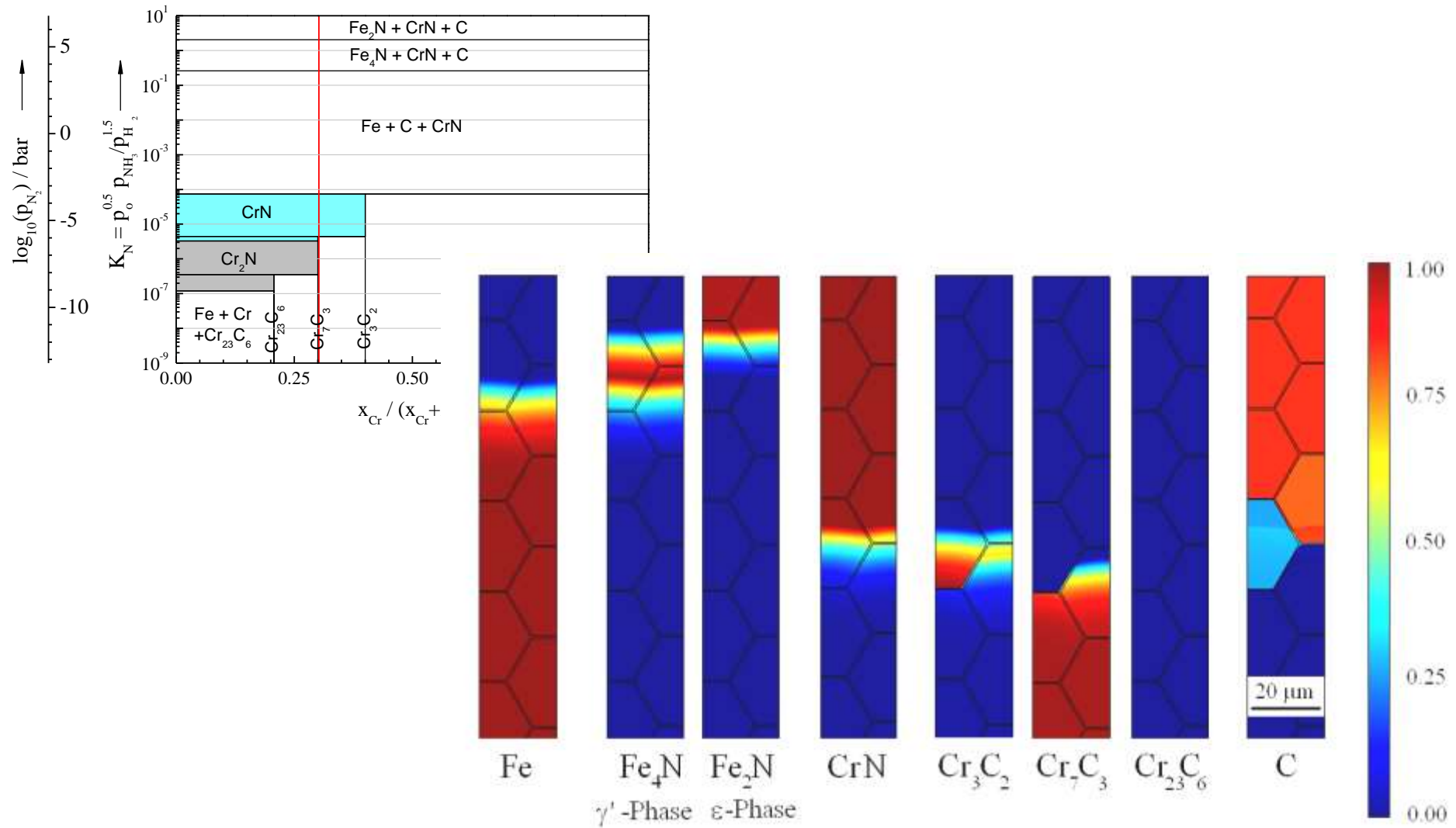


Figure: Spatial phase distribution in an Fe, 1 wt-% Cr, 0.1 wt-% C alloy after gas nitriding at $K_N = 2.4$ and 500 °C for 48 h and phase stability diagram.

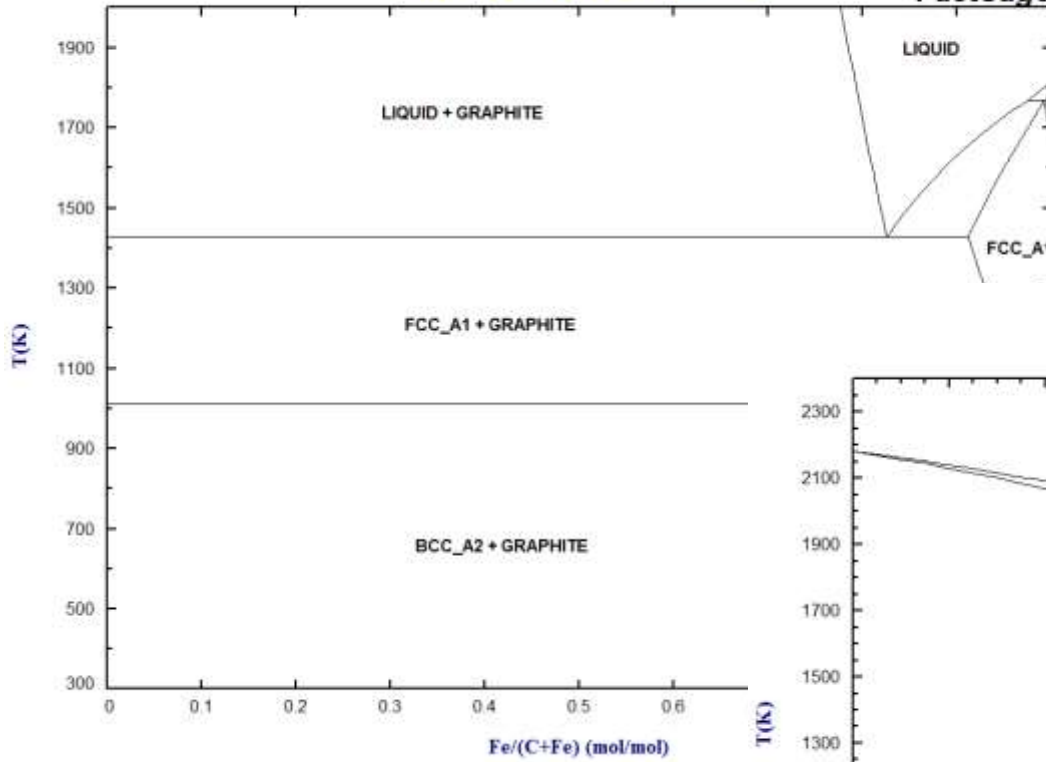
Binary Phase Diagrams



C - Fe

Data from SGTE 2011 alloy database

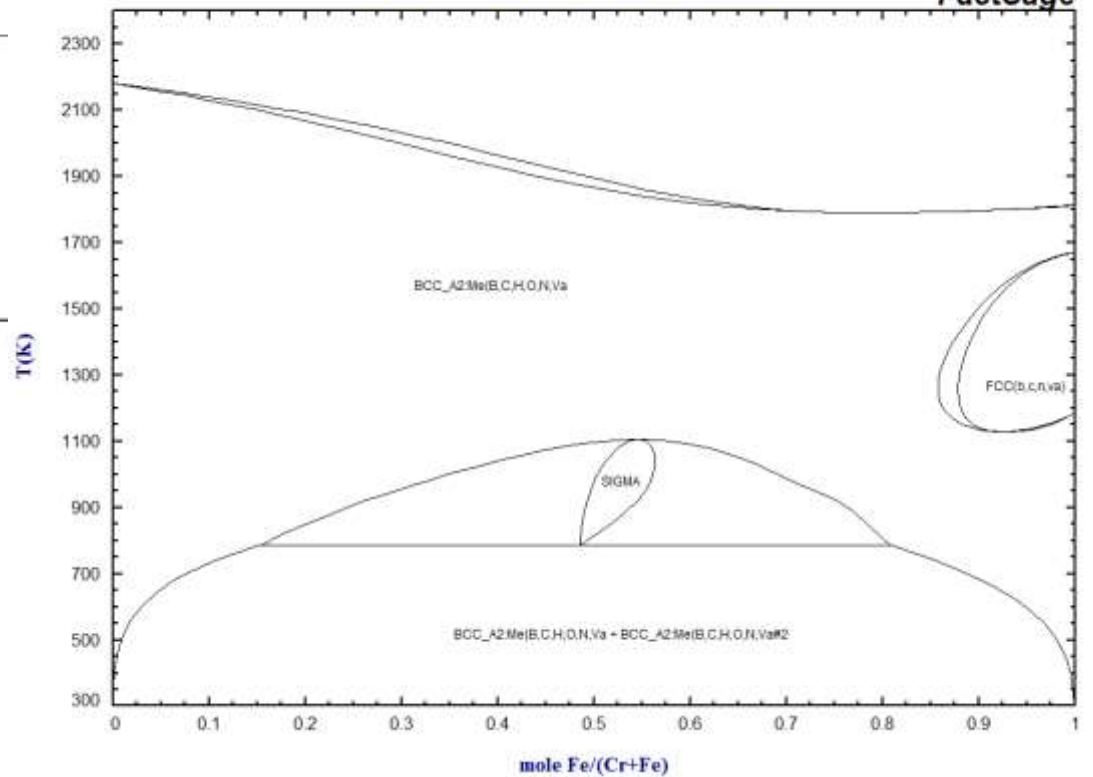
FactSage



Cr - Fe

Data from BINARY (SGTE) alloy databases

FactSage



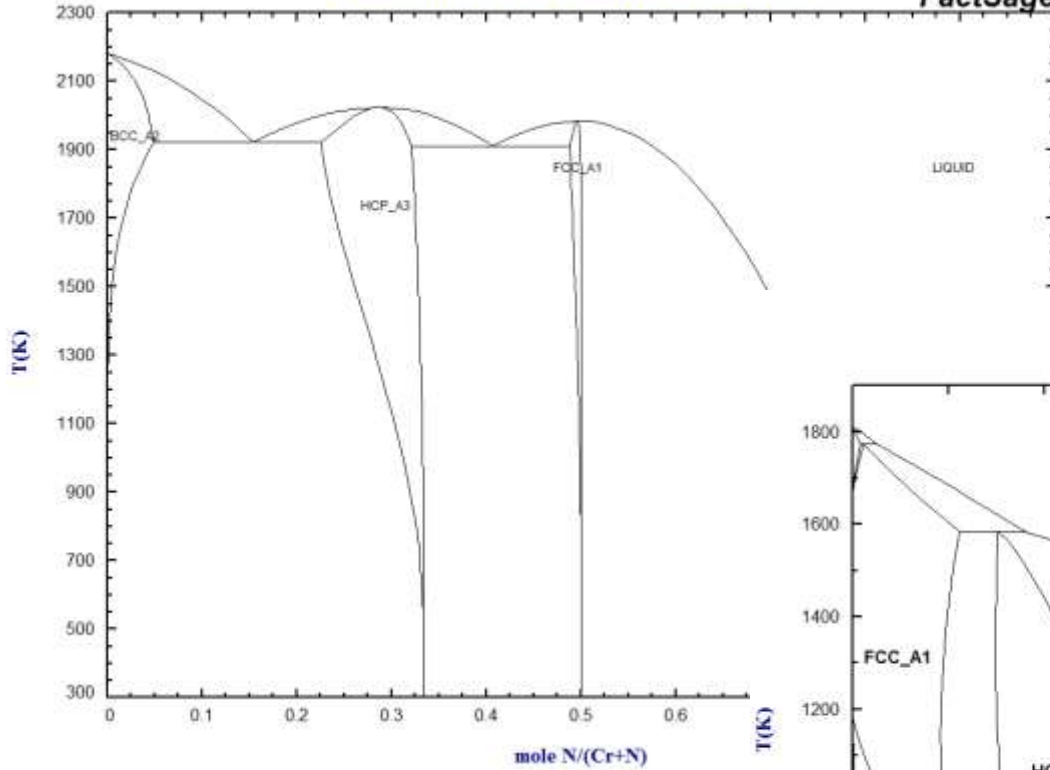
Binary Phase Diagrams



Cr - N

Data from SGTE alloy databases (revised 2004)

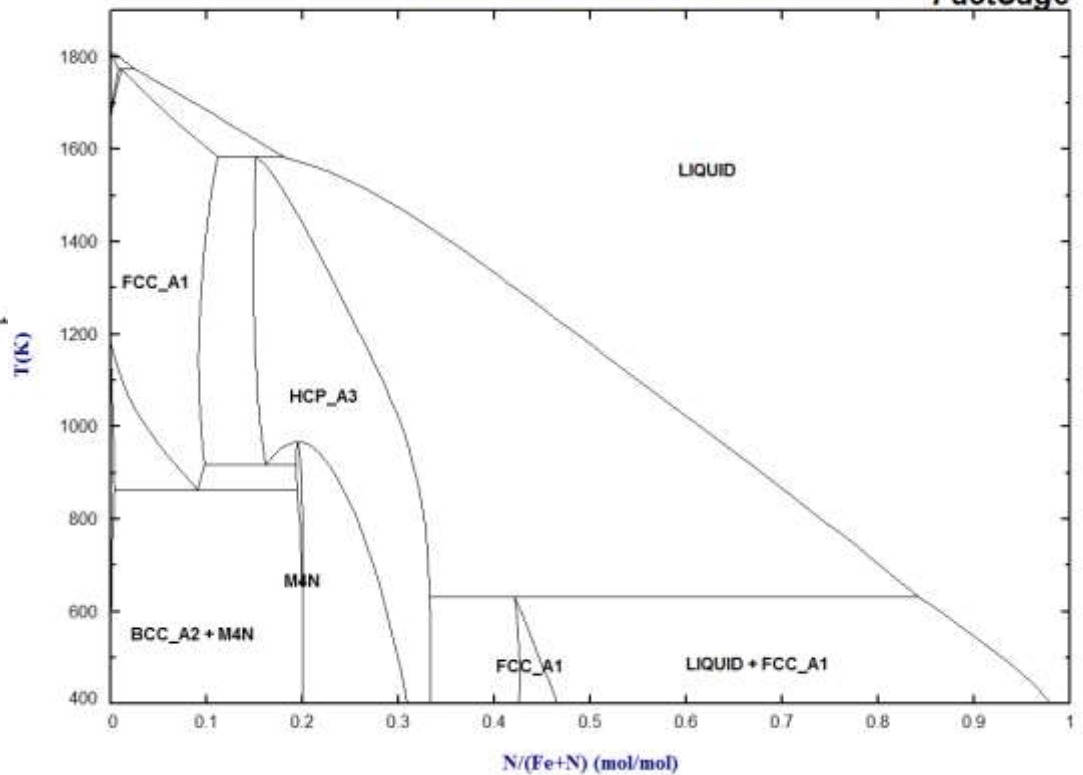
FactSage



Fe - N

Data from SGTE 2011 alloy database

FactSage



The System Iron – Nitrogen

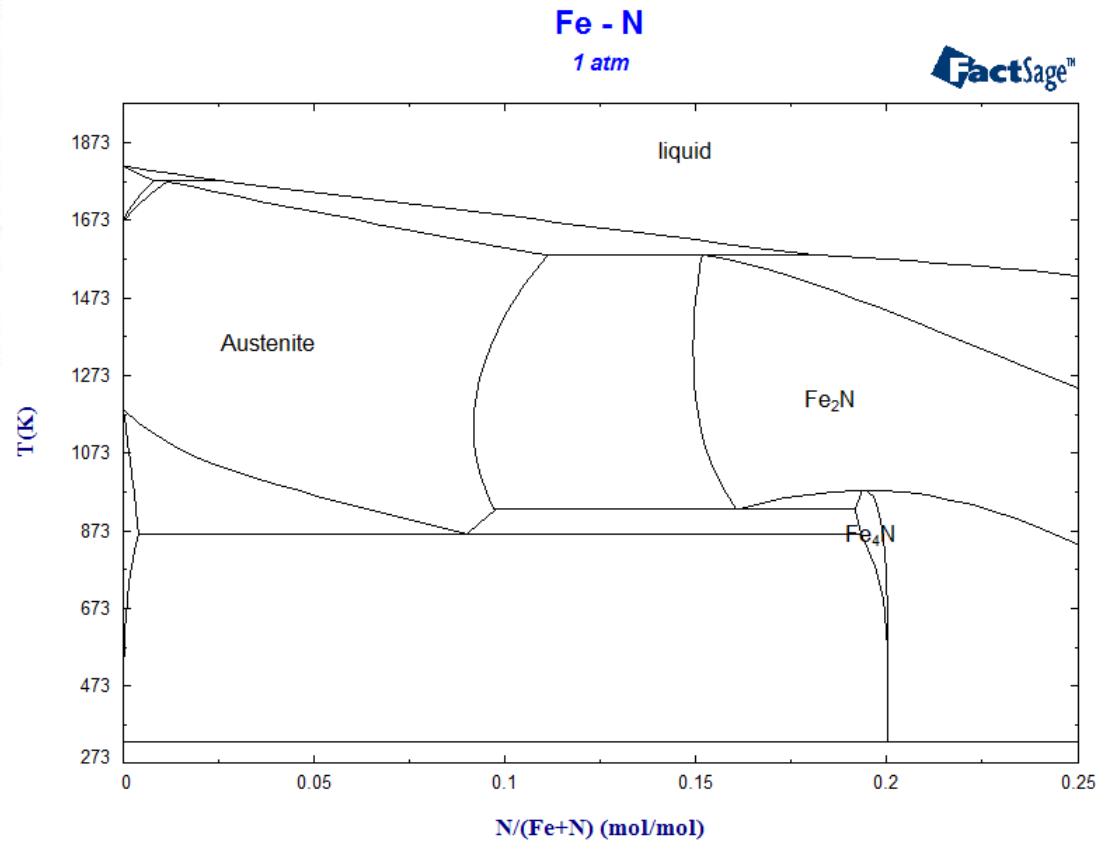
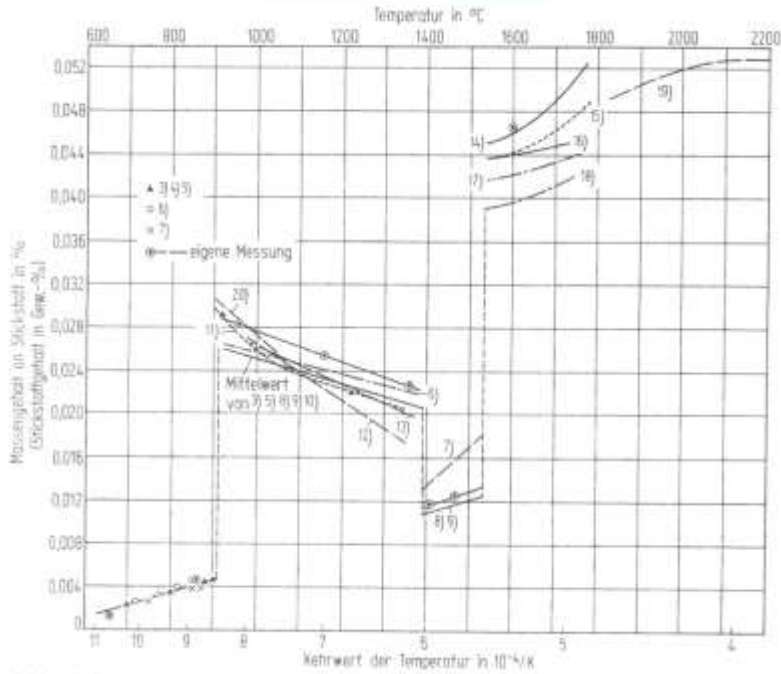


Figure: Nitrogen Solubility in Iron at 1 bar (left) and binary Iron-Nitrogen phase diagram, calculated with FACTSage (right).

The System Iron – Nitrogen

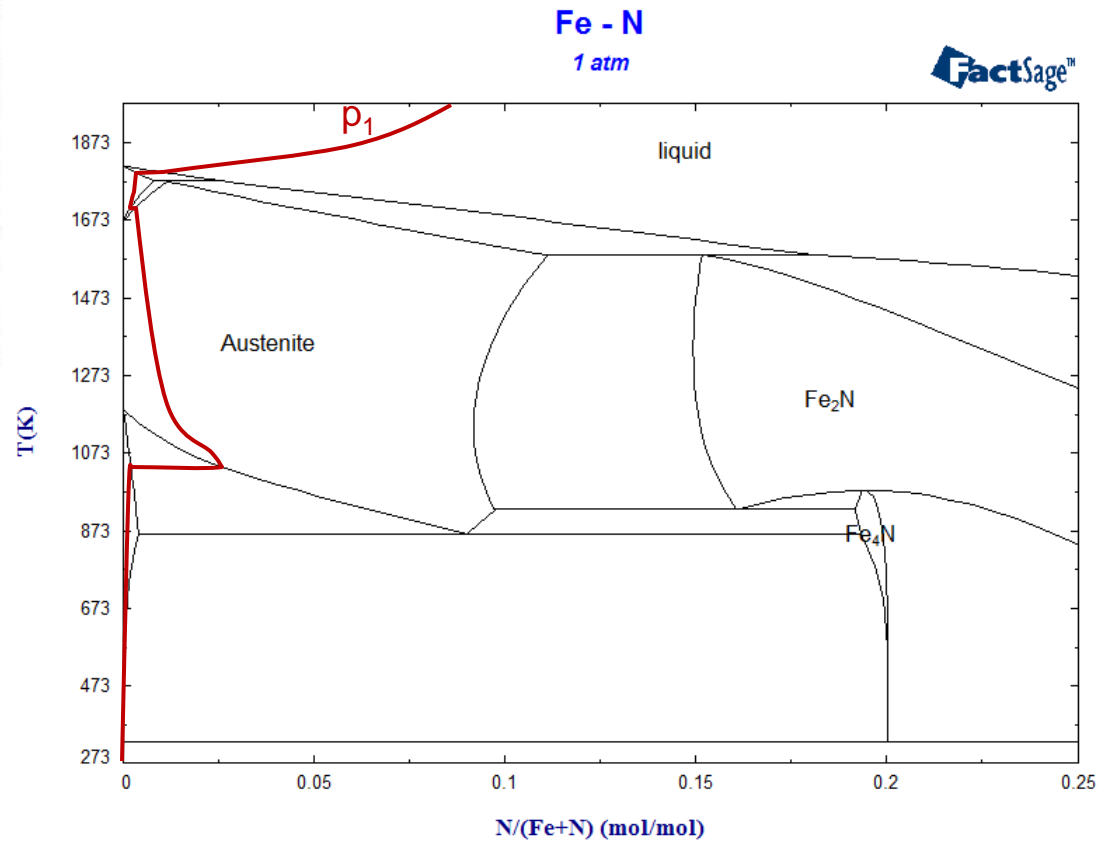
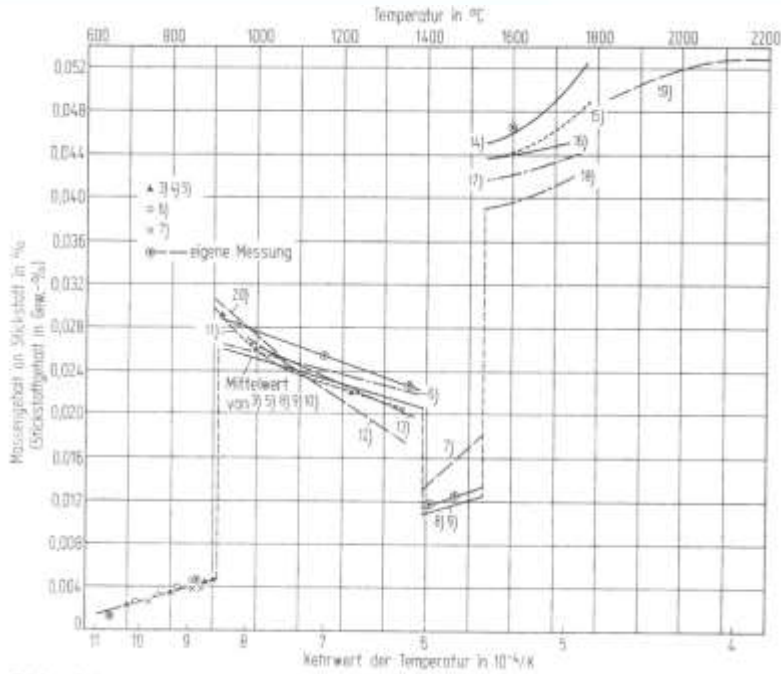


Figure: Nitrogen Solubility in Iron at 1 bar (left) and binary Iron-Nitrogen phase diagram, calculated with FACTSage (right).

The System Iron – Nitrogen

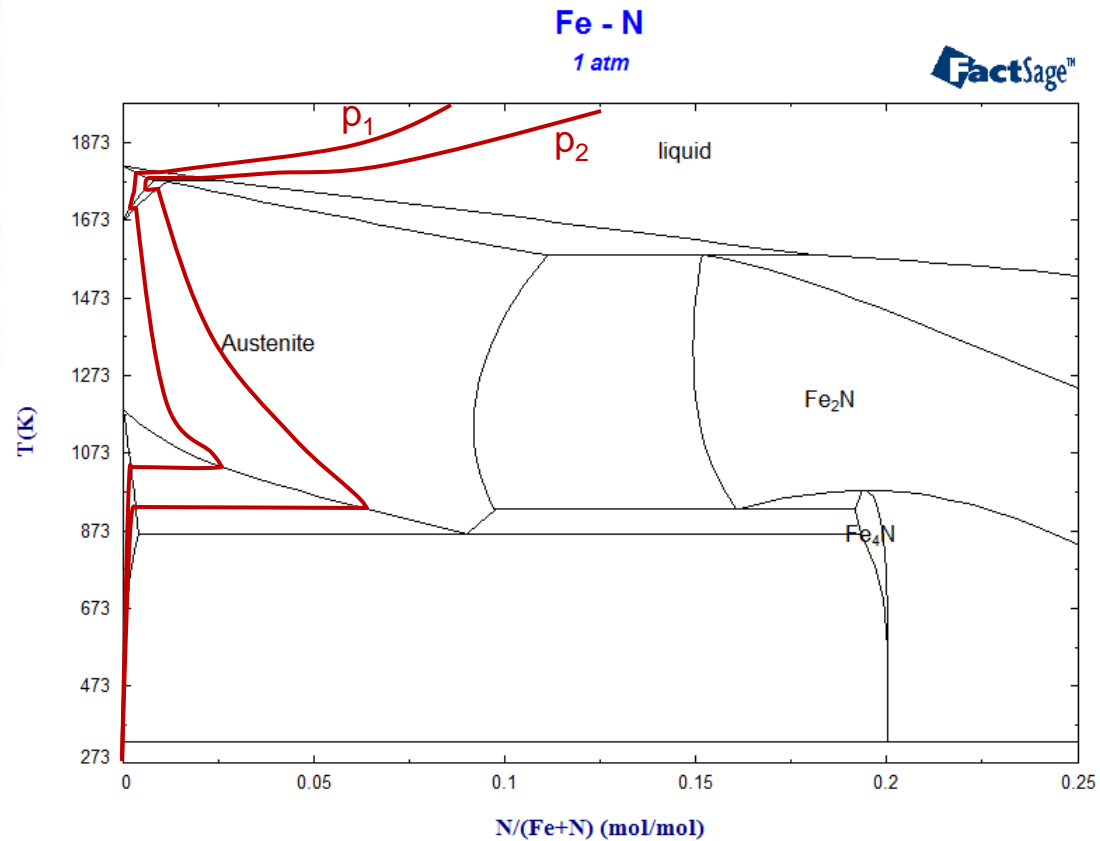
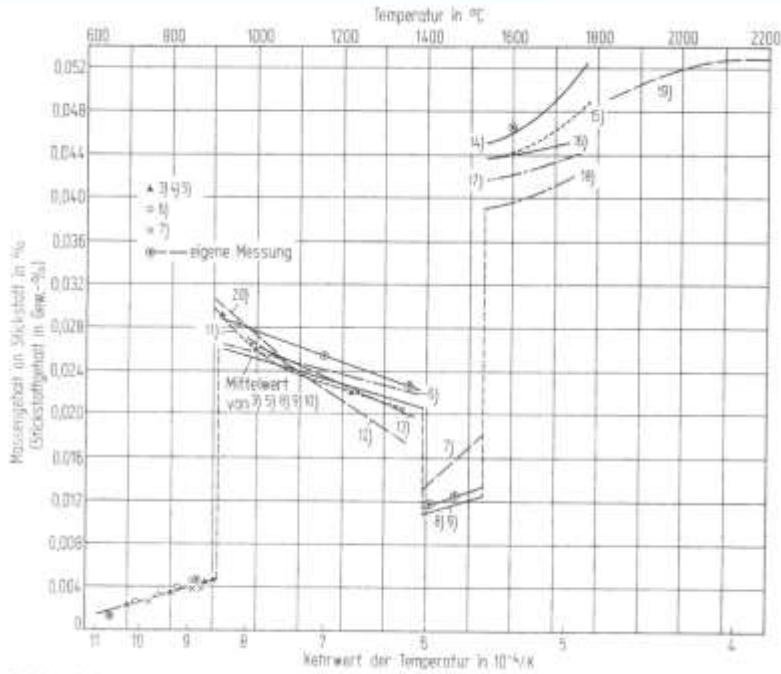


Figure: Nitrogen Solubility in Iron at 1 bar (left) and binary Iron-Nitrogen phase diagram, calculated with FACTSage (right).

Part III

Gaseous Nitriding and Oxidation in the system Fe – Si

Nitriding of Fe, 1 wt-% Si

Conditions: 20 h at 550 °C ($K_N = 1\,000$)

4 h at 550 °C ($K_O \approx 0.01$)

Stability Diagram of Iron – Silicon

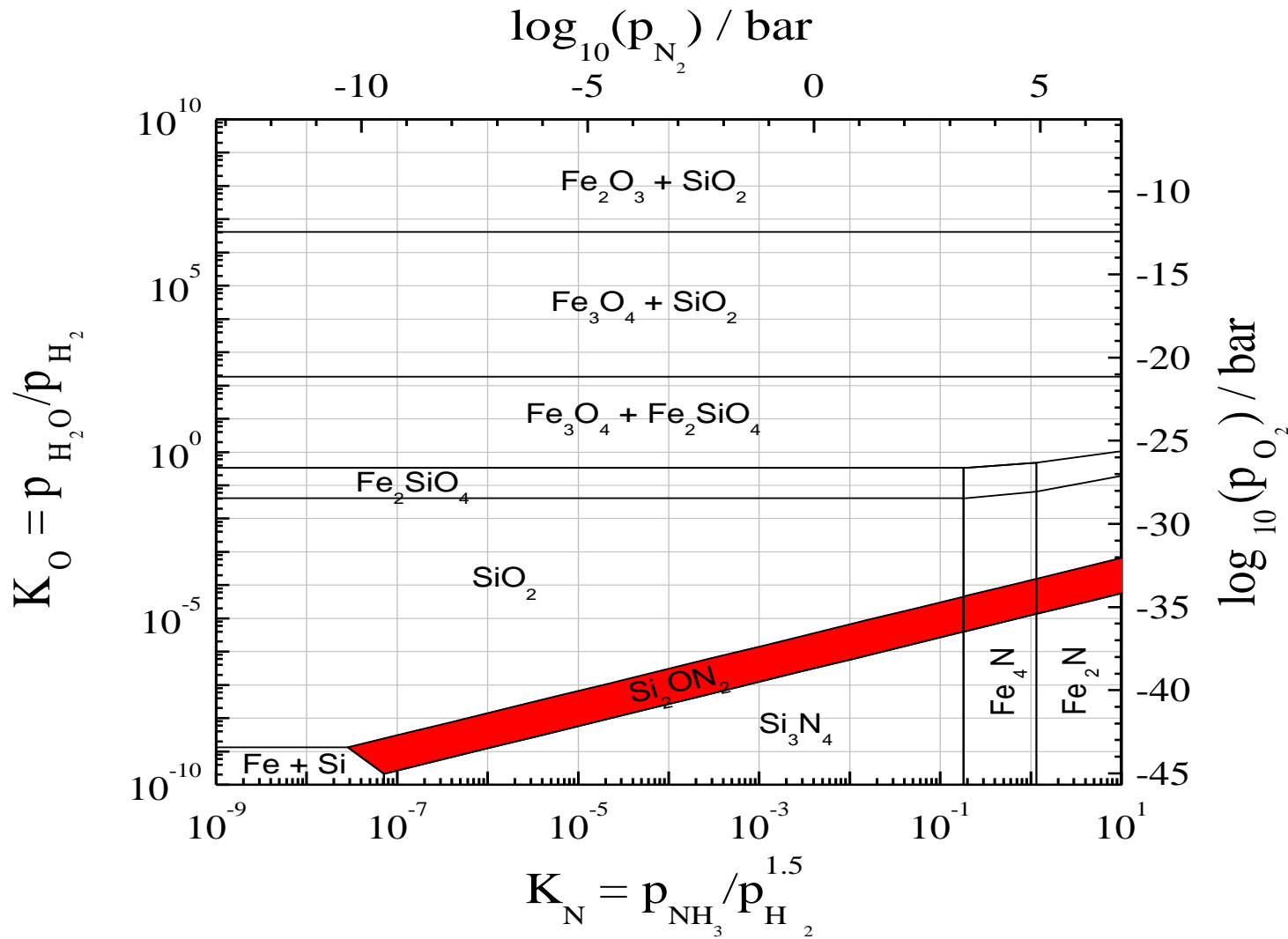


Figure: Stability diagram of an Fe, 1 wt-% Si alloy at 550 °C with respect to the partial pressures of nitrogen and oxygen (SGTE Pure Substance Database).

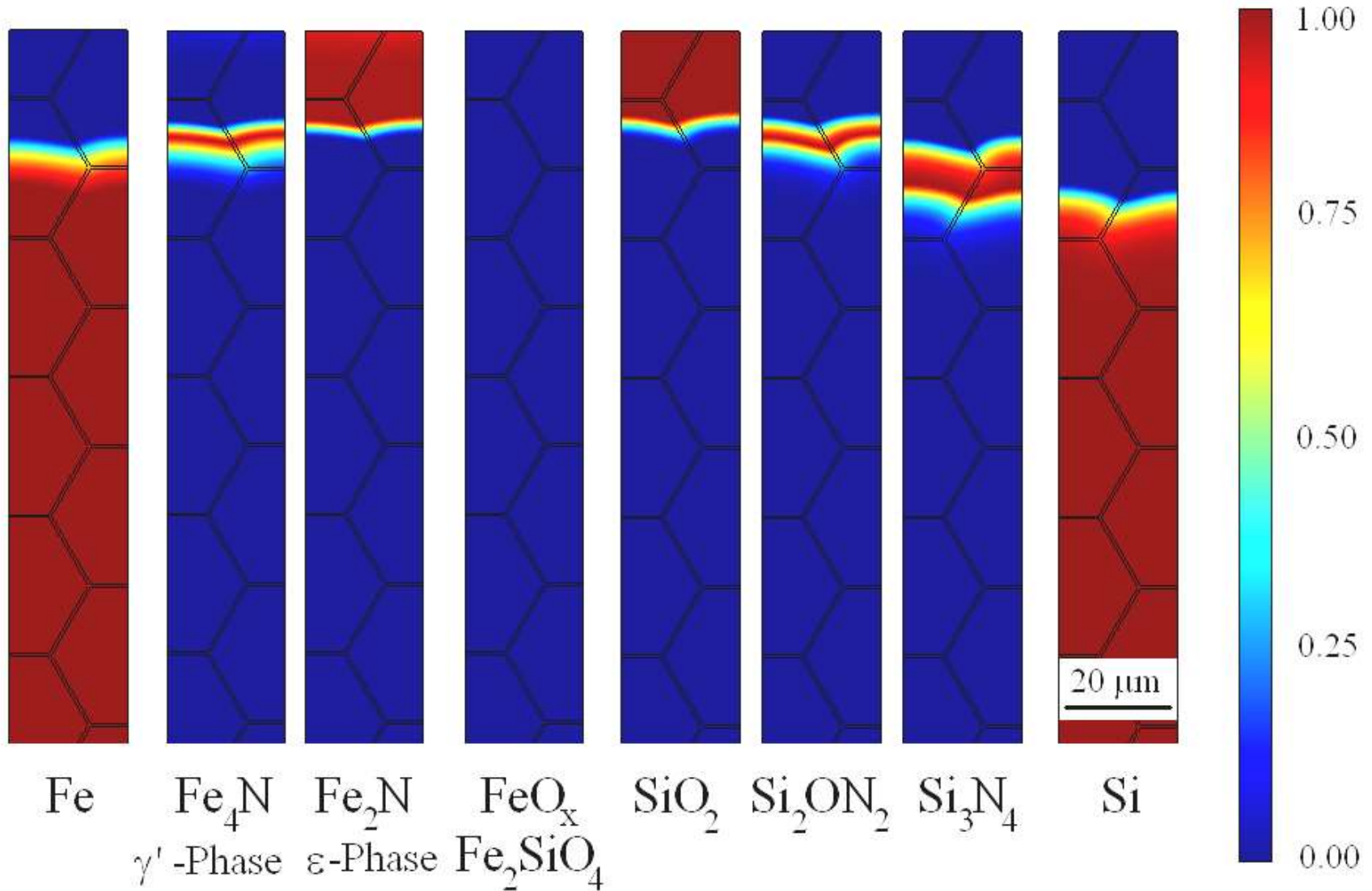
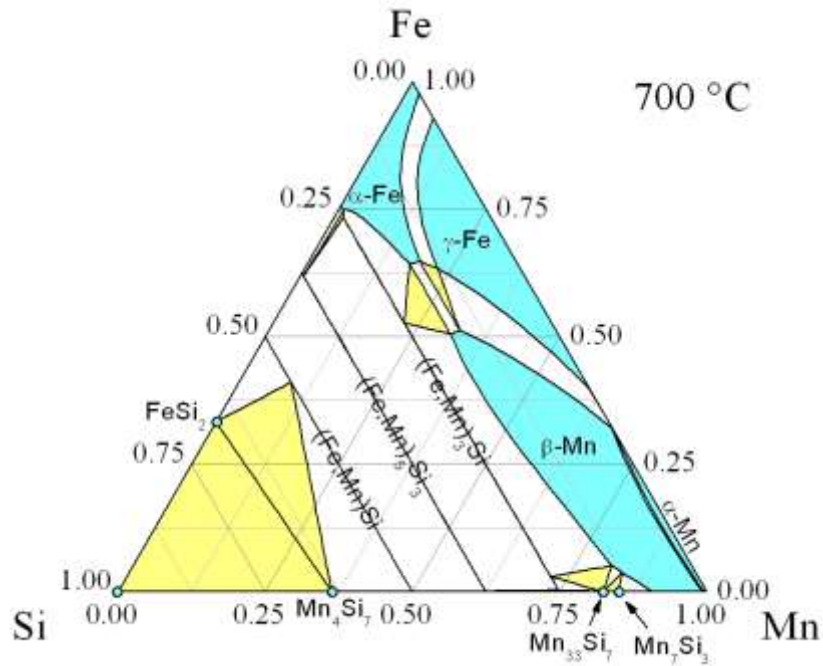


Figure: Spatial phase distribution in Fe, 1 wt-% Si after gaseous nitriding for 20 h at $K_N = 1\ 000$ and oxidation for 4 h and $K_O \approx 0.01$ ($p_{tot} = 1\ atm, 550\ ^\circ C$).

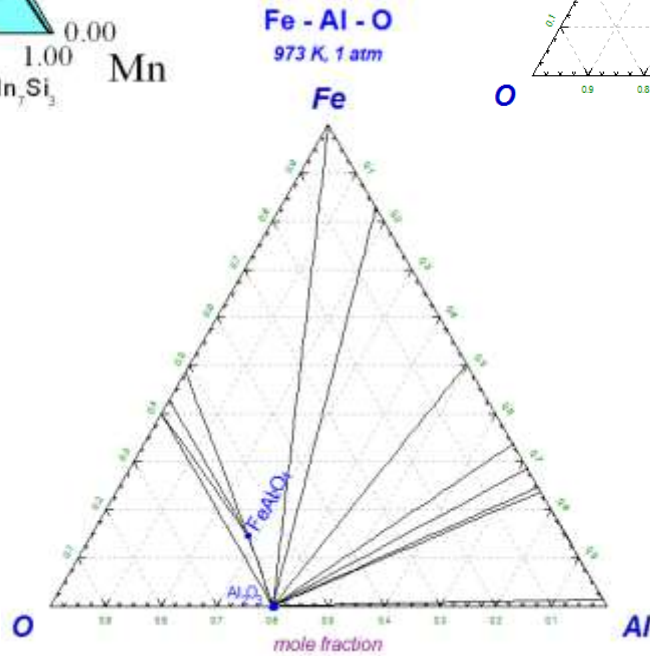
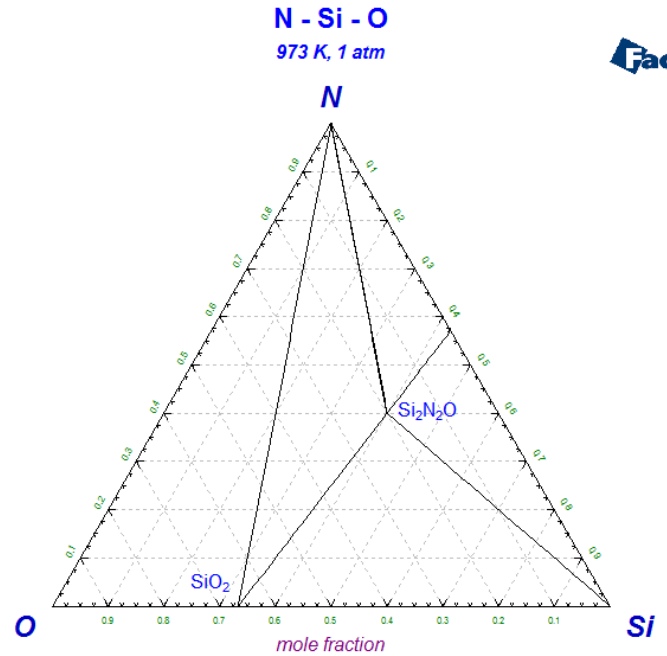
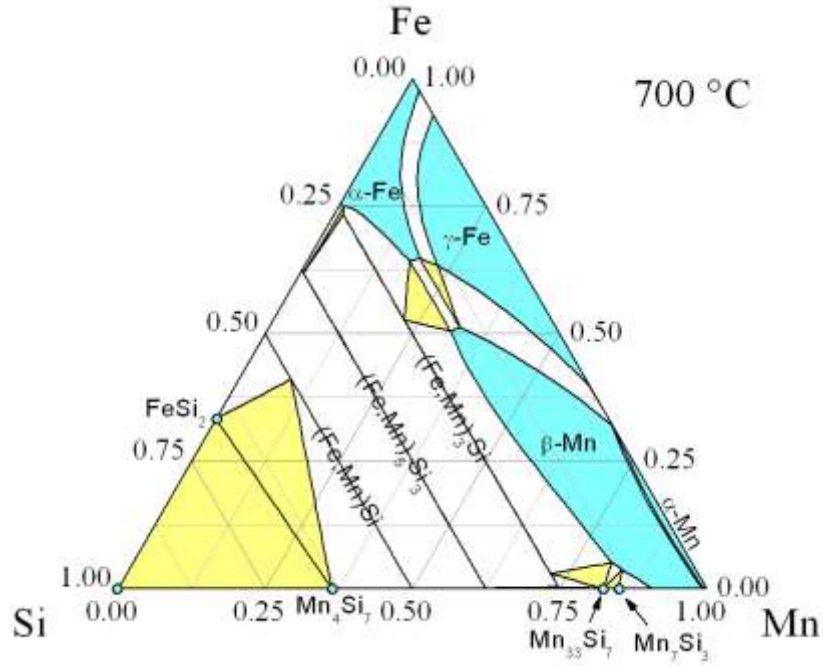
Ternary Phase Diagrams



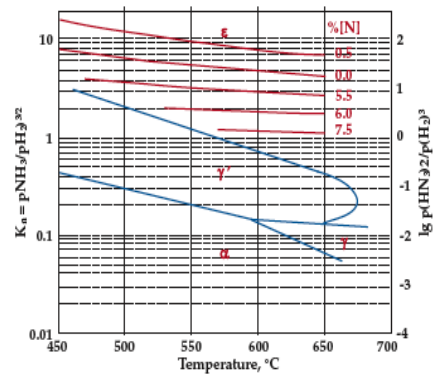
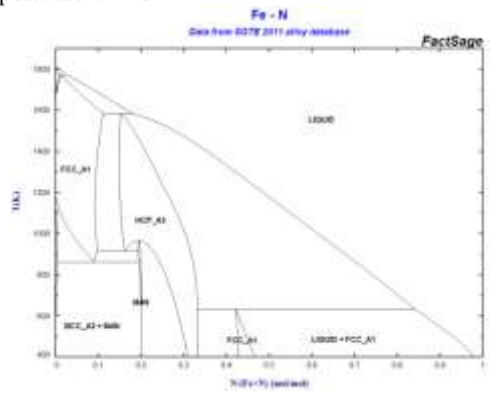
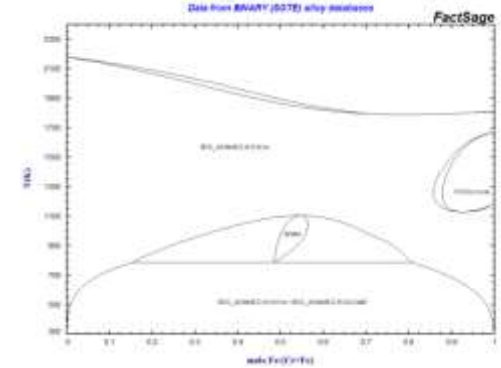
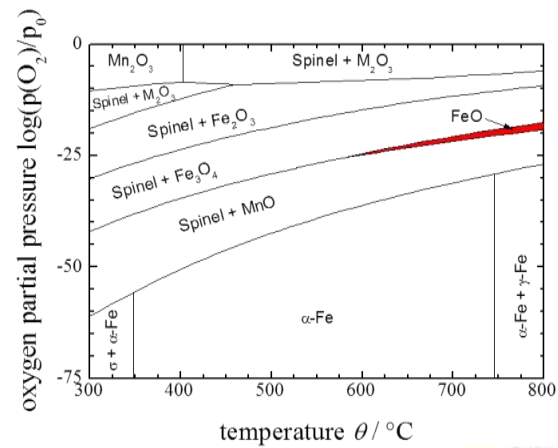
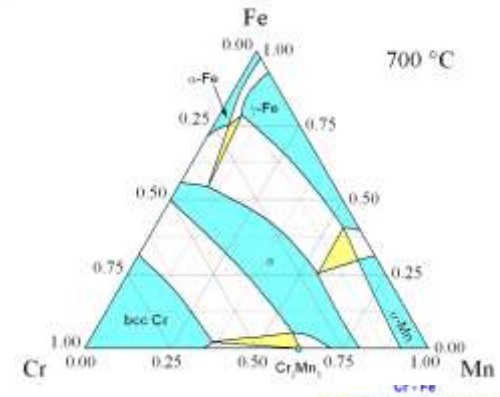
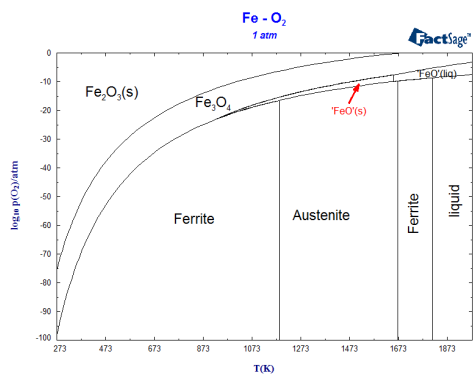
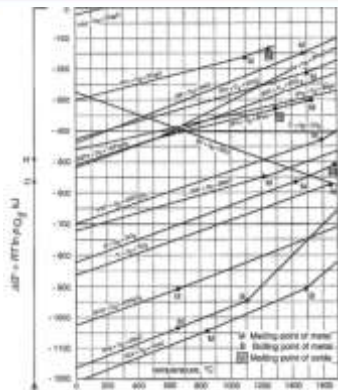
Ternary Phase Diagrams



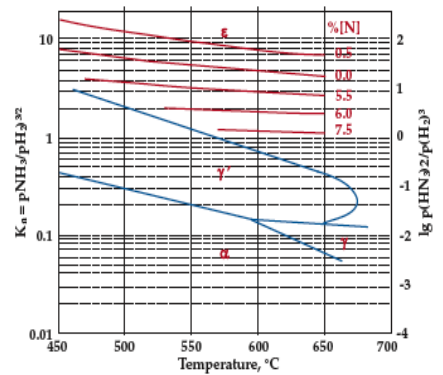
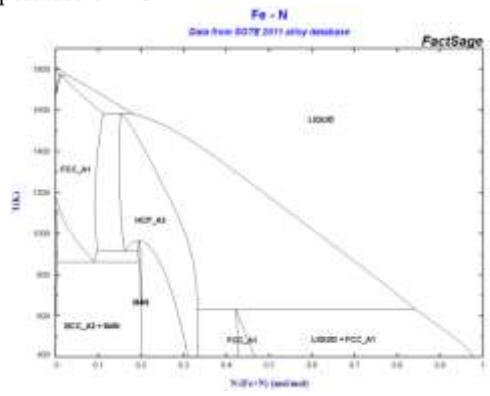
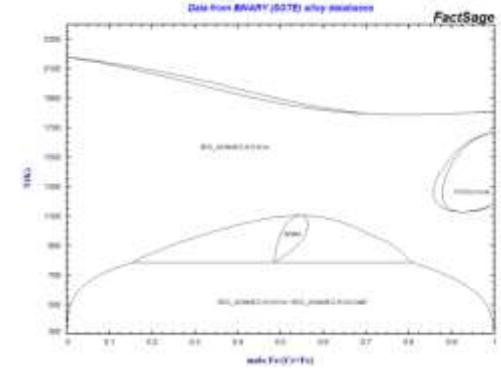
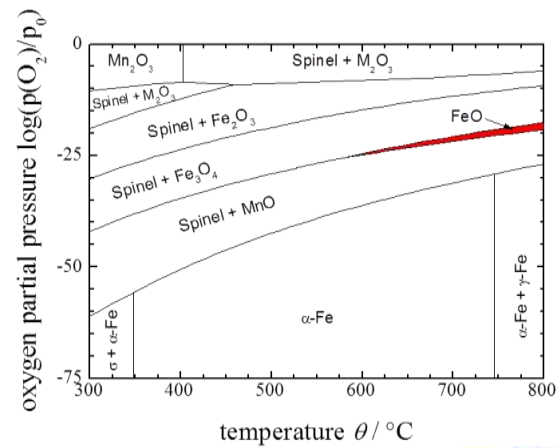
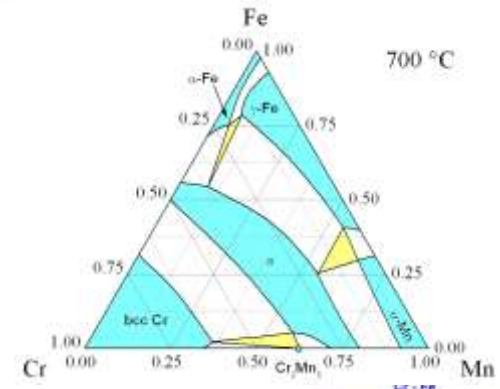
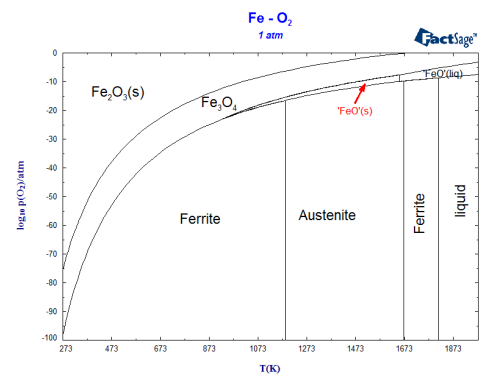
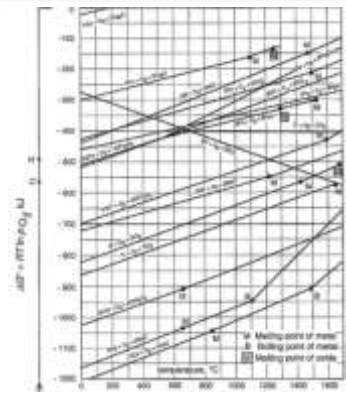
FactSage™



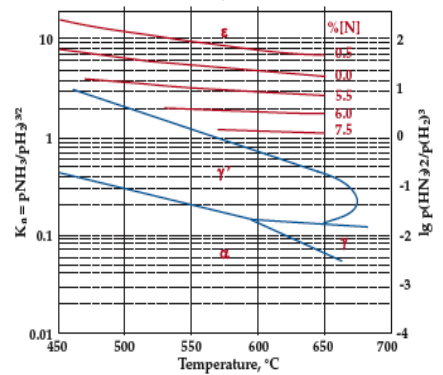
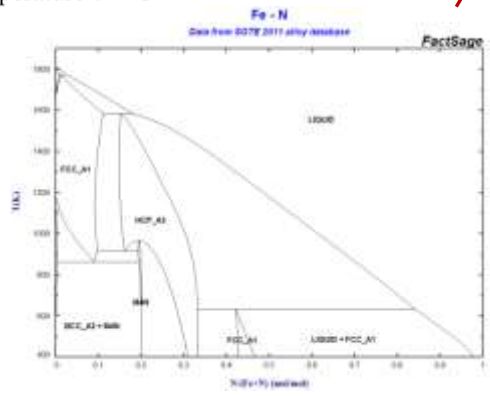
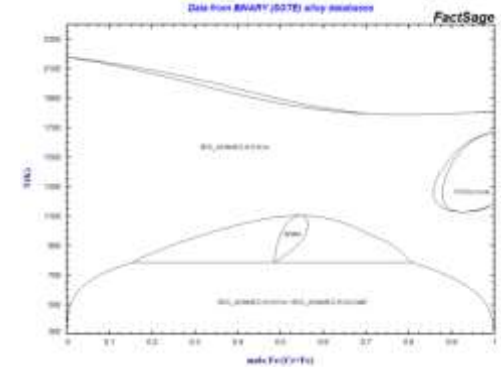
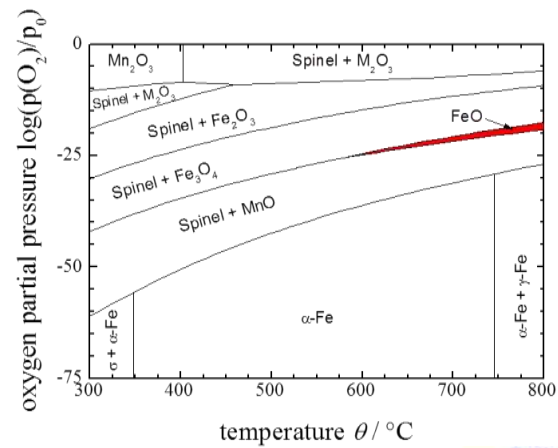
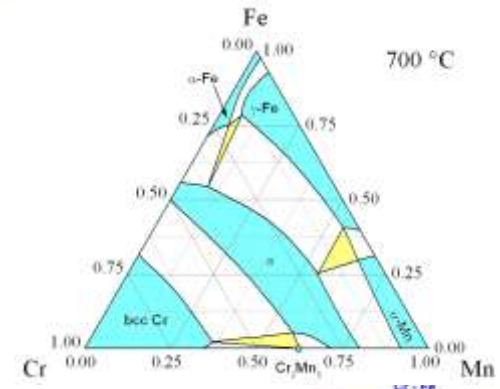
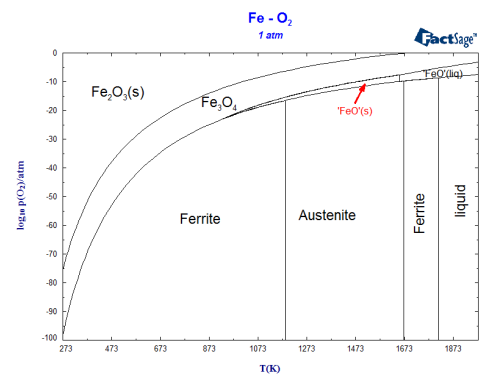
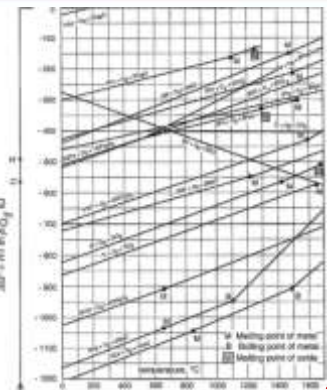
Conclusions - The Problem



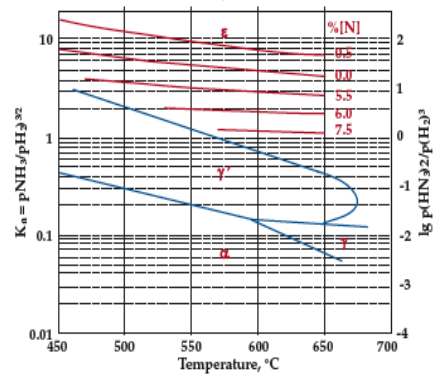
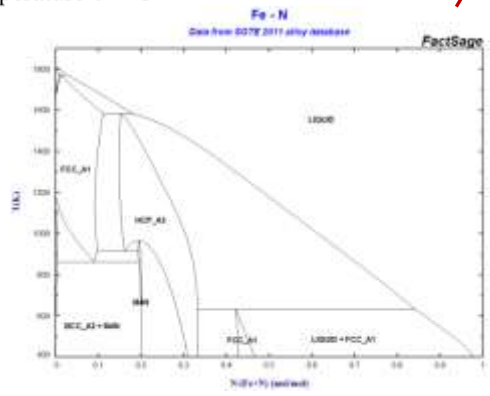
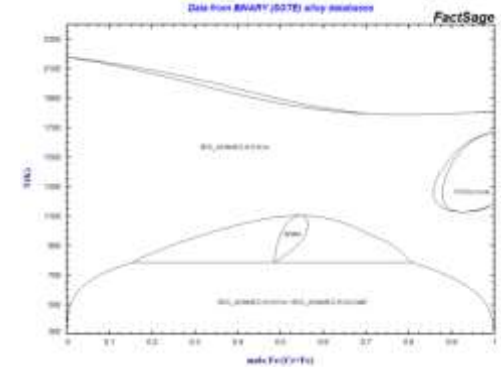
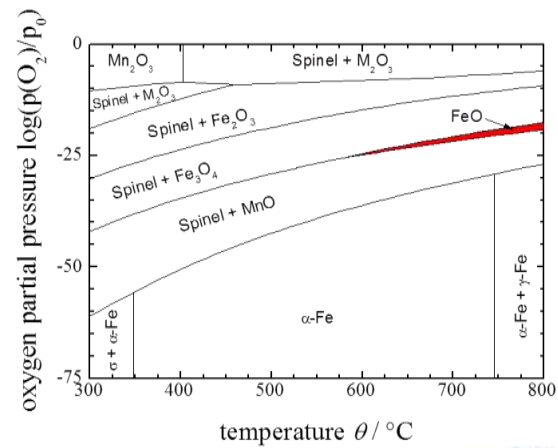
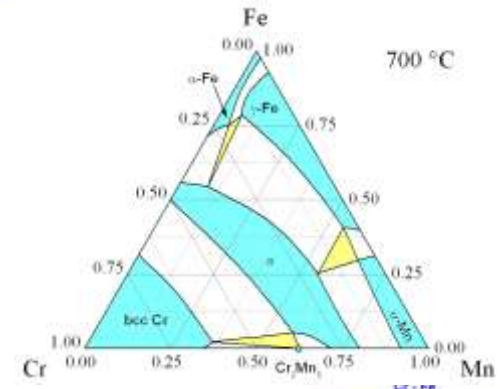
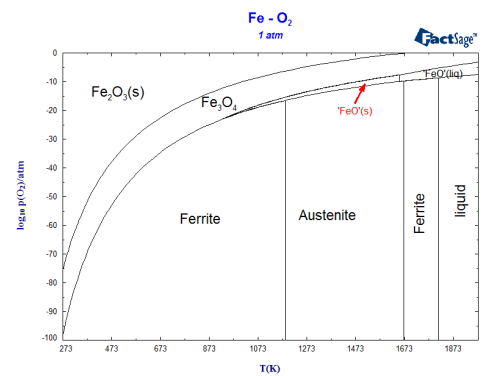
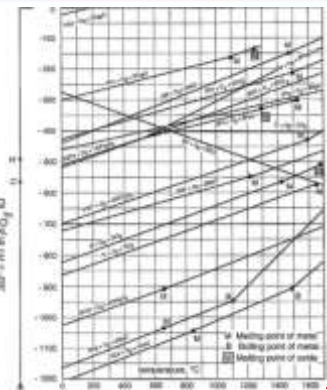
Conclusions – An Effective Solution



Conclusions – An Effective Solution



Conclusions – An Effective Solution





Max-Planck-Institut
für Eisenforschung GmbH

Dirk and Alexandra Vogel,
Else-Marie Müller-Lorenz,
Monika Nellessen



TECHNISCHE
UNIVERSITÄT
WIEN
Vienna University of Technology

Prof. H. Danninger
Vera G. Praig, Markus Holzweber,
Kurt Piplits

voestalpine
EINEN SCHRITT VORAUS.

Dr. D. Paesold
Bernhard Linder, Klaus Rendl,
Andreas Muhr

Funding



Christian Doppler
Forschungsgesellschaft

voestalpine
EINEN SCHRITT VORAUS.







Backup Slides

Additional Slides for the Presentation



Max-Planck-Institut für Eisenforschung GmbH

Head: Prof. Dierk Raabe



Founded in 1917 from the “Kaiser Wilhelm Institute”
by Fritz Wüst.

3 Departments:

Computational Materials Design

Interface Chemistry and Surface Engineering

Microstructure Physics and Alloy Design



Austria

Area: 83 879 km²

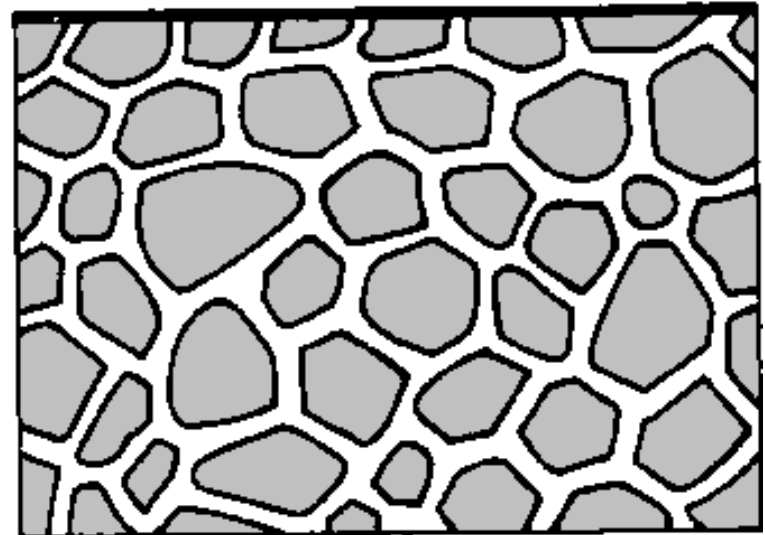
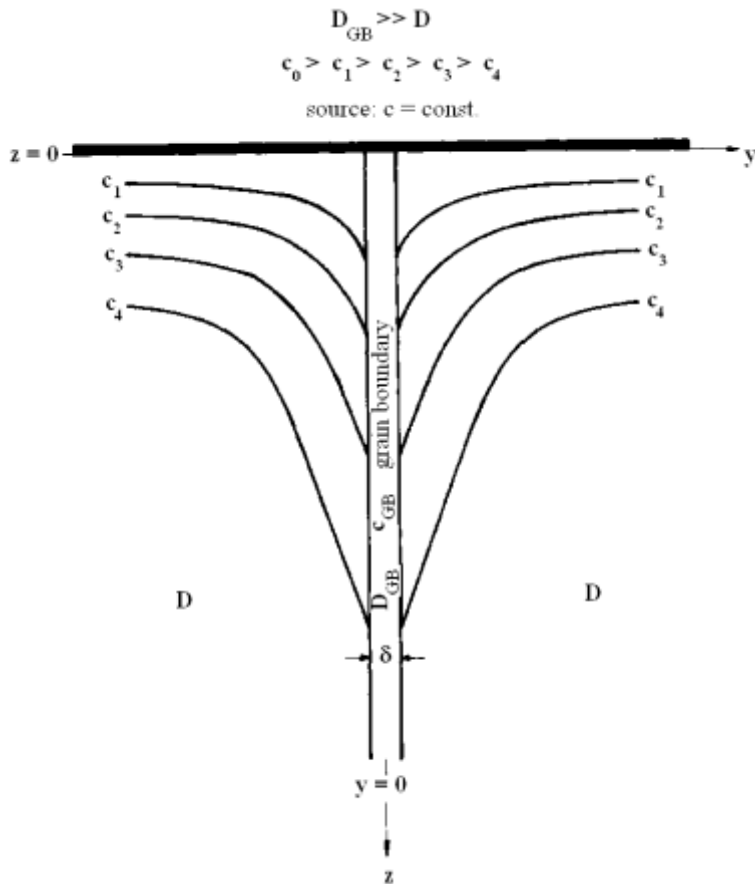
Inhabitants: ~ 8 405 000

Language: German

Capital: Vienna



Fisher's Model of Diffusion



Whipple – Le Claire equation

$$s \delta D_{GB} = 0.3292 \sqrt{\frac{D}{t}} \left(\frac{\partial \log \bar{c}}{\partial z^{6/5}} \right)^{-\frac{5}{3}}$$

Levine – MacCallum equation

$$s \delta D_{GB} = 0.4704 \sqrt{\frac{D}{t}} \left(\frac{\partial \log \bar{c}}{\partial z^{6/5}} \right)^{-\frac{5}{3}}$$



Internal Corrosion of Engineering Alloys: Experiment and Computer Simulation

Ulrich Krupp and Hans J. Christ

(Submitted July 18, 2005)

High-temperature corrosion is generally known as a material degradation process that occurs at the surface of engineering components. In the case of internal corrosion, the corrosive species penetrates into the material by solid-state diffusion leading to the formation of internal precipitates, for instance, oxides (internal oxidation), nitrides (internal nitridation), and carbides (carburation). It is known from numerous publications and technical failure cases that internal corrosion results in a strong deterioration of the properties of a material (i.e., near-surface embrittlement or the dissolution of strengthening phases). The present article introduces the classic theory of internal oxidation and reviews some recent research on internal corrosion phenomena that are closely related to the failure mechanisms of thermally grown protective oxide scales on several commercial high-temperature alloys (e.g., single-crystalline and polycrystalline Ni-base alloys and Cr steels). The mechanisms and kinetics of internal corrosion processes are determined by the temperature, the local chemical composition of the material, the solubility and diffusivity of the corrosive species, as well as the mechanical loading conditions. These influence factors are taken into account by means of a computer model combining a numerical finite-difference approach to solve the diffusion differential equations with the thermodynamic tool ChemApp. Using several examples, it is shown that the model has been applied successfully to simulate the internal nitridation, carburation, and oxidation of high-temperature alloys.



Temperature
 in Ar-H₂-H₂

D.J. Young^a, J. Z...

Depart^a School of Materials Science
^b Forschungszentrum Jülich

ARTICLE IN

Article history:
 Received 11 December 2004
 Accepted 22 February 2005
 Available online 26 February 2005

Keywords:
 A. Steel
 B. TEM
 C. Oxidation

1. Introduction

Internal corrosion is a generic kind of material degradation occurring at high temperatures that is driven by the inward diffusion of a corrosive species (i.e., oxygen, nitrogen, carbon, or sulfur, followed by internal precipitation of the respective oxides, nitrides, carbides, and sulfides).^[1] Contrary to the formation of superficial scales, which in the case of Cr₂O₃ and Al₂O₃ protect the substrate against excessive corrosion attack,^[2] internal corrosion may result in a deep deterioration of the physical properties of the material (e.g., creep resistance and high-temperature fatigue strength).^[3,4] Figure 1 shows an example of internal oxidation (Al₂O₃) and nitridation (AlN; penetration depth ξ = 600 μ m) underneath a thin Cr₂O₃ scale.

The mechanism of internal corrosion depends on the local concentrations and the diffusivities of the corrosive species and the metallic elements in the substrate. For the example shown in Fig. 1, a low oxygen partial pressure, $p(O_2)$, relative to the nitrogen partial pressure $p(N_2)$ in the combustion gas leads to conditions in the material interior, for

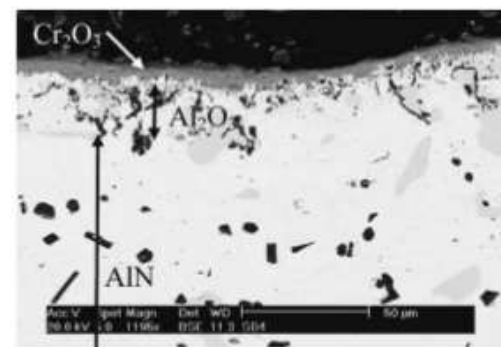


Fig. 1 Internal oxidation and nitridation attack of a failed natural gas burner tube of alloy 601 operated at $T = 1100$ °C

which AlN instead of Al₂O₃ is the thermodynamically most stable compound.*

Even in the case of Al₂O₃-scale-forming Ni-base super-

Oxidation of
 Pergam

INSTITUTE OF PHYSICS
 Modelling Simul

Per
 Dr
 A fini
 profil
 alloy^R

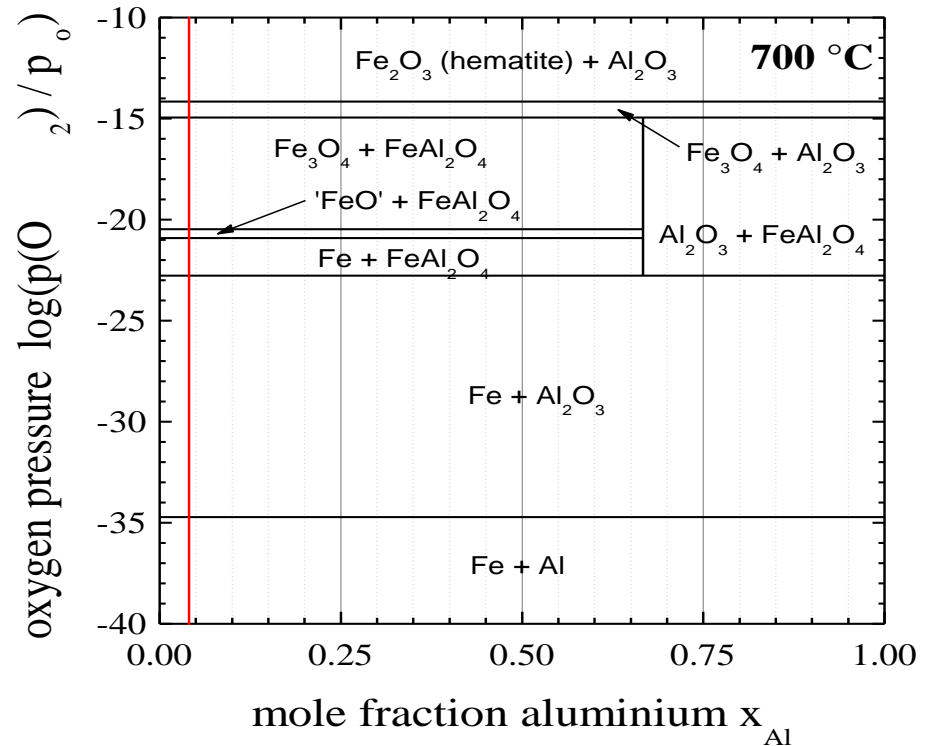
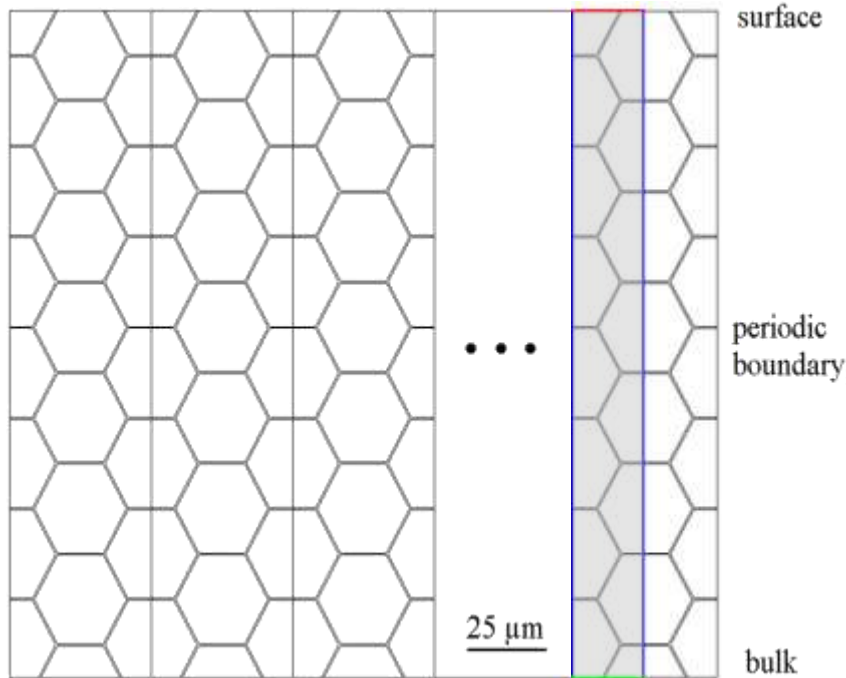
Oxidation
 Sa
 ac-
 an
 yr
 L

ates
 i is
 by
 ig
 it
 t
 This
 re the
 lose to
 t shown
 cal solu-
 tions are
 ortion

element migration

chemical reaction

$$\frac{dc_{i(x,t)}}{dt} = \text{div}(D_{i(x,T)} \cdot \nabla c_{i(x,t)})$$



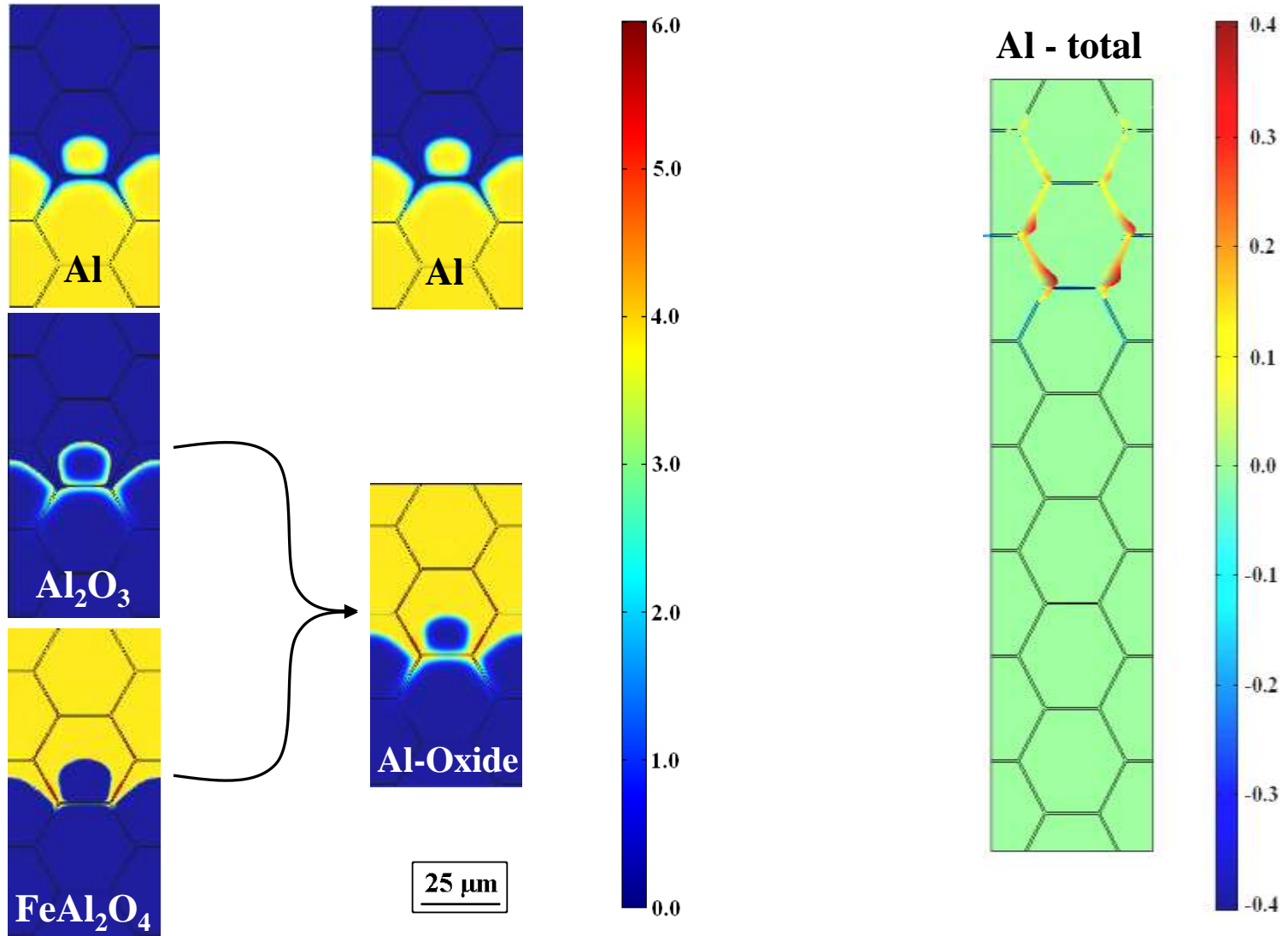


Figure: Spatial phase distributions of Fe, 2 wt-% Al (4.05 mol-% Al) after oxidation at $p(\text{O}_2) = 10^{-22}$ bar for 60 min at 700 °C.

Detail of a Grain Boundary

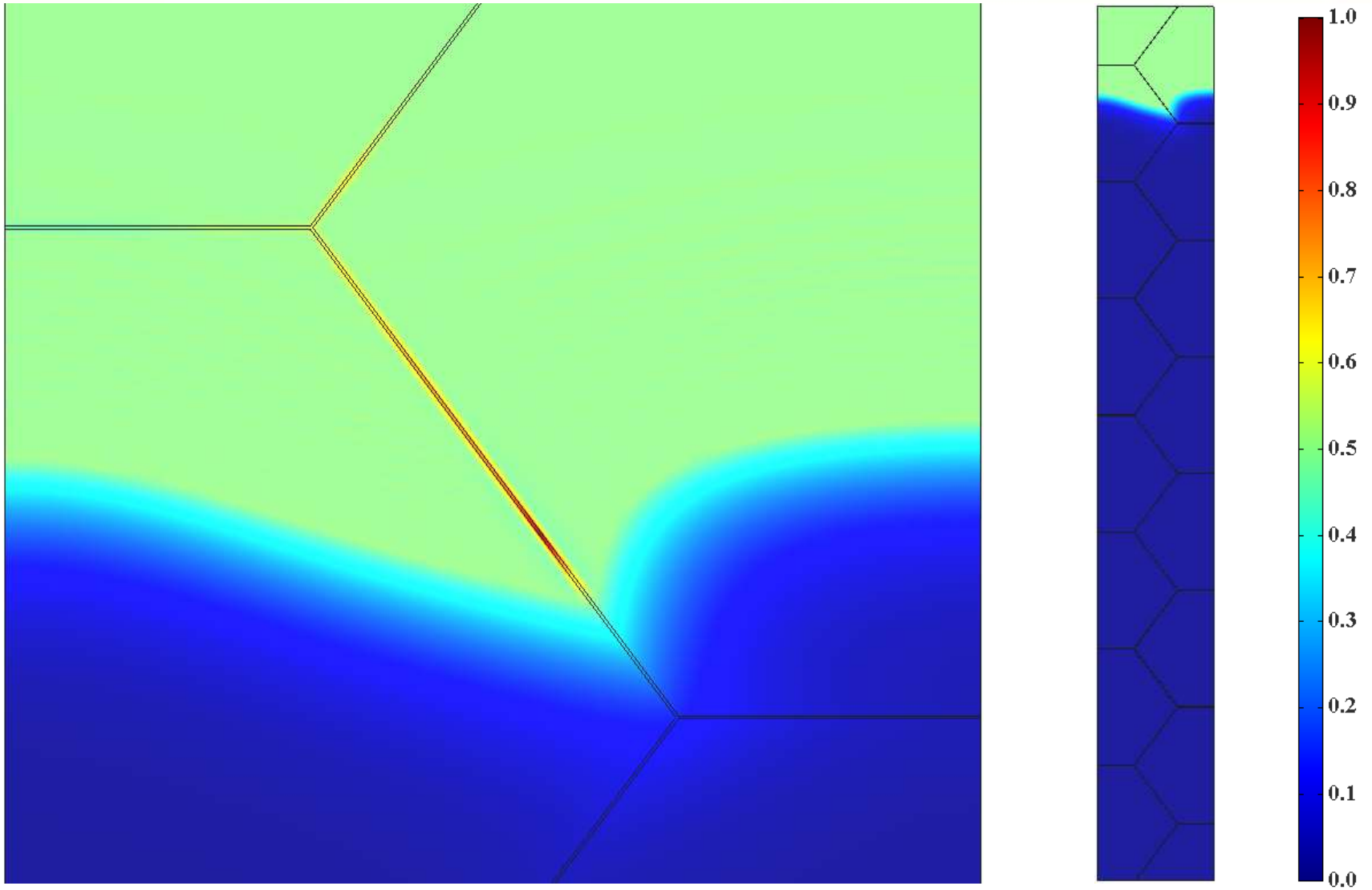


Figure: Spatial distribution of chromium oxides Cr_2O_3 and FeCr_2O_4 along a grain boundary in Fe, 3 wt-% Cr after finished cooling from 650 °C.

Diffusion between different Phases



$$J_A = -D \nabla c$$

$$J_A = -L \nabla \mu$$

$$J_A = -L \nabla \mu = -L \frac{\partial \mu}{\partial c} \nabla c = \dots = -L \underbrace{\frac{RT}{c}}_D \nabla c - L \left(\nabla \mu^o + \frac{RT}{\gamma} \nabla \gamma \right)$$

Figures: Shibuya (渋谷) crossing in Tokyo with green and red pedestrian lights.

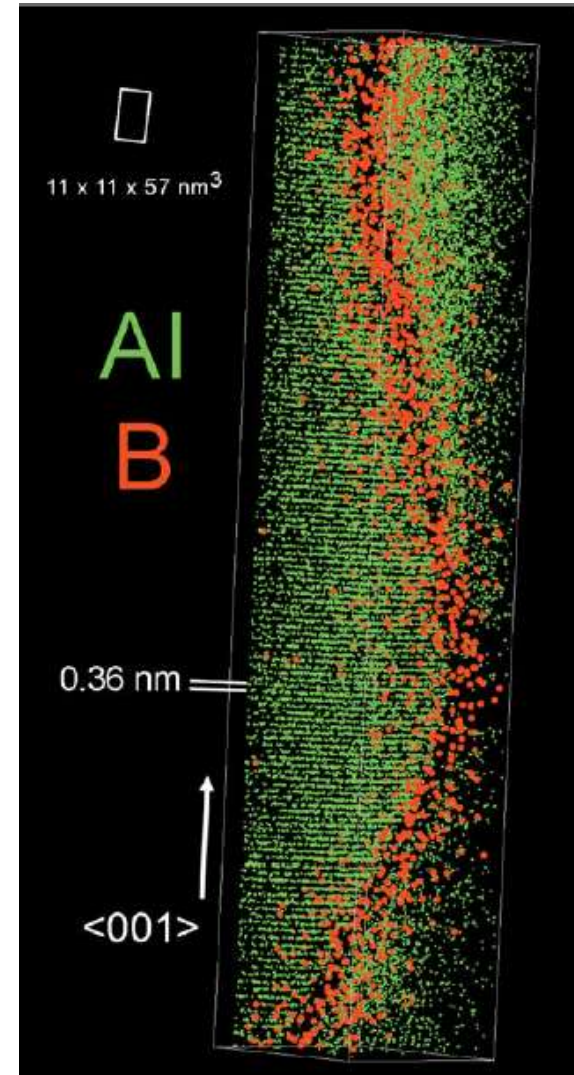
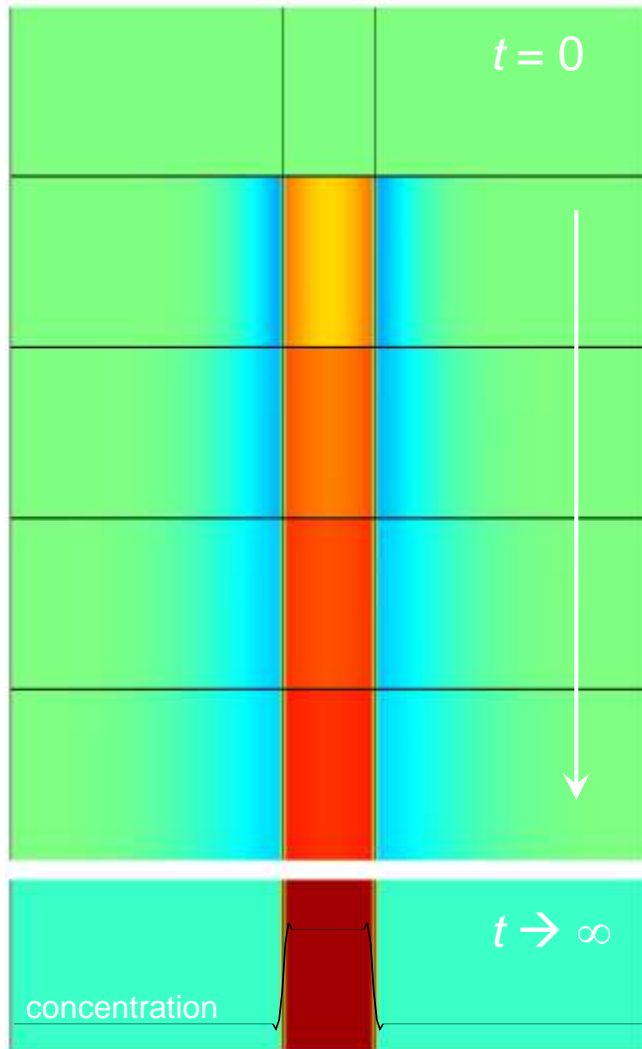
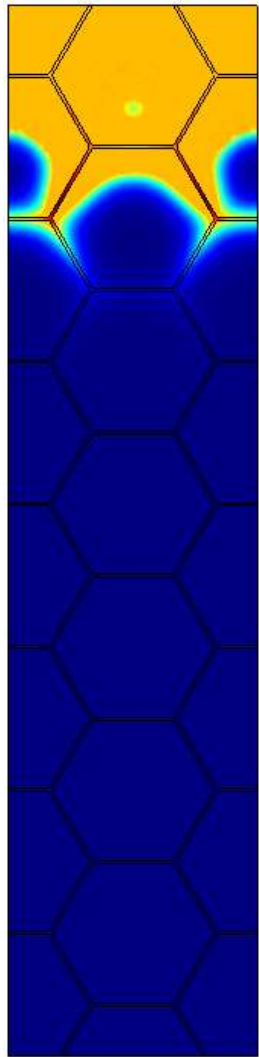
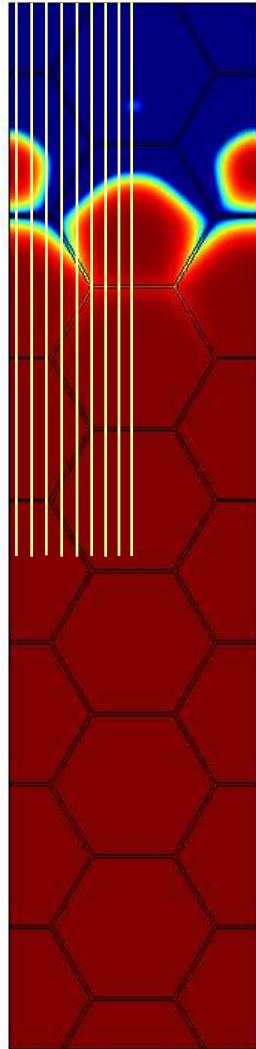


Figure: Numerical simulation of segregation (left) and 3D atom probe tomography of segregated boron atoms along the grain boundary in a NiAl superalloy [1] (right).

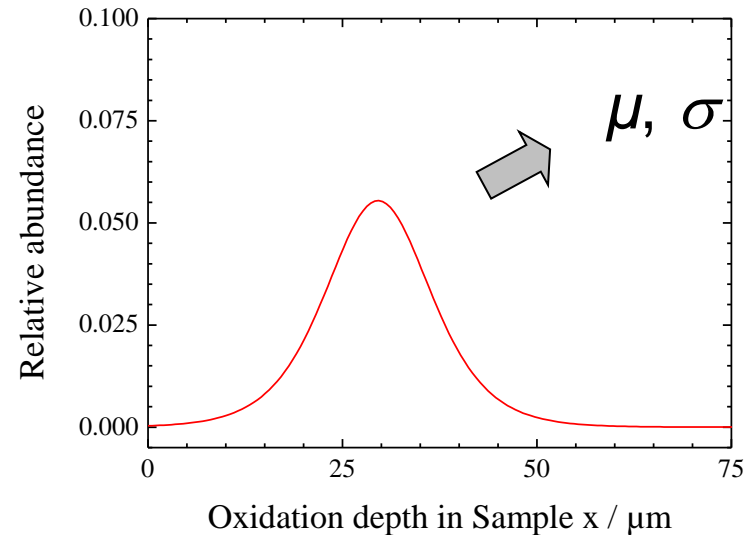
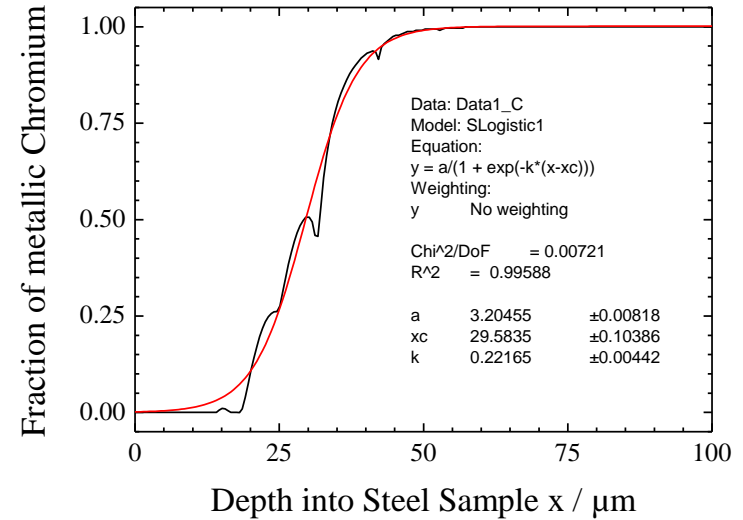
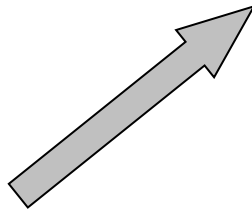
Calculation of the Oxidation Depth



Cr- oxides



metallic Cr



Multikomponentensysteme

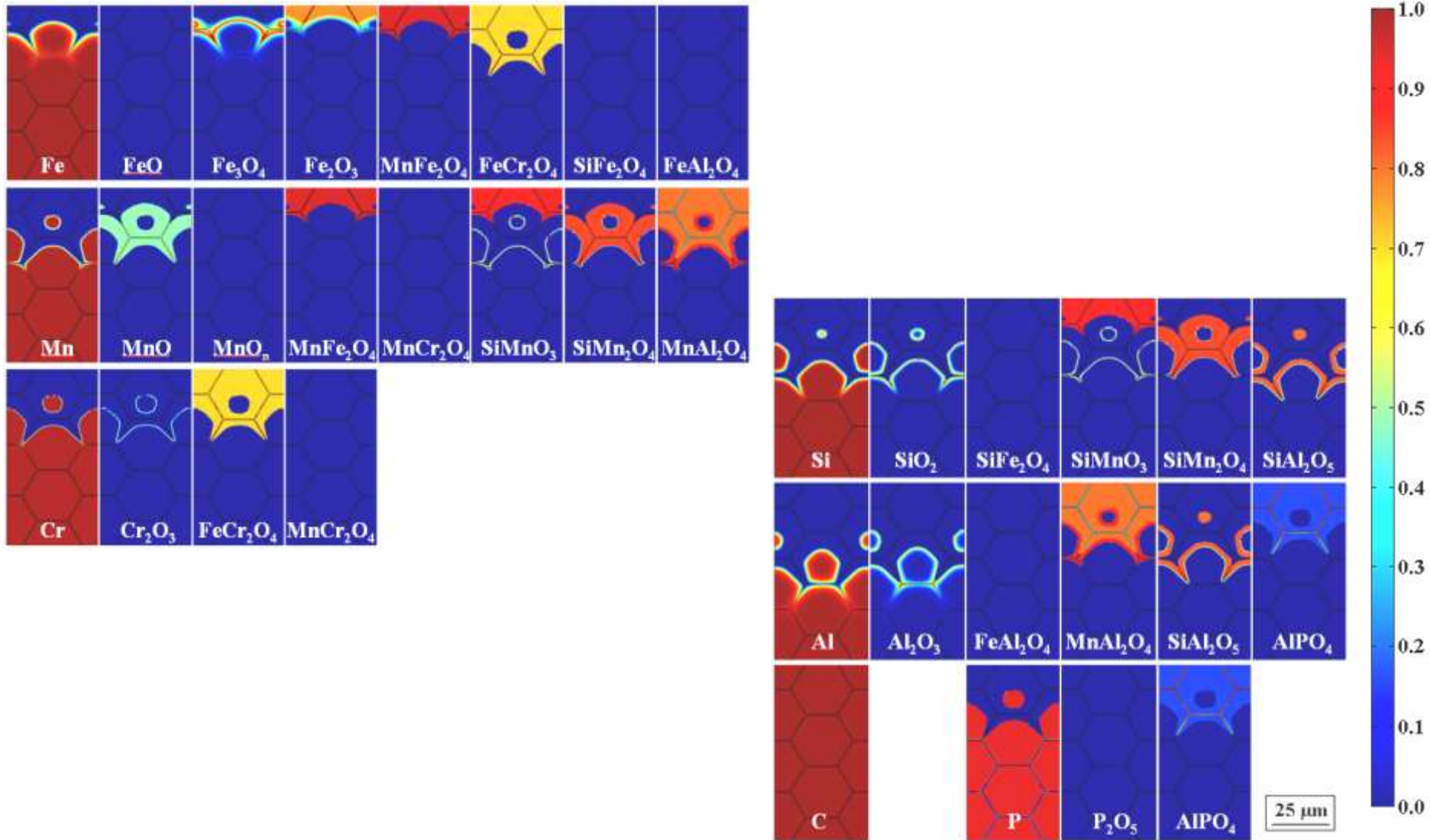
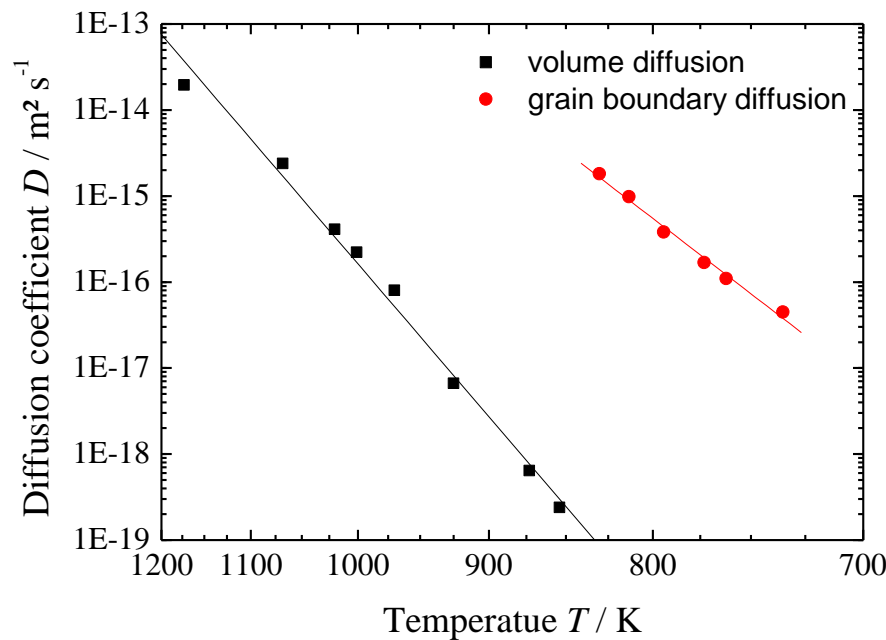


Abbildung: Phasenverteilung einer industrienahen Legierungszusammensetzung nach erfolgter Oxidation bei $p(\text{O}_2) = 10^{-22}$ bar und einer technischen Abkühlkurve.

$$\frac{dc_i(x,t)}{dt} = \text{div}(D_{i(x,T)} \cdot \nabla c_i(x,t)) + f(x,T,c_i(x,t))$$

Diffusion equation



$$D_{i(T)} = D_i^o e^{-\frac{Q}{RT}}$$

Figure: Temperature dependence of phosphorous diffusion in iron.

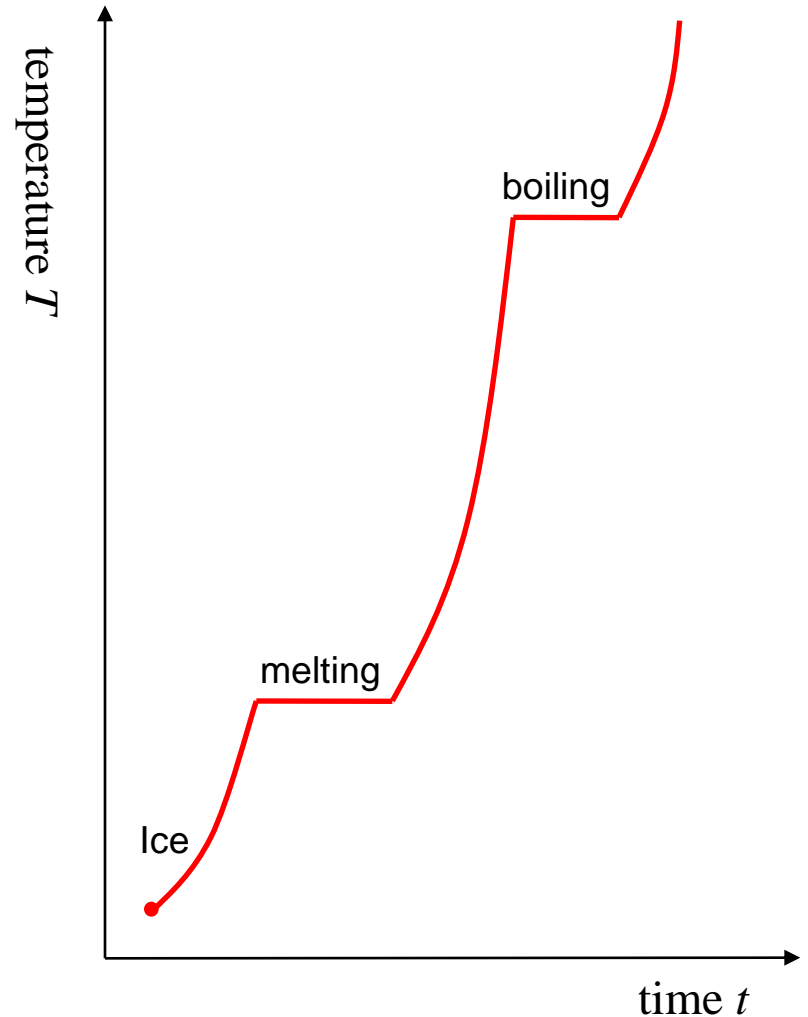
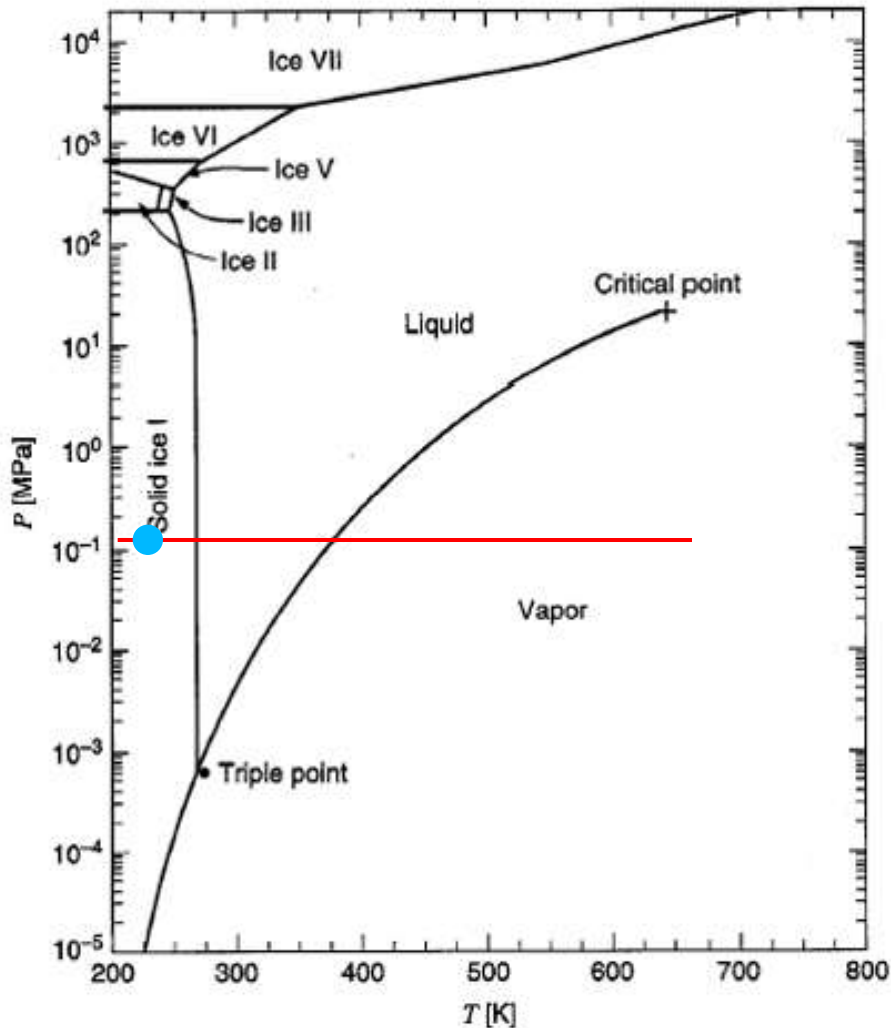
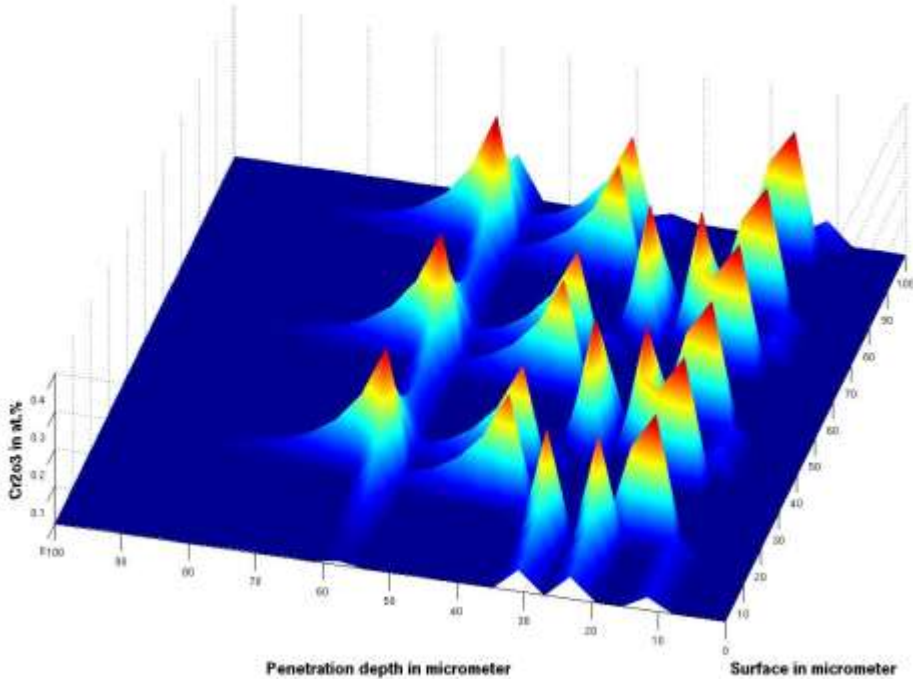
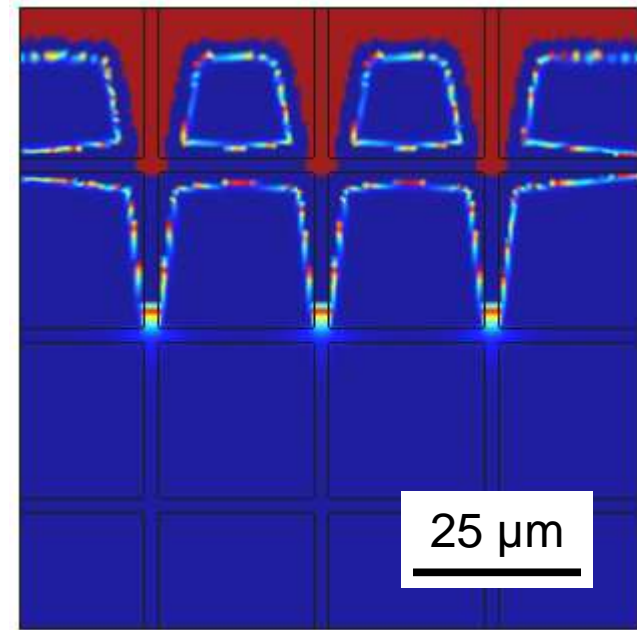


Figure: State diagram of water [2] (left) and schematic temperature evolution with constant heating (right).

Efficiency of the Calculation



300 FEM-points
Calculation time: 90 min



63 000 FEM-points
Calculation time: 120 min

Figure: Distribution of Cr_2O_3 in Fe, 0.67 wt-% Cr at 700 °C after 90 min. Simulation with InCorr (left) and with self-written programme (right).

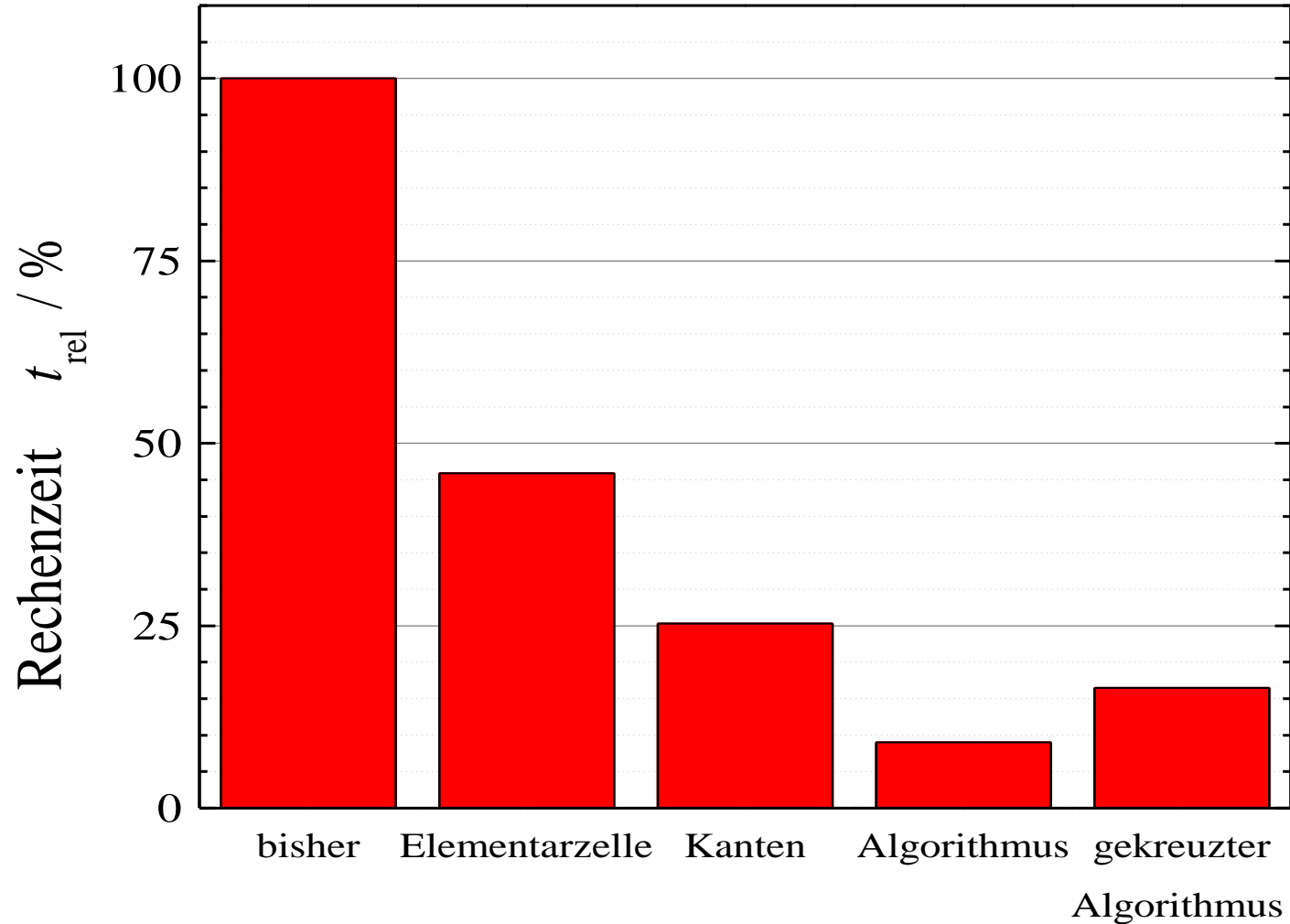


Abbildung: Abhängigkeit der Rechenzeit zur Simulation des Oxidationsverhaltens von Fe, 3 wt-% Cr bei verwendetem Kühlprogramm ab 650 °C (B).

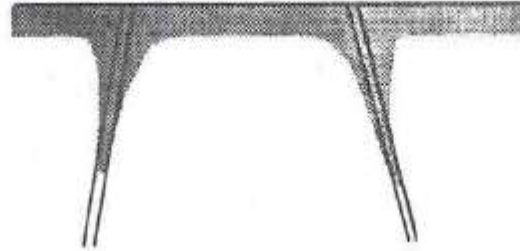
Grain Boundary Diffusion Regimes



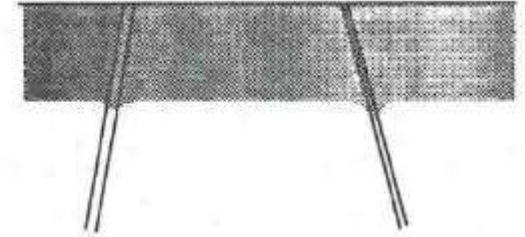
Coarse grained



C – regime

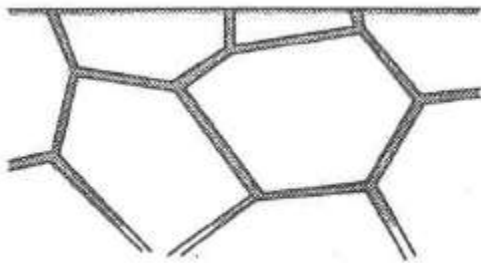


B – regime

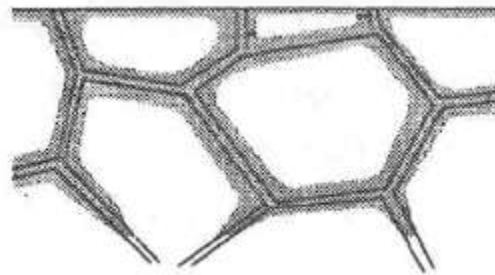


A – regime

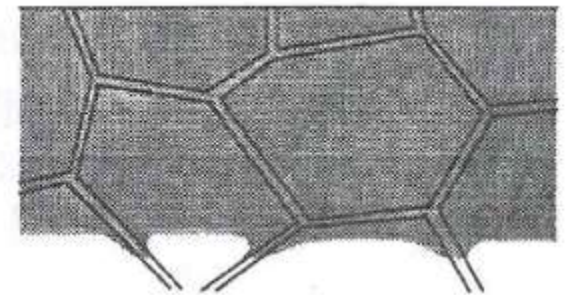
Fine grained



C' – regime



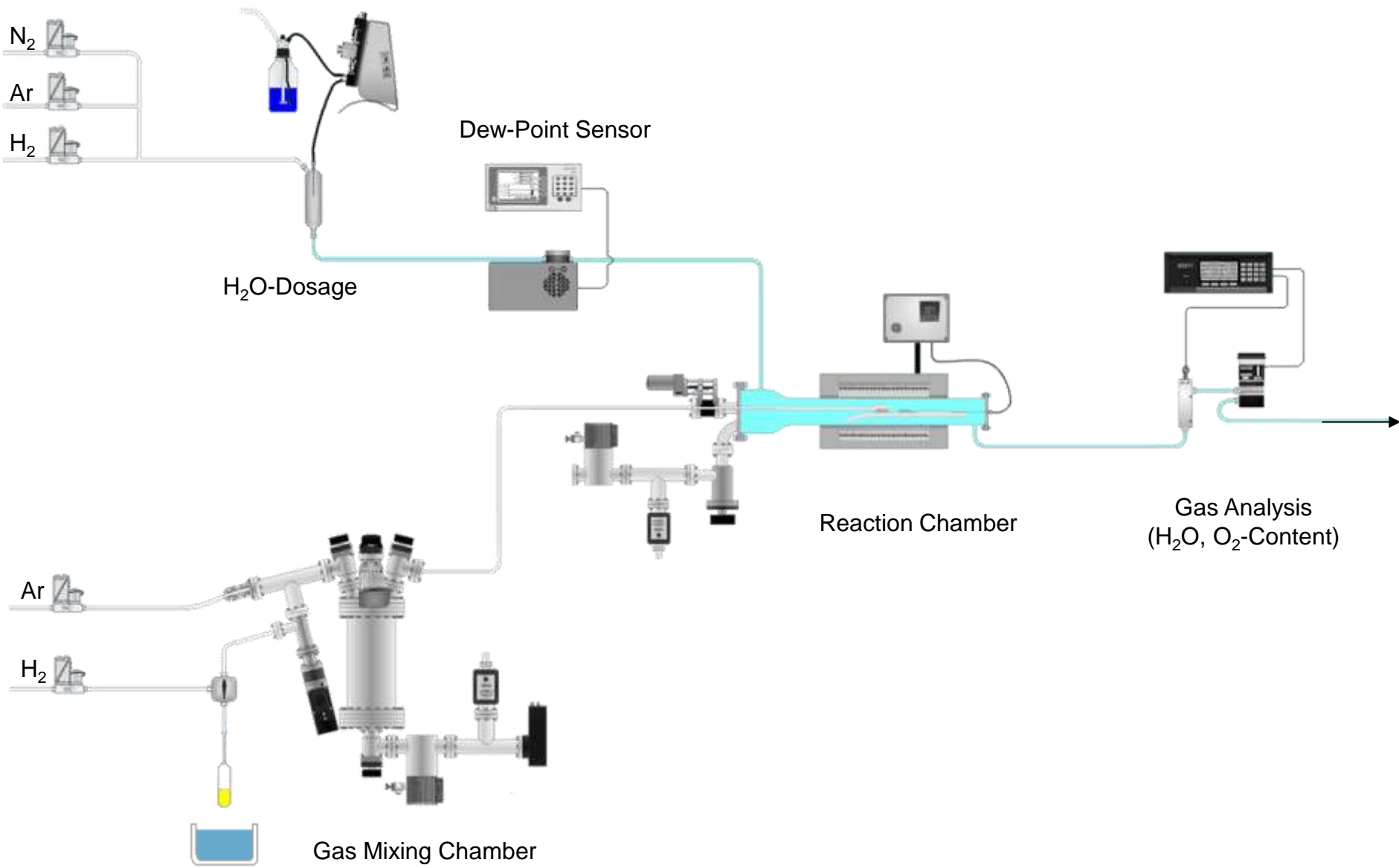
B' – regime



A' – regime

Figure: Illustration of different diffusion regimes, depending on total diffusion time and ratio of D_{GB}/D .

Experimental Set-up





Selective Decarburisation at 800 °C

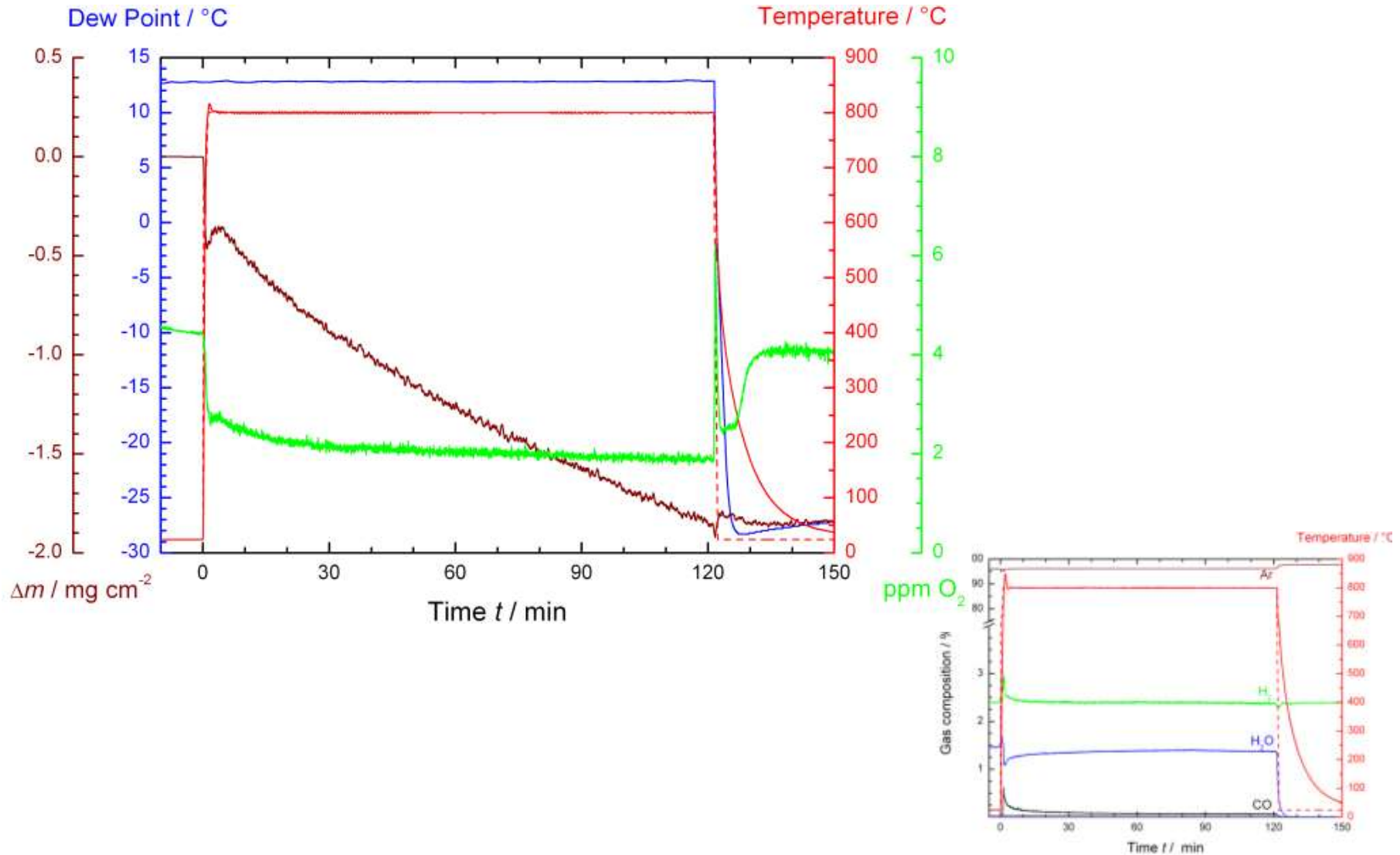


Figure: Experimental parameters during selective decarburisation of Fe, 0.8 wt-% C at 800°C in Ar / 2.5 vol-% H₂ / H₂O.

Selective Decarburisation at 800 °C



Fe, 0.8 wt-%C, 800 °C, Ar/2.5% H₂, DP+13°C

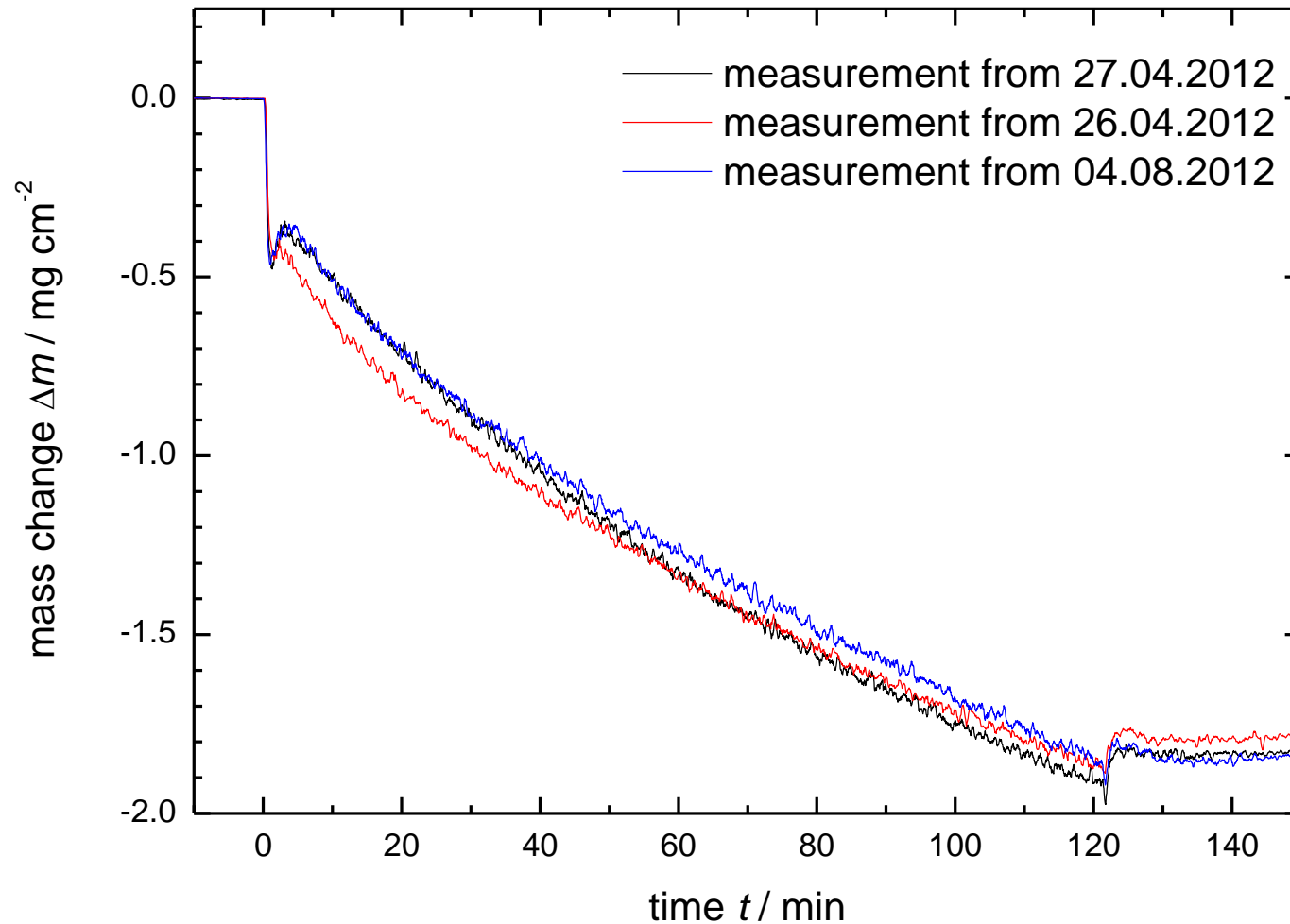


Figure: Mass change during selective decarburisation of Fe, 0.8 wt-% C at 800°C in Ar / 2.5 vol-% H₂ / H₂O.

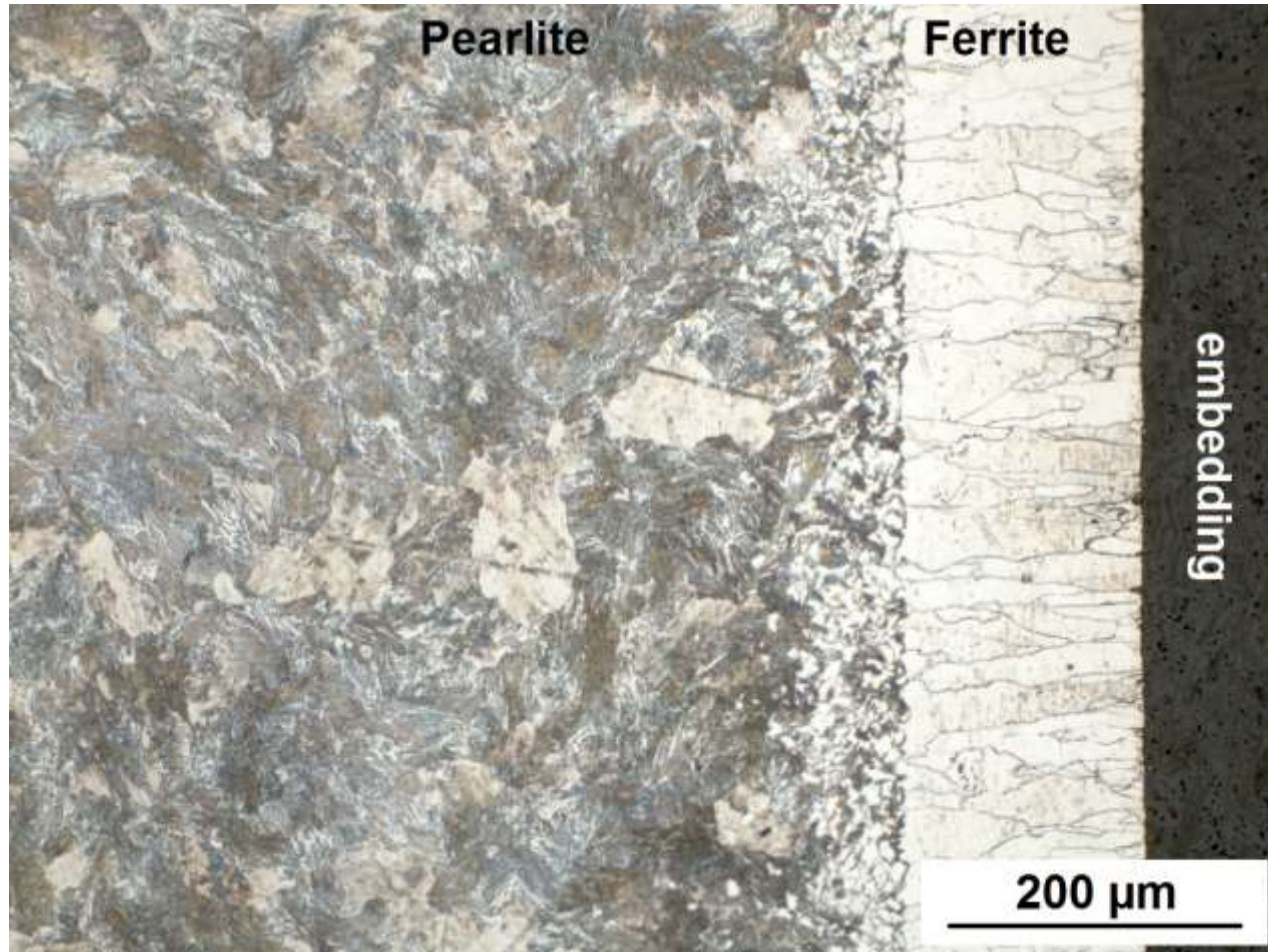


Figure: Cross section of Fe, 0.8 wt-% C after oxidation at 800 °C in Ar / 2.5 % H₂ / H₂O for 60 min. The cross section was etched with 1 % HNO₃ / Ethanol for 15 s.

Selective Decarburisation at 800 °C

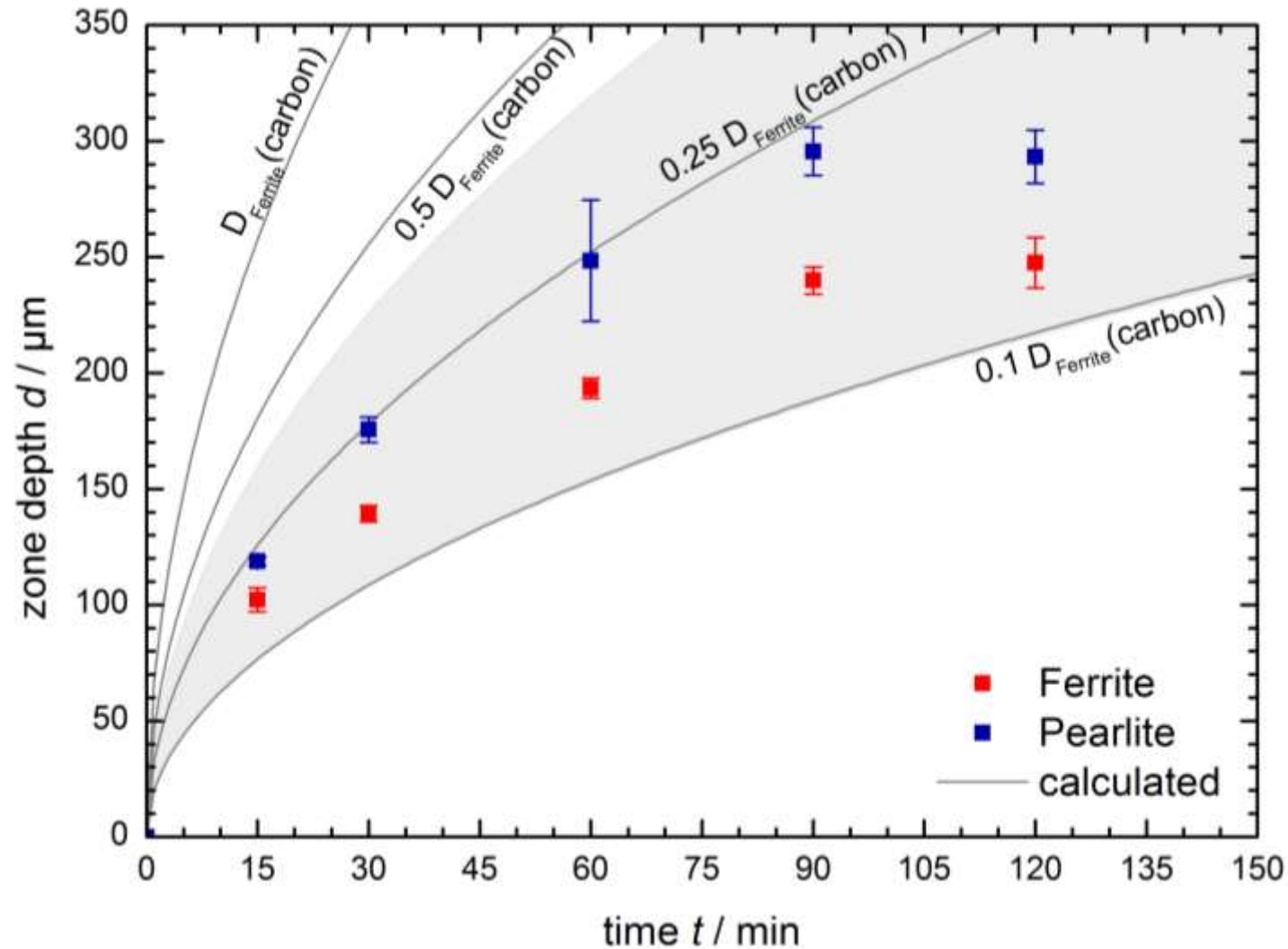


Figure: Evolution of the decarburised zone depth in Fe, 0.8 wt-% C after oxidation at 800 °C in Ar / 2.5 % H₂ / H₂O. The solid lines represent theoretical results.

Selective Decarburisation at 800 °C

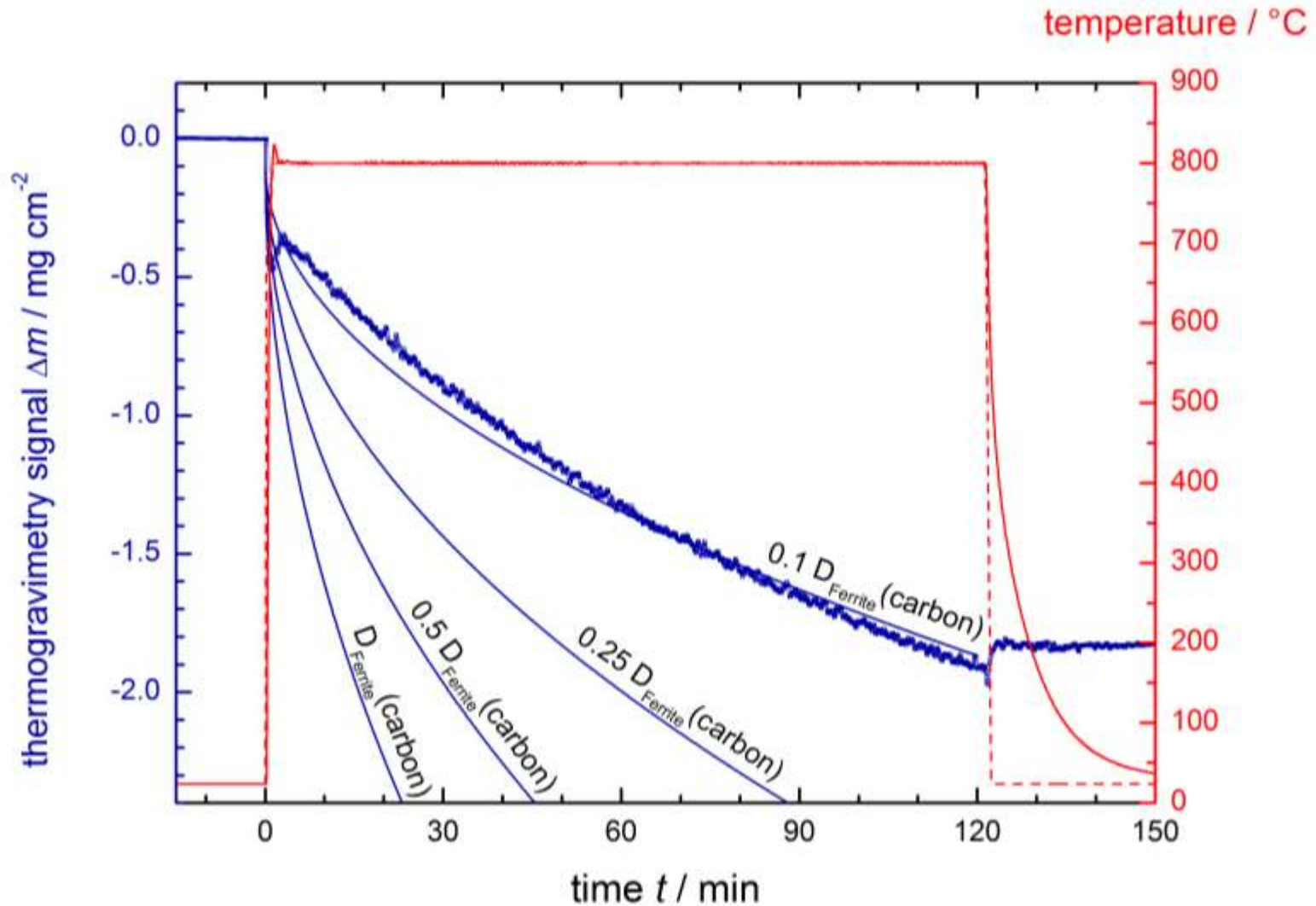
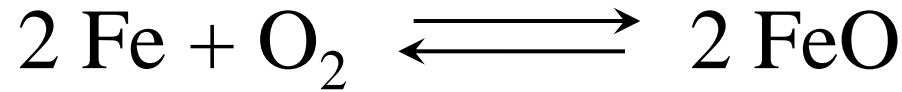


Figure: Evolution of the mass change in Fe, 0.8 wt-% C during oxidation at 800 °C in Ar / 2.5 % H₂ / H₂O. The solid lines represent the theoretical results.



$$\Delta G_{(T)}^{\text{Formation}} \approx 2 \mu_{(T)}^{\text{FeO}} - 2 \mu_{(T)}^{\text{Fe}} - \mu_{(T)}^{\text{O}_2} \stackrel{!}{=} 0$$

$$0 = 2 G_{(T)}^{o, \text{FeO}} + 2 RT \ln(a_{\text{FeO}}) - 2 G_{(T)}^{o, \text{Fe}} - 2 RT \ln(a_{\text{Fe}}) - G_{(T)}^{o, \text{O}_2} - RT \ln\left(\frac{p_{\text{O}_2}}{p_o}\right)$$

$$\Delta G_{(T)}^{o, \text{Formation}} = 2 G_{(T)}^{o, \text{FeO}} - 2 G_{(T)}^{o, \text{Fe}} - G_{(T)}^{o, \text{O}_2} = -RT \ln\left(\frac{p_{\text{O}_2}}{p_o}\right) + 2 (RT \ln(a_{\text{FeO}}) - RT \ln(a_{\text{Fe}}))$$

$$\underbrace{2 G_{(T)}^{o, \text{FeO}} - 2 G_{(T)}^{o, \text{Fe}} - G_{(T)}^{o, \text{O}_2}}_y = -R \ln\left(\frac{p_{\text{O}_2}}{p_o}\right) T + \underbrace{0}_d$$



Nitride Stability

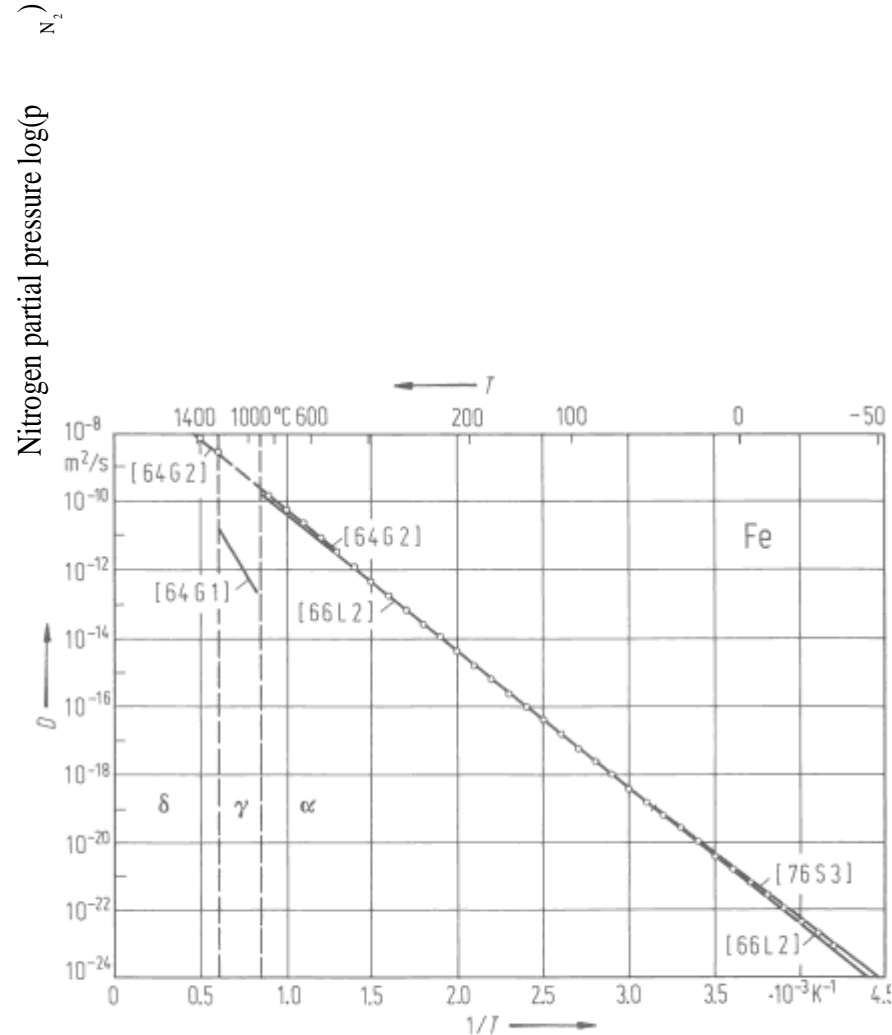
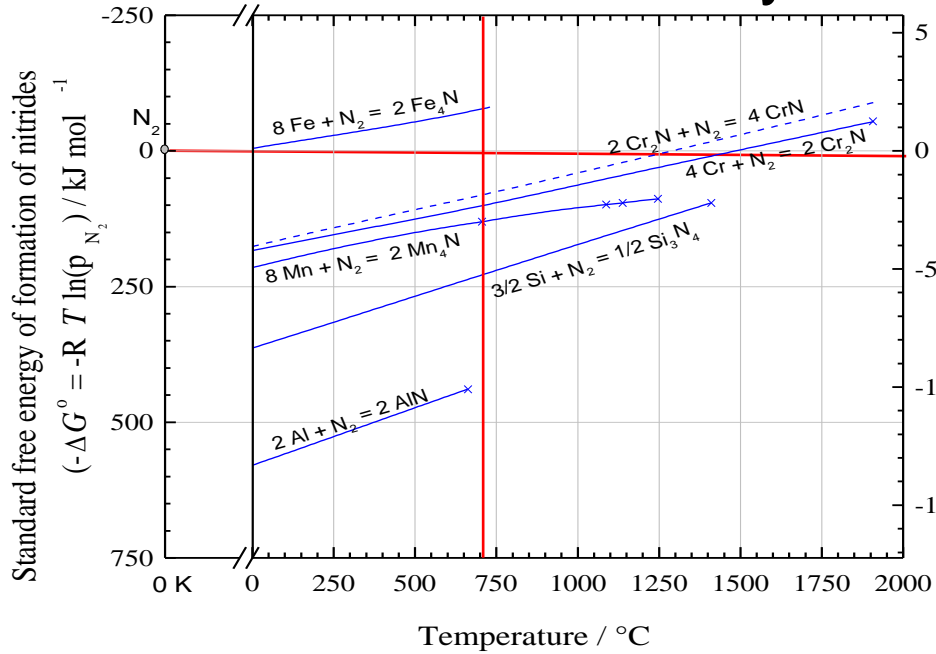
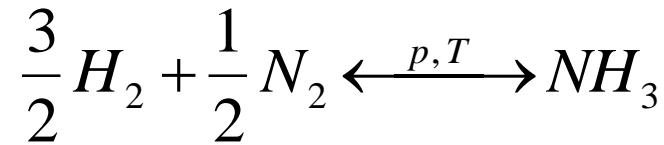


Fig. 22. Fe. Diffusion coefficient for N diffusion in α , γ and δ -phase Fe vs. (reciprocal) temperature. Circles: calculated from equation quoted from [76S3].



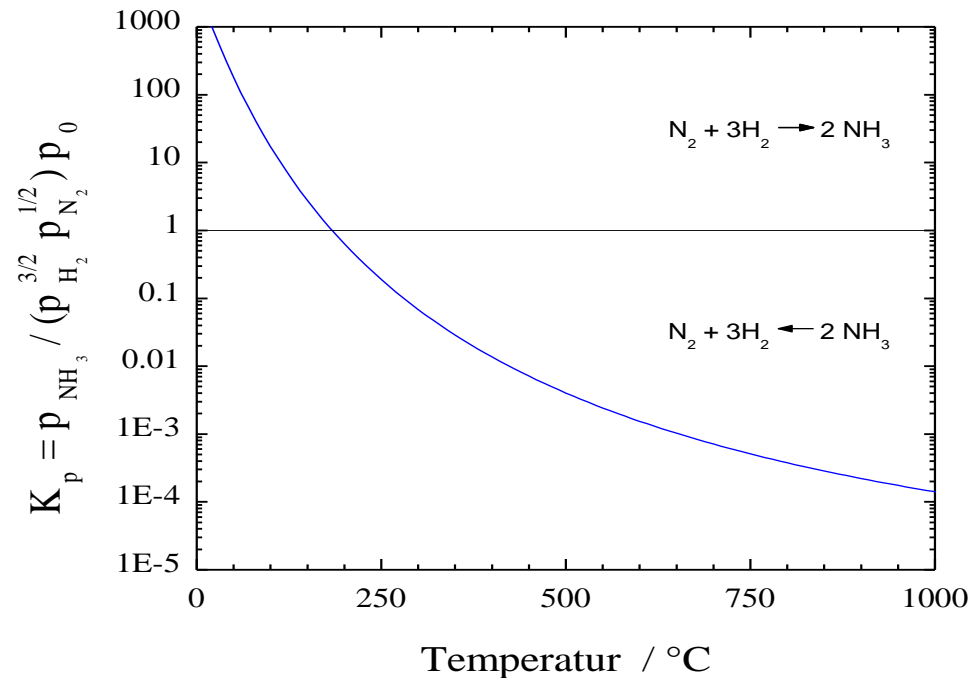
$$G_{(T)}^{NH_3} - \frac{3}{2} G_{(T)}^{H_2} - \frac{1}{2} G_{(T)}^{N_2} \stackrel{!}{=} 0$$

$$K_{p(T)} = e^{-\frac{G_{NH_3, (T)}^{\circ} - \frac{3}{2} G_{H_2, (T)}^{\circ} - \frac{1}{2} G_{N_2, (T)}^{\circ}}{RT}}$$

$$K_{p(T)} = \frac{p_{NH_3}}{p_{H_2}^{1.5} p_{N_2}^{0.5}} p_0$$

$$K_N \stackrel{!}{=} \frac{p_{NH_3}}{p_{H_2}^{1.5}} \sqrt{p_0}$$

$$K_N = \sqrt{p_{N_2}} \frac{K_{p(T)}}{\sqrt{p_0}}$$



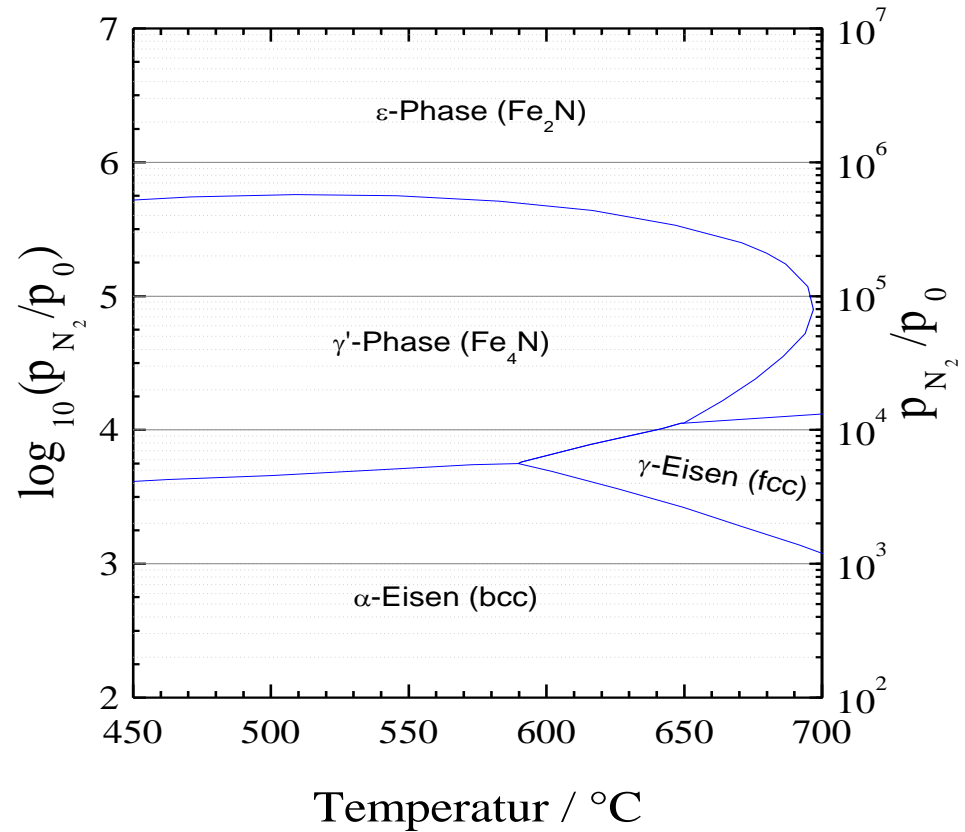
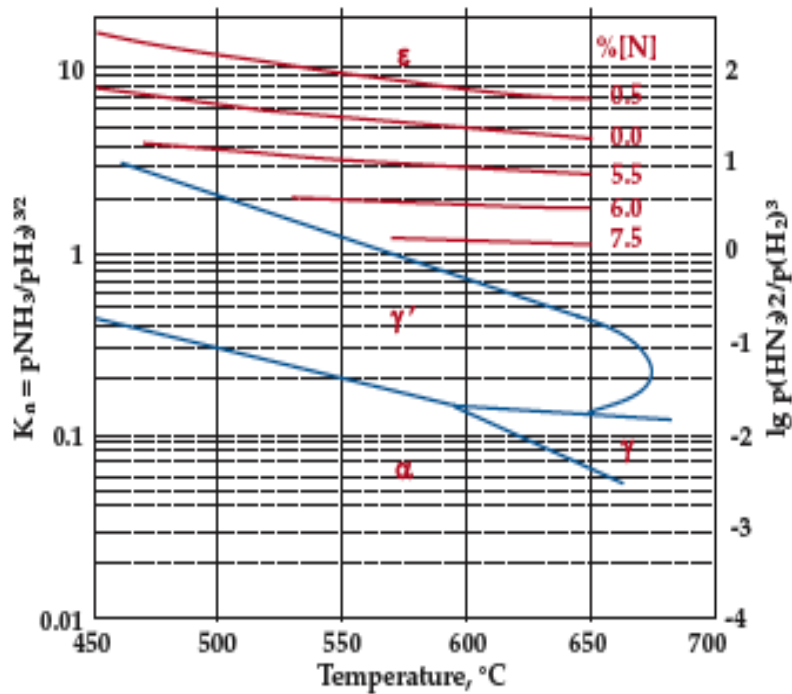


Figure: Lehrer-Diagramm of iron nitrides according to literature (left) and stability diagram calculated with the programme FactSage (right).