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AACHEN KNOW-HOW CENTRE RESOURCE TECHNOLOGY

Selected fields of application for FactSage-Modelling in nonferrous metallurgy

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DIE METALLURGEN

IME – Research in nonferrous metallurgy

General

Institute of RWTH Aachen University

30 Researchers, 30 technical/administrative staff

30 BSc- and 20 MSc-thesis per year

> 500 publications since 1999

Recycling-Metallurgy

Process development and Scale Up

Pyro- and Hydrometallurgy

Minimization of emissions, waste material recycling

Process technology for metallic materials

Vacuum metallurgy

Purification of metals and alloys

Nano powders

Services and consulting

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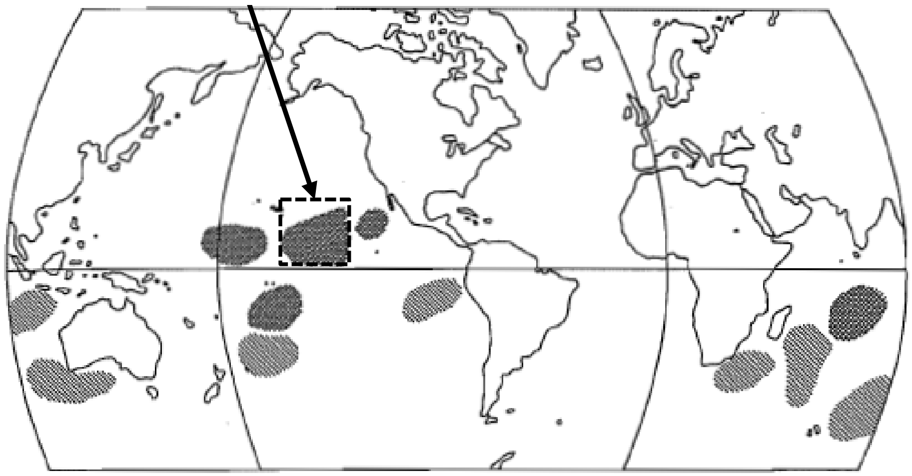
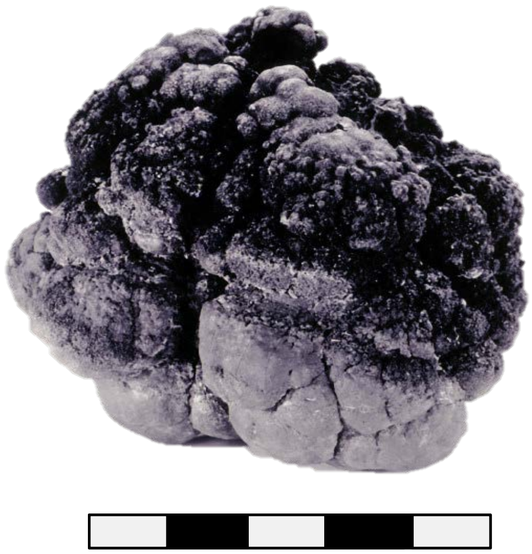
Study I: Smelting and carbothermic reduction of manganese nodules

Goals:

- Simulation of ocean nodule smelting
- Approximation of the liquidus temperature of the molten slag
- Influence of SiO_2 content on the liquidus temperature
- Simulation of the carbothermic metal reduction from liquid slag
  ➔ Can Mn and Fe content be separated from metal values (Ni, Cu, Co, Mo, V)?

Nodule occurrence with current research licenses





Study I: Smelting and carbothermic reduction of manganese nodules

Model simplifications:

- All metals in ocean nodules occur as simple oxides (see table below)
- Oxides of P, Ba and Sr are not considered, since the slag solution database (FToxid) does not contain data
- 15 component system, elements < 500 ppm are not considered
- Influence of the atmosphere during smelting is omitted

Reality:

- Metals occur as complex oxidic, hydroxidic, carbonate or phosphate minerals (e.g. $Na_4Mn_{14}O_{27}$•$21H_2O$)
- Approximately 0.7 wt.-% P+Ba+Sr in ocean nodules
- Nodules contain nearly all elements of the periodic table
- Smelting in an open electric arc furnace

Metal oxides considered in model [wt.-%] of 100%

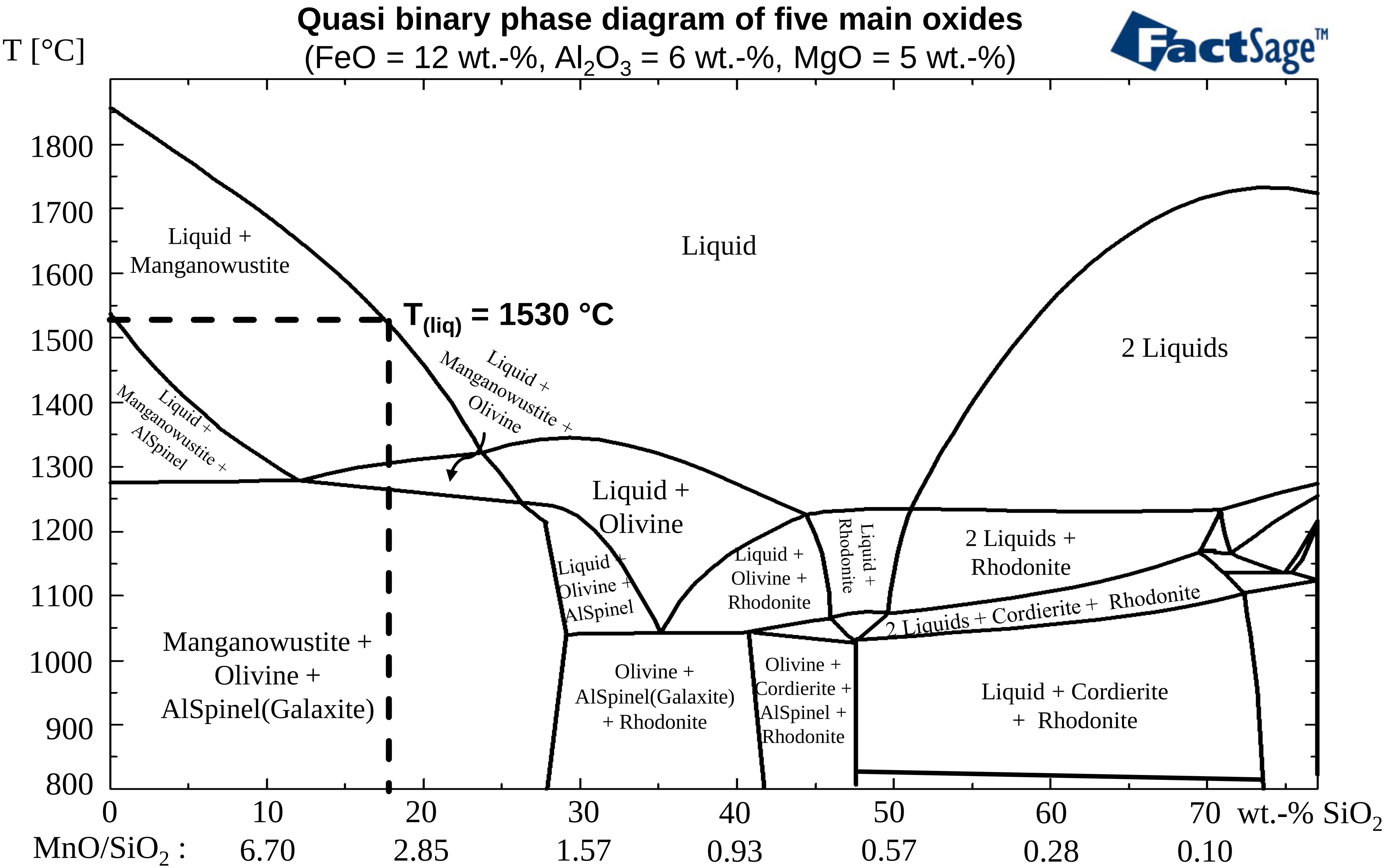
Average of 206 BGR samples → heavy fluctuation in composition

MnO	SiO_2	FeO	Al_2O_3	MgO	Na_2O	CaO	NiO	CuO	K_2O	TiO_2	CoO	ZnO	V_2O_5	MoO_3
51.2	16.1	10.1	5.44	4.05	3.47	2.88	2.19	1.86	1.50	0.54	0.27	0.24	0.13	0.12

Databases:

- FactPS
- FToxid (liquid slag and solid solutions)
- SGTE (liquid alloy)

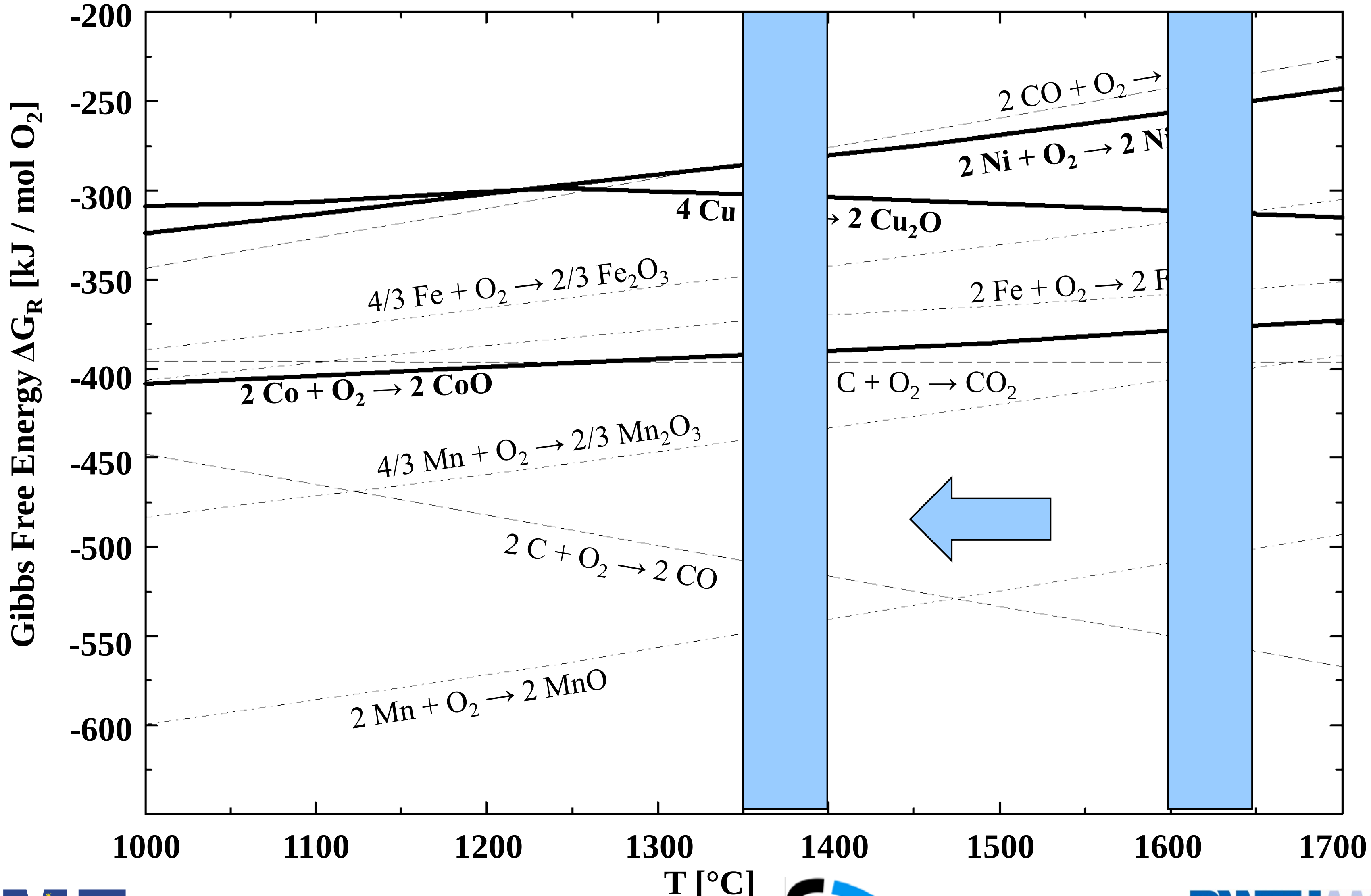
Study I: Smelting and carbothermic reduction of manganese nodules



Study I: Smelting and carbothermic reduction of manganese nodules

Activity adjusted Ellingham diagram

(activites of oxides in slag from equilib model)



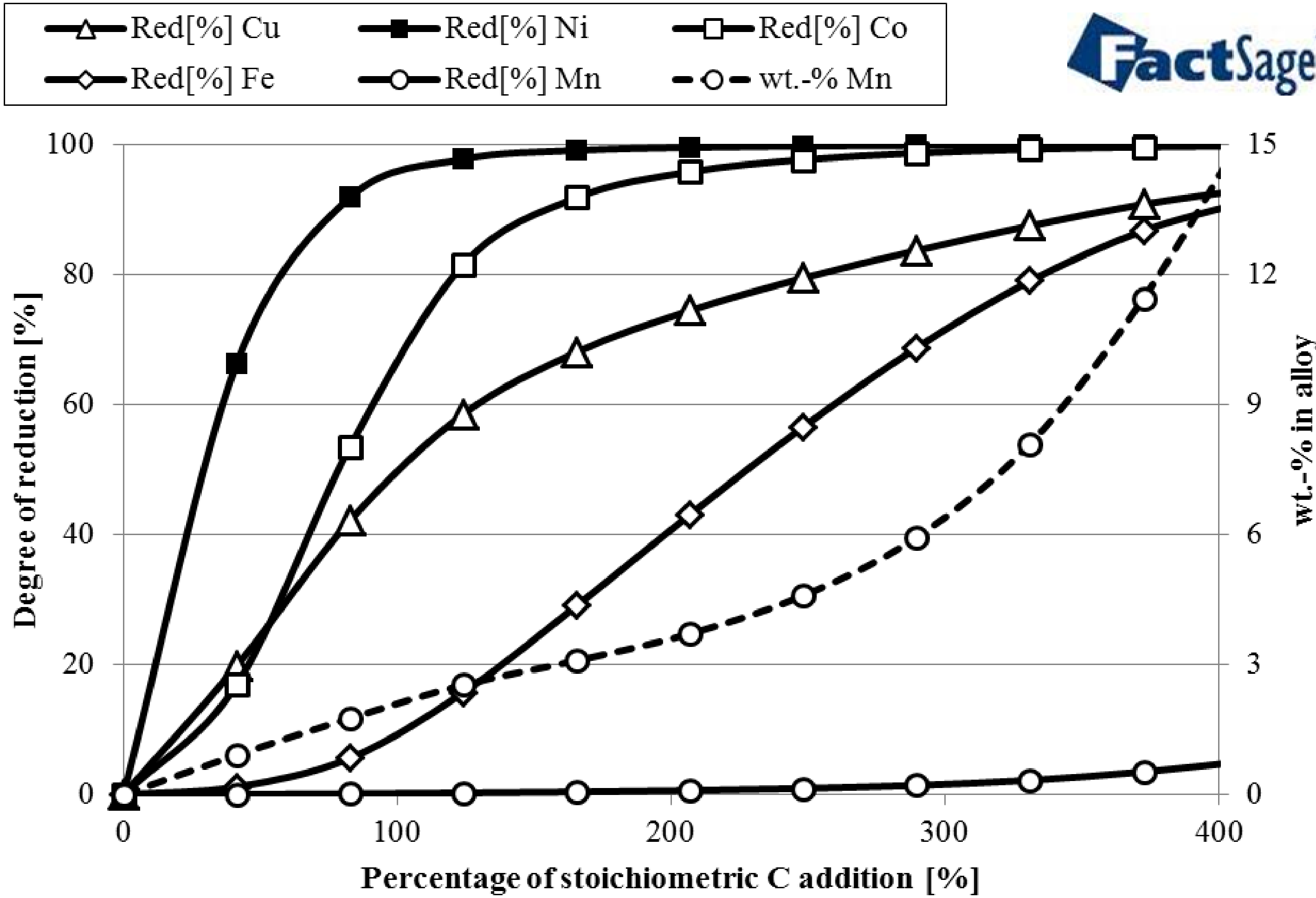
Study I: Smelting and carbothermic reduction of manganese nodules

Equilib model of metal reduction

No SiO_2 addition

MnO/SiO_2 = 3.2

➔ T = 1650 °C



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Study I: Smelting and carbothermic reduction of manganese nodules

Equilib model of metal reduction

High SiO_2 addition ➔ 351.54 g/kg SiO_2

MnO/SiO_2 = 1

➔ T = 1400

Results:

- SiO_2 addition decreases liquidus temperature significantly
- Metal reduction may be carried out at lower temperature
- Mn reduction becomes thermodynamically adverse
- Fe reduction cannot be avoided thermodynamically

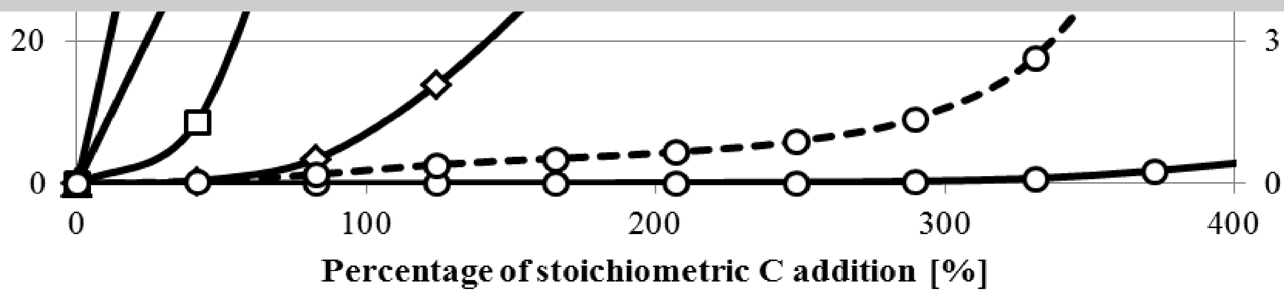
Key points from model for experiments:

➔ MnO/SiO_2 ratio should be between 1.5 and 1

➔ Control of reduction is critical to attain low Mn-content in alloy

➔ Complete separation of Mn in slag is improbable because of the reduction of Mn_2O_3

➔ Trade-off between undesired Fe reduction and valuable metal recovery is necessary



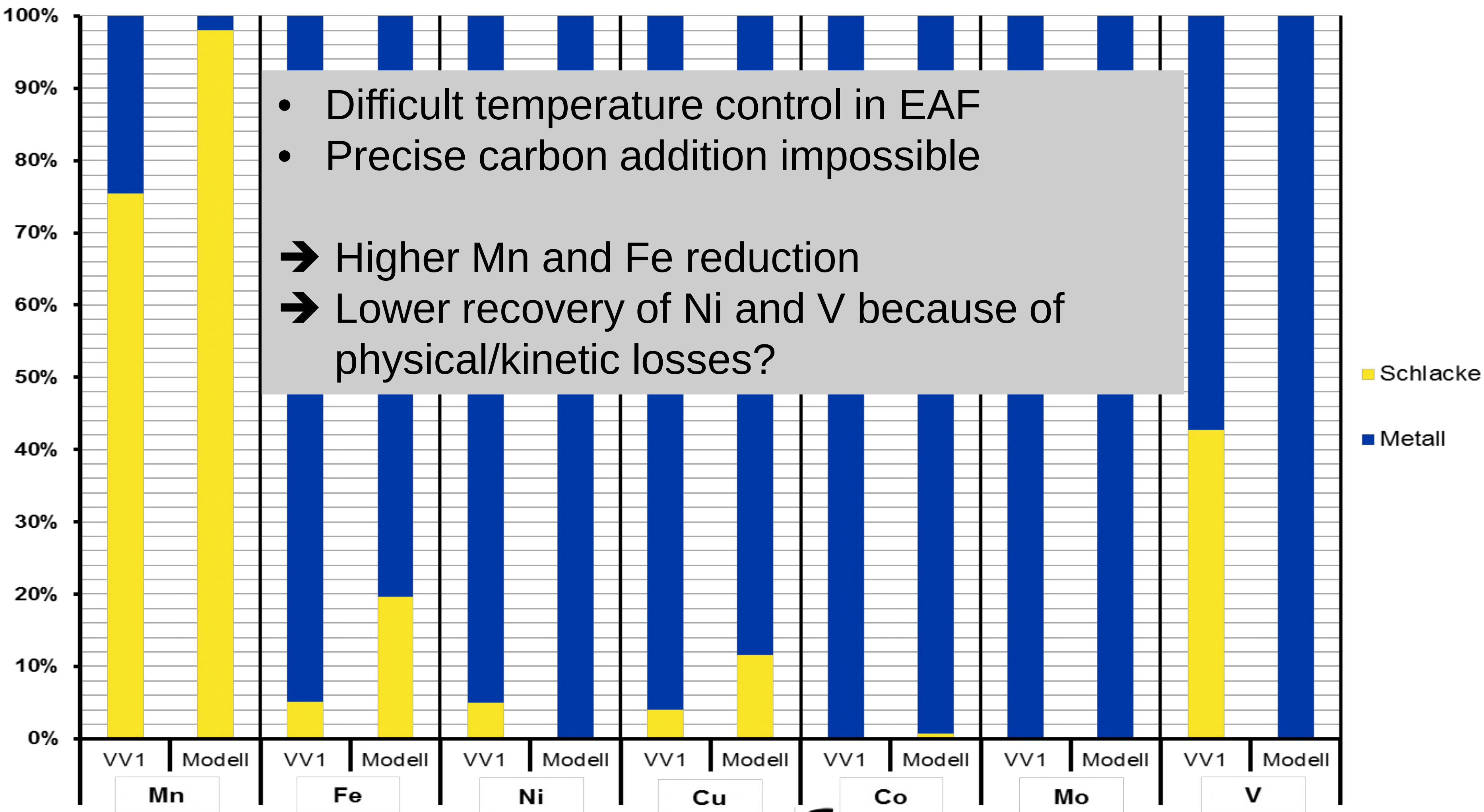
Study I: Smelting and carbothermic reduction of manganese nodules

Study I: Smelting and carbothermic reduction of manganese nodules

Comparison of model and experiments:

No silica addition ~1650 °C

Phase distribution comparison



- Difficult temperature control in EAF
- Precise carbon addition impossible

➔ Higher Mn and Fe reduction
➔ Lower recovery of Ni and V because of physical/kinetic losses?

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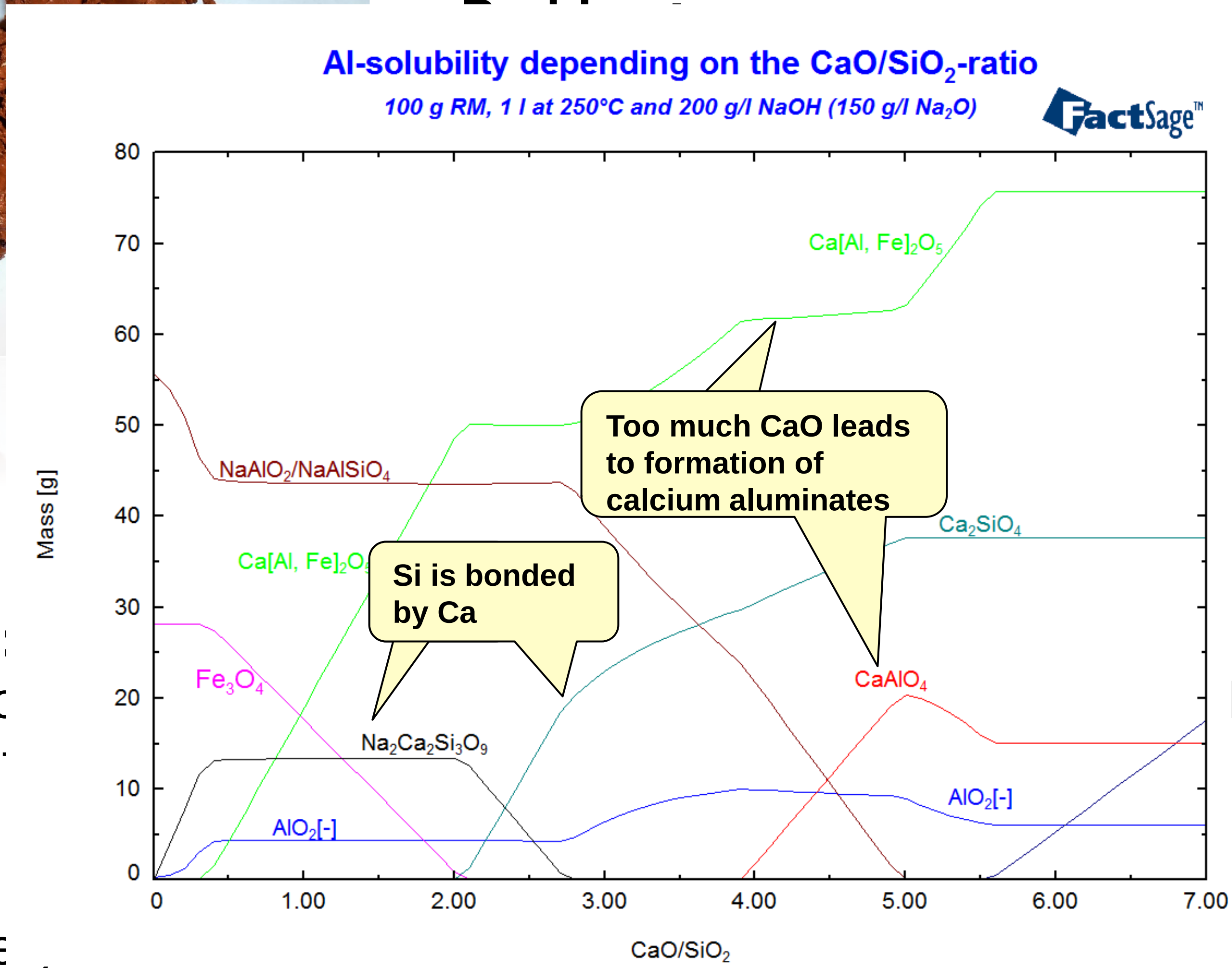
Study II: Recovery of valuable metals Al and Fe from red mud



Approach:

Recovery c … he Bayer

process wi

Goal:

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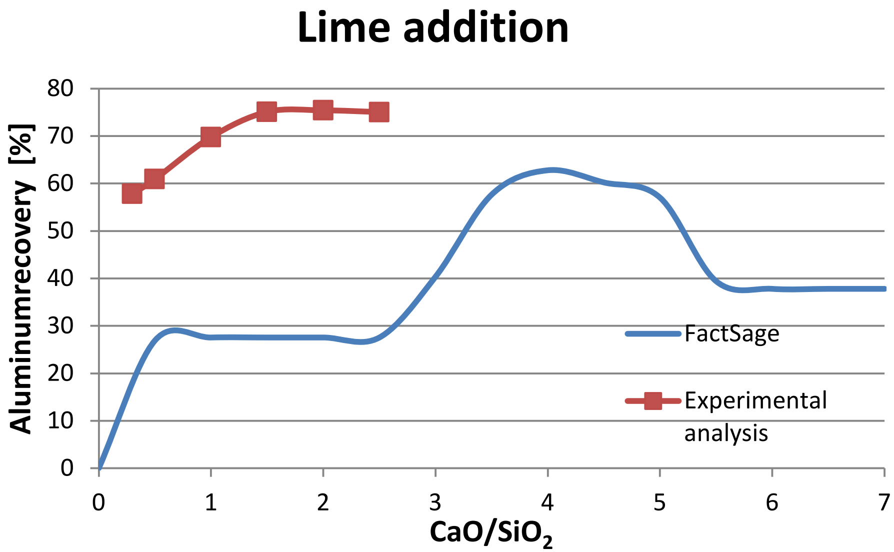
Study II: Comparison of FactSage and experiments

Maximum recovery in FactSage at 64% for CaO/SiO_2 of 4

Experiments verify the trend of significantly higher recoveries:



Problem:

- FactSage -> Equilibrium calculation
- Reality
  - ⇨ existence of other phases ($Al(OH)_3$)
  - ⇨ 250°C slow kinetics for equilibrium

➔ Delayed recovery increase and plateau at CaO/SiO_2 ~1.5 and higher recoveries through readily soluble $Al(OH)_3$

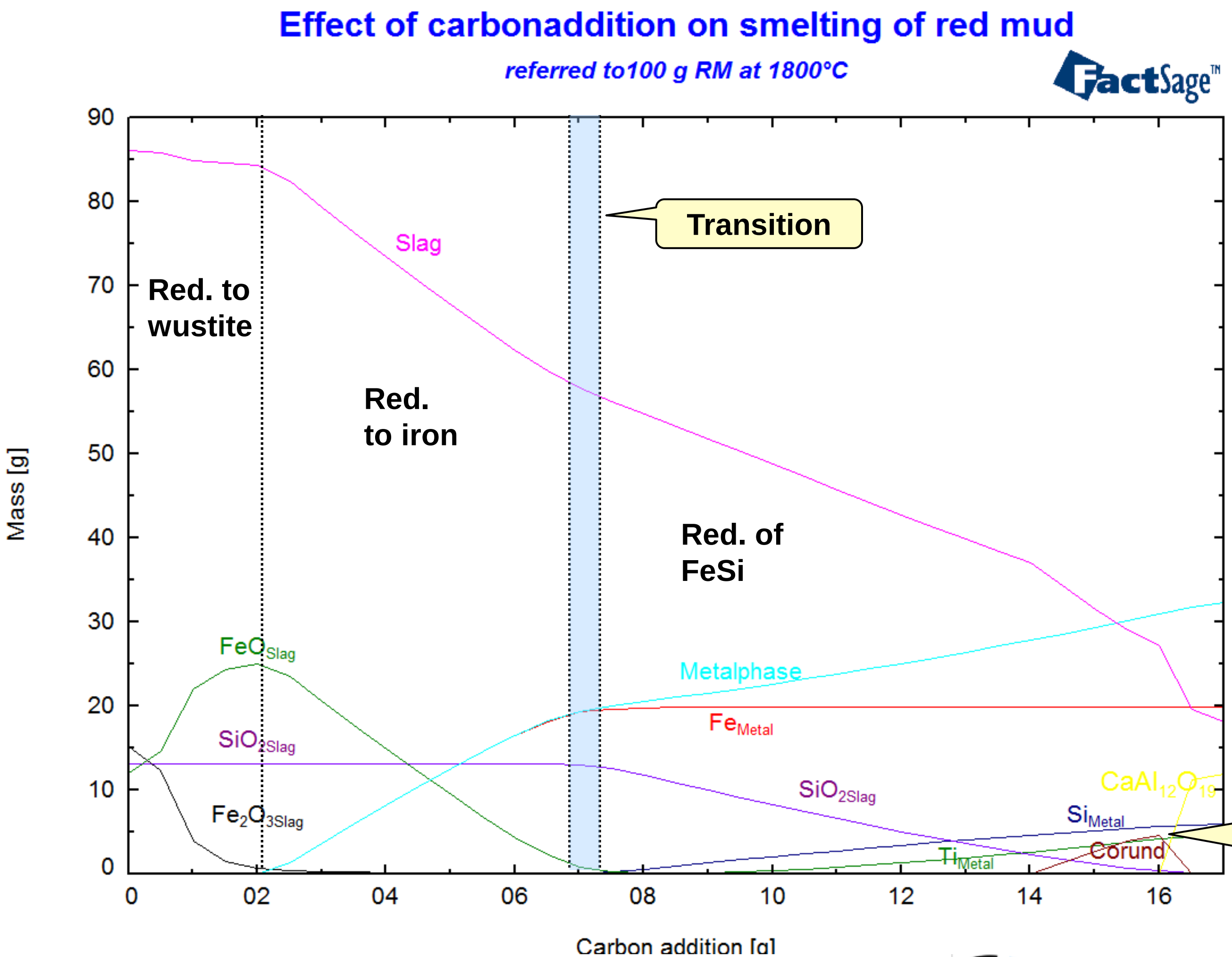
Future approach:

Preheating of the experimental mixture at 900°C to reach equilibrium and subsequent leaching

Study II: New approach: Si-separation in electric arc furnace (EAF)

- Recovery of iron and silicon through carbothermic reduction
- Enrichment of (soluble) Al in slag

→ Avoiding the necessity for massive landfills for Red Mud (~ 100M t per year)



Recovery of iron at a carbon addition of 75 g/kg red mud

Recovery of Fe18Si16Ti at a carbon addition of 165 g/kg red mud

Reduction of Ti and precipitation of first solid phases

Study II: Comparison of FactSage and experiments (Fe Reduction)

“Selective” iron reduction at 1600°C

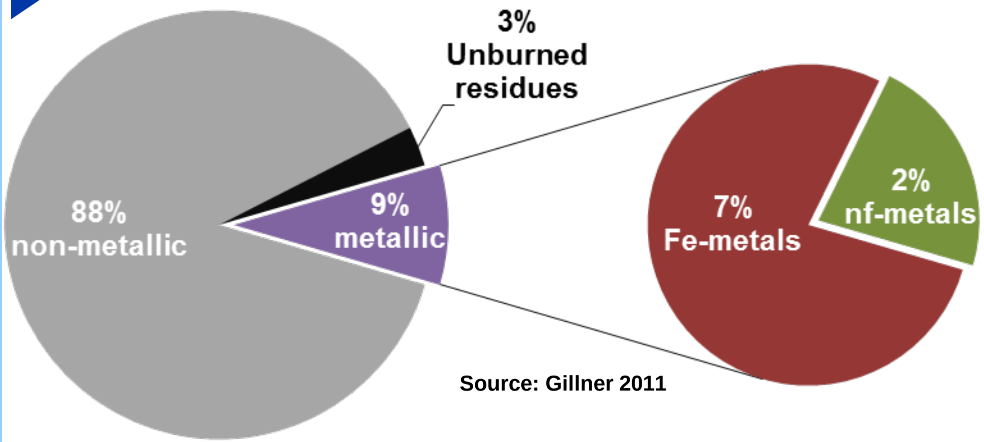
Slight hyperstoichimetric carbon addition (9 instead of 7 g/100g RM and CaO addition of 3.5 g/100g RM)

Metal [wt.-%]	Fe	C	Si	Ti	Al
FactSage	90,7	2,7	4,4	0,2	0,002
Experiment	93,7	4,4	0,04	0,2	0,000

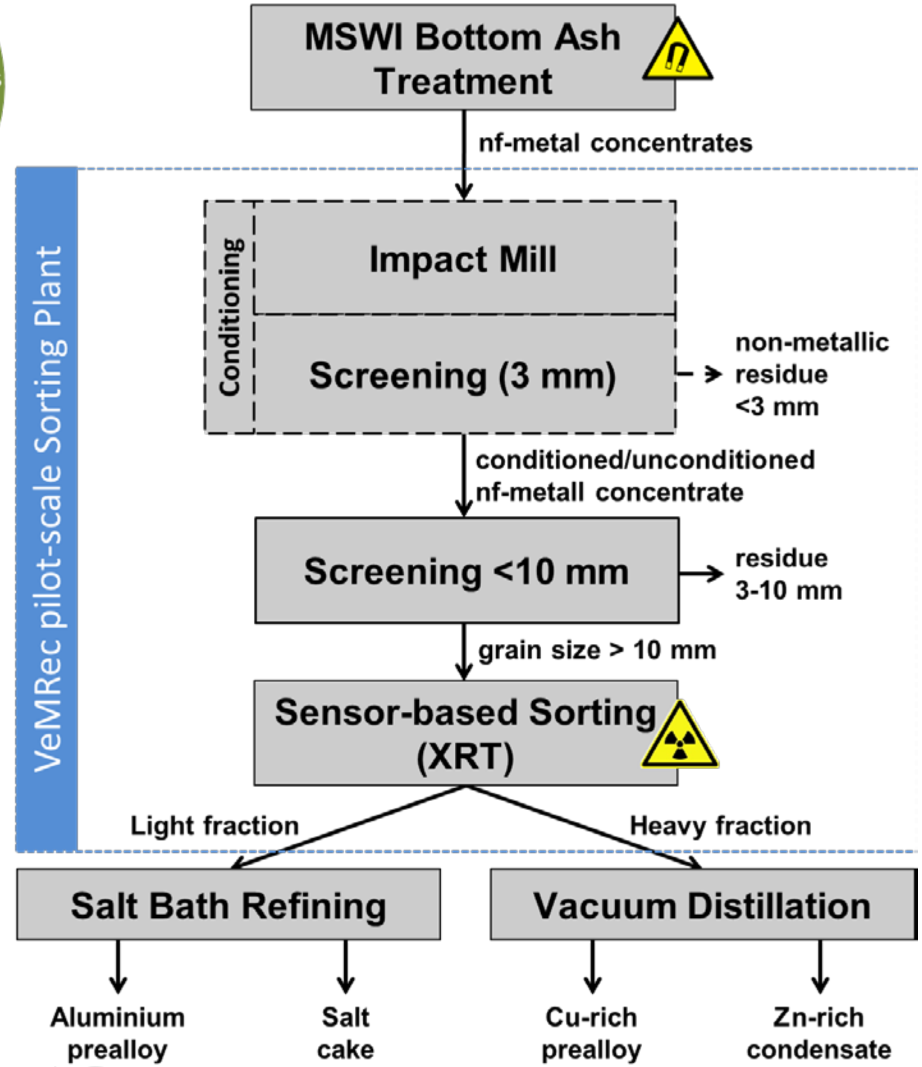
Slag [wt.-%]	Al_2O_3	SiO_2	CaO	Na_2O	TiO_2	Fe_2O_3
FactSage	49,2	19,4	13,2	8,3	11,7	0,02
Experiment	47,8	22,7	11,5	9,4	13,6	0,7

- **Si-equilibrium not reached**
- **Slag composition is in very good accordance with calculated model**

Study III: Non-ferrous(nf) metal recycling from MSWI bottom ash



1. **Separation of nf-metals by conventional MSWI bottom ash treatment**
2. **Sensor-based Sorting of nf-metal concentrates for the production of light and heavy metal fractions**
3. **Development of metallurgical evaluation methods, e.g. by *FactSage***



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Study III: Non-ferrous(nf) metal recycling from MSWI bottom ash

Light fraction
10-40 mm
conditioned

Heavy fraction
10-40 mm
conditioned

Study III: Metallurgical evaluation of nf-metal fractions

Treatment of light fraction through salt refining is relatively basic

→ High Al containing alloy (> 90 wt.-%)

Treatment of heavy fraction much more challenging

→ High Al, Si , Fe content which is undesired in metal

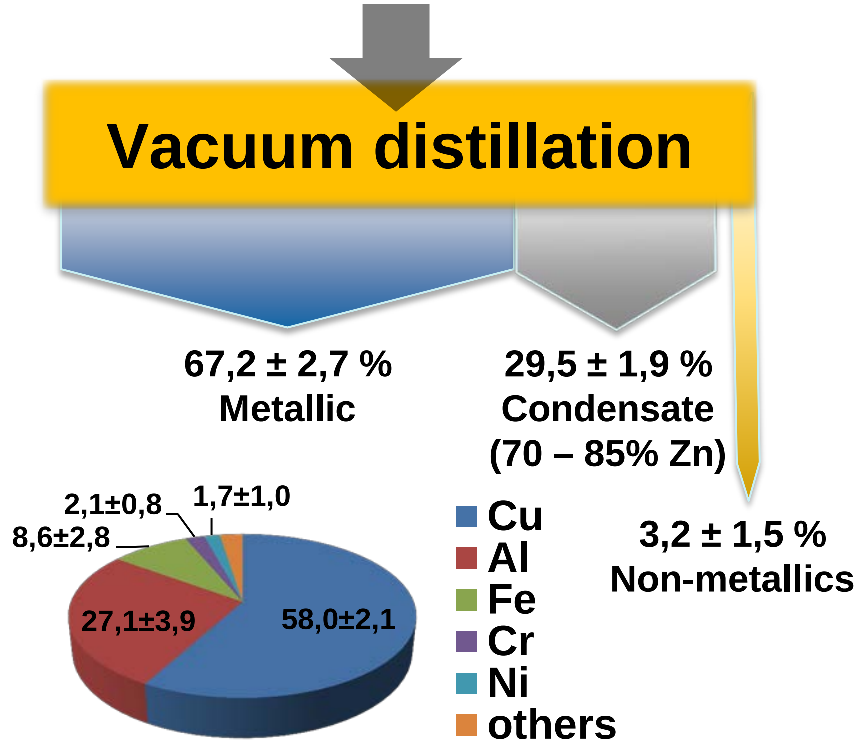
→ Zn distillation as first step

Average Composition of the waste's heavy fraction [wt.-%]

Cu	Zn	Al	Pb	Fe
37.7 ± 4	19.6 ± 5	25.7 ± 2	0.85 ± 0.5	8.33 ± 5

Si	Ni	Cr	Mn
1.48 ± 0.2	1.8 ± 1.5	2.05 ± 1.7	0.38 ± 0.2

mech. conditioned heavy metal fraction 10-40 mm



- **Contamination with light metals, stainless steel and non-metallics critical for heavy metal recycling**

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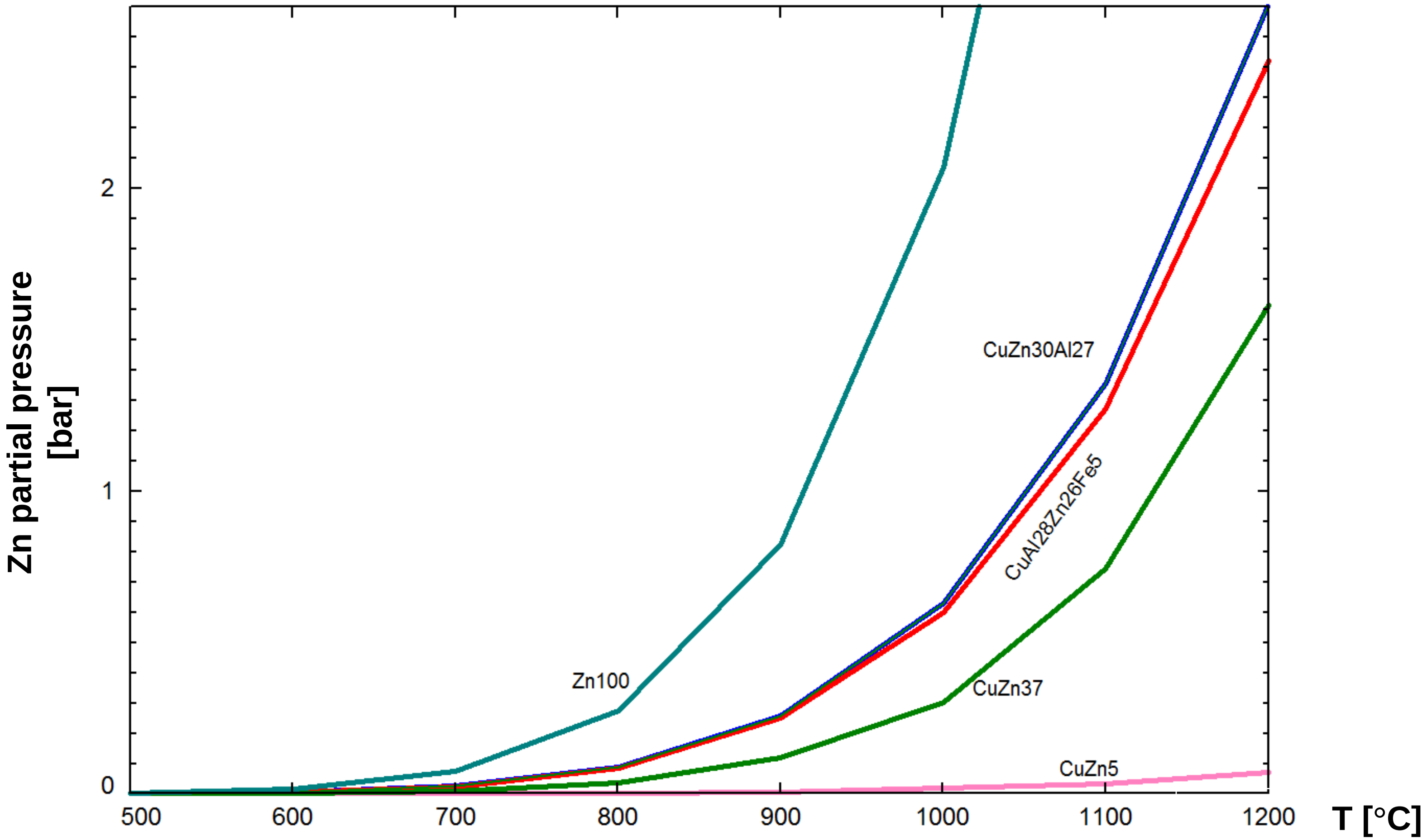
Study III: Thermochemical modelling with *FactSage*

For the recycling of heavy metal fraction:

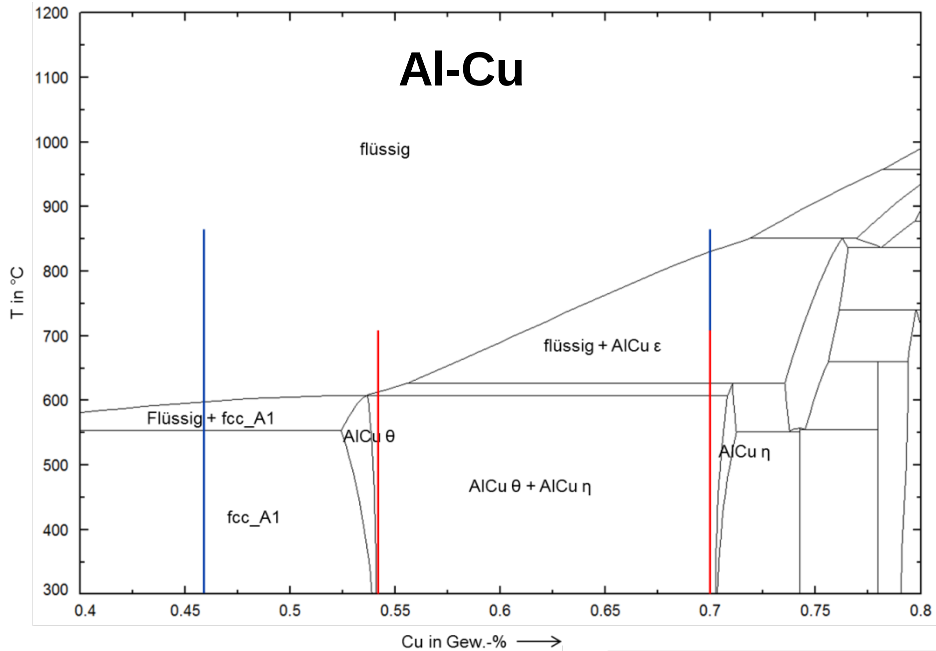
- Evaluation of vapour pressure for Zn and Zn-containing alloys with complex composition
- Calculation of binary phase diagrams for the identification of possible (intermetallic) product phases in the Cu-rich prealloy
- Selective oxidation of ignoble accompanying elements in de-zinced metal by different oxidation agents

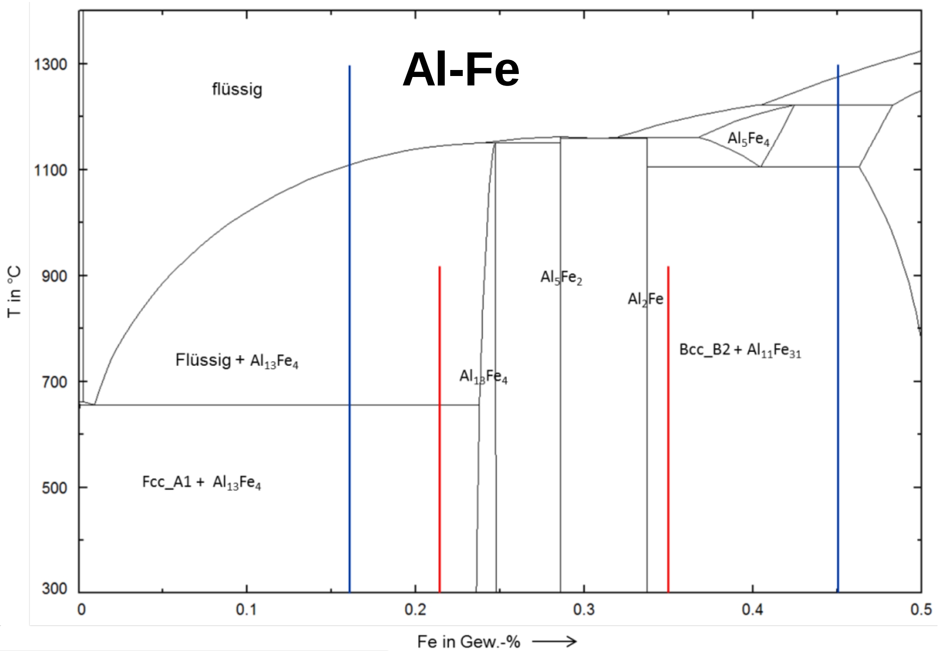
Study III: Vapour pressure of alloys

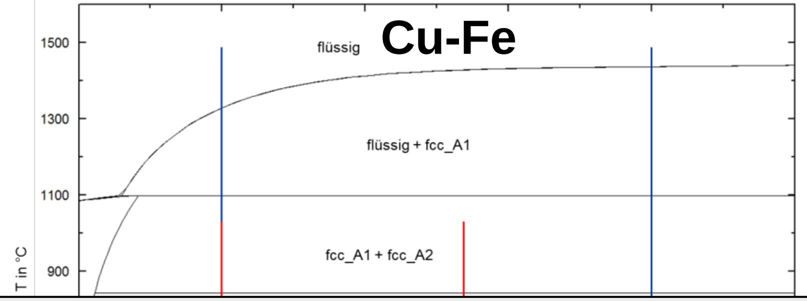


- Zinc partial pressure changes with the activity of zinc, which is higher for Cu-Zn-Al and Cu-Zn-Al-Fe than for Cu-Zn systems (SGPS-SGTE)

Study III: Binary edges of de-zinced heavy metal







- **Binary edges indicate, that intermetallics are predominant for Al-Cu and Al-Fe system, while demixing is typical for Cu-Fe system (FScopp-SGTE)**

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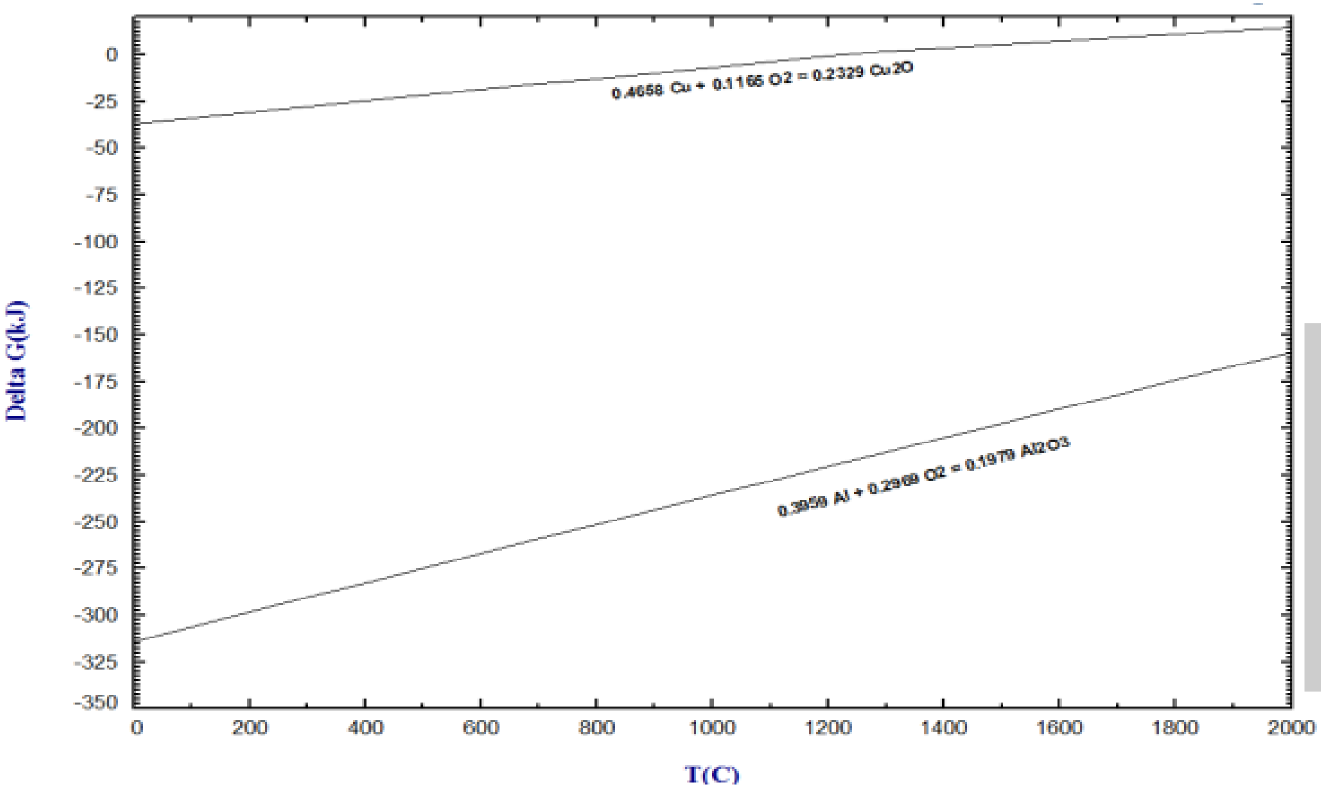
Study III: Activity-fitted Ellingham-diagrams for oxidative treatment

1. **Calculation of activities for the composition in de-zinced heavy metal in equlibrium at 1300 °C**

2. **Compilation of activity-fitted Ellingham-diagrams for the estimation of the selectivity of oxidative treatment**



Future research:

Selective Oxidation of Al and Si in metal through use of a high Cu_2O containing slag

Summary and outlook

FactSage Modelling is very helpful in our research:

- Theoretical support of experimental results
- Feasibility checking of an idea without or in addition to experiments
- Quick verification of a new approaches / ideas

Future / additional research involving FactSage:

- Modelling of aluminothermic metal production
- Simulation of different salt compositions for aluminum recycling
- Liquid salt electrolysis of REE

"Need to have / nice to have" additions to FactSage:

- Rare Earth Element databases:
  - slags with REE-oxides → further addition to FToxid
  - other chemical REE-species (e.g. carbides)
  - additional data for phase diagrams
- Database involving the combustion of organic materials (simulation of pyrolysis of different wastes)
- System Ti-Al-O in contact with different slag systems (e.g. CaF_2-CaO-Ca) for TiAl deoxidation in ESR

Thank you for your attention!

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