METALLOTHERMIC SCANDIUM SYNTHESIS –

A THERMOCHEMICAL STUDY

Part I: Phase equilibria of ScF₃ reduction with Ca and Ca-Zn alloy investigated by triangulation and tetrahedration methods

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ABSTRACT

In this paper, the results of a thermochemical study on metallothermic scandium synthesis using calcium and calcium-zinc alloys as reduction agents are presented. Equilibrium system components, reaction mechanisms, concentration ratios of charge components, as well as choice of temperature ranges for those multicomponent systems, are investigated by triangulation and tetrahedration. Those calculations are supported by thermochemical software *FactSage®,* with which the existence of quasi-binary lines in investigated systems is confirmed. With this method an overview of possible reduction reactions and their products in whole investigated system is obtained, giving the information on every reactant/product with desirable composition.

The conditions for maximum scandium yield ScF_3 compounds are derived to compare potentials of scandium production processes. ScF_3 is fully converted using elementary calcium, but all products will be in solid state at considered temperature of 1300 K. Nevertheless, it is recommended to use a Ca-Zn alloy as reductant in order to obtain liquid phases, but scandium content in the product decreases with increasing zinc proportion in the reducing alloy.

Metallothermische Scandiumsynthese:

Eine thermochemische Studie

Teil I: Untersuchung der Phasengleichgewichte der ScF₃ Reduktion mit Ca und Ca-Zn Legierungen mittels Triangulation und Tetrahedration

In diesem Beitrag werden die Ergebnisse einer thermochemischen Studie zur metallothermischen Scandiumgewinnung unter Einsatz von Calcium und Calcium-Zink Legierungen als Reduktionsmittel vorgestellt. Komponenten der Gleichgewichtssysteme, Reaktionsmechanismen,

Konzentrationsverhältnisse der Einsatzmaterialien und mögliche Temperaturbereiche für diese Multikomponentsysteme werden mittels Triangulation und Tetrahedration untersucht. Diese Berechnungen werden mit der thermochemischen Software FactSage® unterstützt, mit welcher die Existenz quasibinärer Linien in den untersuchten Systemen bestätigt wird.

Die Bedingungen für maximale Scandiumausbeute aus ScF_3 werden bestimmt, um Potentiale für Produktionsprozesse des Scandiums abzuleiten. ScF_3 wird vollständig durch elementares Calcium reduziert; jedoch befinden sich alle Produkte im festen Zustand bei den betrachteten Temperaturen von 1300 K. Aufgrund dessen wird empfohlen Ca-Zn als Reduktionsmittel einzusetzen, um flüssige Phasen zu erzielen, obwohl der Scandiumgehalt im Produkt mit steigendem Zinkgehalt in der Reduktionslegierung abnimmt.

Keywords: phase equilibria; calciothermy; scandium; triangulation; tetrahedration.

1   Introduction

Scandium became one of the important rare earth metals of today as its application in modern technology increases, such as in PC memory, medical devices, but especially as alloying element for strengthening aluminum in aerospace industry [1–4]. Nevertheless its high price impedes further utilization due to small concentration in ores and quite complex and costly production techniques.

Scandium (Sc) metal was firstly extracted by electrolysis of $ScCl_3$ in a KCl-LiCl melt [5], but this technology is up to now abandoned due to many disadvantages. Currently, scandium is extracted from ScF_3 or $ScCl_3$ metallothermically by reduction with calcium [6] or magnesium [7] in an argon atmosphere, but due to the hygroscopic nature of chlorides, their high evaporation pressure and necessity for additional hydrometallurgical purification steps, reduction of $ScCl_3$ is not preferred. Therefore, this paper have focus on ScF_3 as raw material for scandium production by metallothermy. Reduction is carried out in tantalum (Ta) or molybdenum (Mo) crucibles, sometimes in graphite crucibles with inner Mo sheet lining. After metal-slag separation, Sc is remelted in vacuum (ca $1,33 \cdot 10^{-3}$ Pa) in order to remove volatile accompanying elements, especially calcium. Further purification from tantalum is done by sublimation. An intermediate alloying is suggested to lower reduction temperature by addition of elements that form an alloy or compound with Sc, reducing the amount of crucible material dissolved. An Mg-Sc alloy is desired when using Mg, whereas Zn is added to the charge when Ca is used, due to the fact that Ca does not form an alloy with Sc. For lowering the melting temperature of the slag, addition of LiF is proposed, specified by the following reduction reaction (eq. 1) [8]:

$$2\ ScF_3 + 3\ Ca + 8\ Zn + 12\ LiF = 2\ (Sc \cdot 4Zn) + 3\ (CaF_2 \cdot 4\ LiF) \tag{1}$$
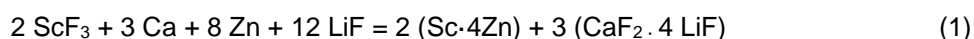
All published reports depict solely experimental results and all methods are based on empirical indications. Considerations concerning reduction mechanisms, explanations for the concentration ratios of charge components, as well as reasons for the choice of temperature ranges, are missing.

In the present study, all these aspects for reduction of ScF_3 by Ca and CaZn alloy are addressed. The thermochemical equilibrium of multicomponent systems is calculated and explained by triangulation and tetraedation. The conditions for maximum possible yield from expensive scandium compound is derived to compare potentials of scandium production process.

2   Methodology of investigations

In order to conduct a thermochemical calculation of a reaction correctly, it is necessary to know which compounds constitute the reactants and products of the reaction. The definition of multicomponent compounds of accompanying elements as well as the identification of reactions of these compounds with system components and their resulting reaction products is mandatory to assess the rate of these reactions within the system. Phase diagrams illustrate the mentioned relations graphically.

The "Klärkreuze" method was suggested by W. Guertler already in 1920 to clarify which reactions occur in a ternary system (stability condition) and which products are formed [9]. This method divides the concentration triangle using quasi-binary lines. Thus, the ternary system disintegrates into a series of secondary subsystems from which every subsystem displays equilibrium conditions of basic substances (compounds) [10]. This partition of a ternary system into a series of secondary subsystems is called triangulation. The historical development of this method for multicomponent systems is published in [11–14], in which triangulation of the ternary systems was carried out first. For quaternary systems, the partition of a concentration tetrahedron into a series of secondary quaternary systems is called tetrahedration. The tetrahedron space of a quaternary system is divided in secondary tetrahedrons by quasi-ternary planes allowing conclusions about possible products forming in multicomponent systems. As it was suggested by [14], the assessment of the metallurgical Sc-Me1-Me2-F system by triangulation and tetrahedration is conducted, where all thermochemically stable connection lines and planes between all elements and all congruently as well as incongruently melting components were calculated using *FactSage® 7.0,* depending on the formation temperature which allowed determination of those quasi-binary tie lines and quasi-ternary planes. This method has been already successfully applied by the authors for lead refining [15–17] and for clarification of Mg removal from Al alloys by SiO_2 addition [18]. Taking into account that thermochemical data on scandium compounds is scarce, the method presented describes an approach that neglects some properties of a system. However, for an idealized first attempt at understanding the properties of the system, triangulation and tetrahedration promises to be a suitable technique. Due to the lack of thermochemical data on scandium compounds this methodology is used for determination of existing phases and their stability in simplified/ideal systems without consideration of mixed phases.

3   Thermodynamic considerations

The chemical affinity of scandium to fluorine is presented in Table 1. The table lists elements in decreasing fluorine affinity order. Furthermore, each element is attributed with the $-\Delta G^{298}$ value for its forming fluoride, related to kJ/mol oxide, kJ/mol F_2, kJ/g-eq F_2 and kJ/g-atom. Every element listed is capable of reducing the fluorides of the respective element standing below it, due to the values of kJ/g-atom. The $-\Delta G^{298}$ values for kJ/mol fluoride and kJ/mol F_2 are overlapping, which hinders the evaluation

of the reductive potential of individual elements, whereas kJ/g-eq F_2 doesn't show the meaningful tendency. The $-\Delta G^{298}$ values related to kJ/g-atom reflect best the reduction potential order of fluorides of individual elements. Therefore, they are considered for an estimation of reduction feasibility. Lanthanum exhibits the highest Gibbs free energy value for fluorination and would therefore be able to reduce all fluorides listed below as an element considering pure substances. Note that scandium has smaller affinity to fluorine than calcium, indicating that a reduction to scandium metal using calcium is possible at standard conditions. Likewise, Al and Mg do not seem to be suitable reducing agents when pure substances are considered.

Table 1:   Fluorine affinity of selected elements at standard conditions [19]

Reducing agent	Fluoride	$-\Delta G_{298}$			
		kJ/mol fluoride	kJ/mol F_2	kJ/g-eq F_2	kJ/g-atom F
La	MeF_3	1654.0	1102.6	551.3	413.5
Y	MeF_3	1647.0	1098.0	549.0	411.7
Th	MeF_4	2002.0	1001.0	500.5	400.4
Ce	MeF_3	1601.0	1067.3	533.6	400.2
Sr	MeF_2	1181.0	1181.0	590.5	393.6
Ca	MeF_2	1176.0	1176.0	588.0	392.0
Sc	MeF_3	1540.0	1026.6	513.3	385.0
Zr	MeF_4	1810.0	905.0	452.5	362.0
Al	MeF_3	1540.0	954.0	477.0	357.7
Mg	MeF_2	1071.0	1071.0	535.5	357.0
Li	MeF	588.0	1176.0	588.0	294.0

ScF_3 can be reduced by Ca (and even five other metals), where all reaction products are in their solid state. This will lead to challenges in phase separation later. Since the values of Gibbs free energy of CaF_2 and ScF_3 do not differ significantly, the positive effect of Sc compound formation with Zn will be investigated.

4   Triangulation of boundary Sc-Ca-Zn-F system and tetrahedration

Boundary system triangulation of the quaternary Sc-Ca-Zn-F systems as well as tetrahedration of the quaternary systems gives information on reactants and reaction products of a possible Sc-compound reduction.

In order to perform triangulation of a ternary system, the compounds formed within this system were identified (Table 2).

Table 2:   Most relevant compounds of the Sc-Ca-Zn-F system

System	Compound	Melting point [K]	Melting behavior	Reference
Ca-F	CaF_2	1691	congruent	[20]
Ca-Sc		Segregation at 1751		[21,22]
Ca-Zn	$CaZn_2$	977	congruent	[23]
	$CaZn_5$	968	congruent	
	$CaZn_{11}$	997	congruent	
	Ca_3Zn	667	incongruent	

	Ca$_5$Zn$_3$	687	incongruent	
	CaZn	712	incongruent	
	CaZn$_3$	915	incongruent	
	CaZn$_{13}$	942	incongruent	
Sc-Zn	ScZn	1503	congruent	[24,25]
	ScZn$_2$	1298	incongruent	
	Sc$_{13}$Zn$_{58}$	1093	incongruent	
	Sc$_3$Zn$_{17}$	1088	incongruent	
	ScZn$_{12}$	748	incongruent	
Sc-F	ScF$_3$	1825	congruent	[26,27]
Zn-F	ZnF2	1145	congruent	[28]

Triangulation of boundary systems of the Sc-Ca-Zn-F systems is conducted as described in methodology of investigations (section 2). Tie lines shown in Figure 1 are quasi-binary according to calculations with thermochemical program *FactSage® 7.0*, except for tie lines in the CaZn$_2$-ZnSc-Zn system in temperature range between 1100 – 1298 K. Tie lines in this system didn't show distinctive equilibrium results and were conflicted with triangulation norms. Possible reasons for this could be incomplete data in software or/and change in equilibrium due to boundary solubility of Ca, Zn and Sc which is not considered in this method of investigation. As thermochemical calculations involving Zn$_2$Sc were not reliable tetrahedration was conducted at T > 1300 K, in order to neglect this compound. During tetrahedration (Figure 2), incongruently melting compounds Ca$_3$Zn (667 K), Ca$_5$Zn$_3$ (687 K), CaZn (712 K), ScZn$_{12}$ (748 K), CaZn$_3$ (915 K), CaZn$_{13}$ (942 K), Sc$_3$Zn$_{17}$ (1088 K) and Sc$_{13}$Zn$_{58}$ (1093 K) were neglected as well, since they are non-existent in the investigated temperature range (T > 1300 K).
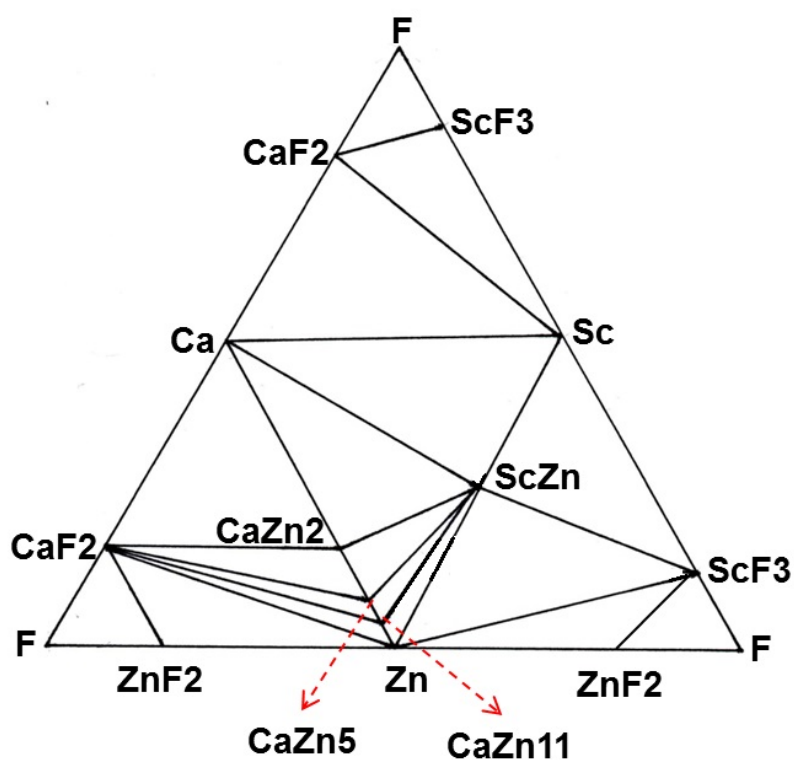

Figure 1: Boundary system triangulation of the quaternary Sc-Ca-Zn-F system

In addition, within the quaternary Sc-Ca-Zn-F system another quasi-binary tie line CaF_2-ScZn is formed. The entire system is divided into sub-systems by quasi-ternary planes passing through quasi-binary tie lines of boundary systems and through space of quasi-binary CaF_2-ScZn tie line. Figure 2a show that the connecting lines between ScF_3 and the reducing agent (Ca-Zn alloy) cross several sub-systems as a function of the added amount of reducing agent. Thereby, every crossed sub-system depicts the final product that is formed at the corresponding addition of Ca-Zn alloy to ScF_3. As it can be seen in this figure, in the Sc-Ca-Zn-F tetrahedron a series of quaternary systems is formed sharing the ternary or binary boundary systems. One system includes ScF_3 as component while the other does not, showing that the shared ternary/binary boundary systems reflect the products of complete ScF_3 reduction. At calculation temperature of 1300 K, compounds $CaZn_2$, $CaZn_5$ and $CaZn_{11}$ are in liquid state and therefore, the four sub-systems CaF_2-Ca-$CaZn_2$-ScZn, CaF_2-$CaZn_2$-$CaZn_5$-ScZn, CaF_2-$CaZn_5$-$CaZn_{11}$-ScZn and CaF_2-$CaZn_{11}$-Zn-ZnSc can be illustrated in one sub-system CaF_2-Ca-Zn-ScZn (Figure 2b).

Plane CaF_2-Sc-ZnSc is shared by ScF_3-CaF_2-Sc-ZnSc and CaF_2-Ca-Sc-ZnSc subsystems, planes CaF_2-Zn-ZnSc and ScF_3-CaF_2-ZnF_2 are shared by ScF_3-CaF_2-Zn-ZnSc and CaF_2-Ca-Zn-ZnSc subsystems, whereas plane CaF_2-Ca-ZnSc is shared by CaF_2-Ca-Sc-ZnSc and CaF_2-Ca-Zn-ZnSc subsystems (Figure 2b). These faces depict the end products of ScF_3 and (nCa+mZn) reaction depending on the (nCa+mZn) amount and show their composition in case that the connecting line ScF_3-(nCa+mZn) passes through them.
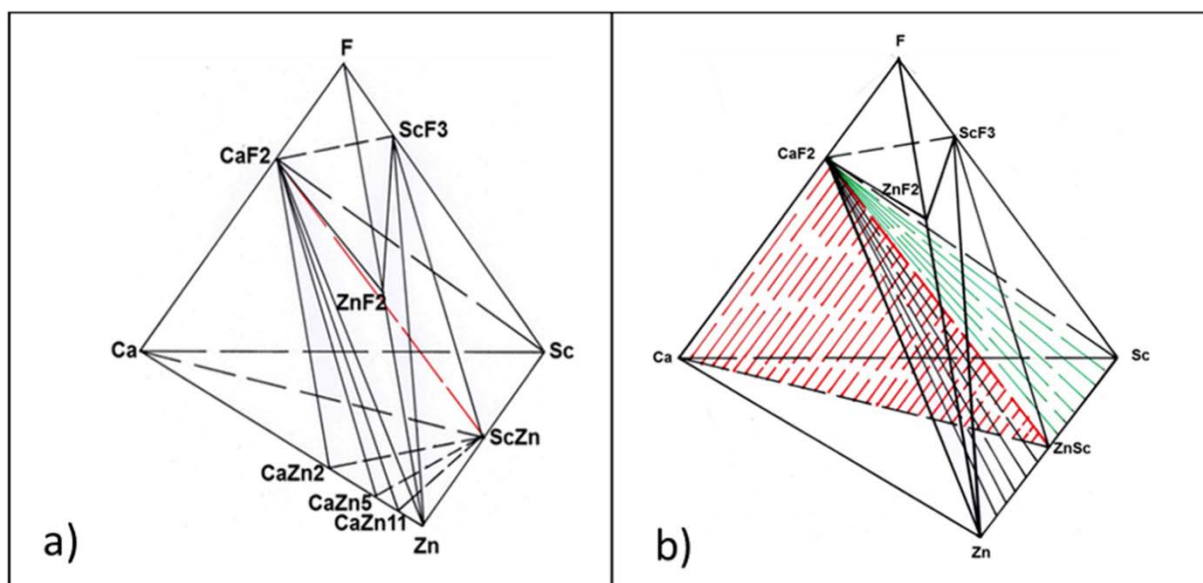

Figure 2: a) and tetrahedration of the system Sc-Ca-Zn-F at T > 1300 K b) stable components and tetrahedration of the system Sc-Ca-Zn-F at T > 1300 K without consideration of $CaZn_2$, $CaZn_5$, $CaZn_{11}$; quasi-ternary planes (red, green and black marked) as faces shared by two sub-systems

4.1   Resume of triangulation and tetrahedration

Application of triangulation and tetrahedration for understanding scandium reduction mechanisms gives insight into possibilities for reaction paths. It proves the implication that ScF_3 reduction with Ca is thermochemically favorable. Furthermore, using different ratios of Ca:Zn as reducing agent is feasible as well, leading to Sc-Zn compounds melting at lower temperatures than pure Sc making it possible to lower treatment temperatures. The exact process variables need to be considered still and are the target of the considerations on equilibrium calculations in the following section.

5   Reduction equilibrium calculations,

As mentioned from tetrahedron the end products can be determined depending on subsystem in which they are present. This method is proven by using the "Equilib" module of thermochemical program *"FactSage 7.0",* where equilibrium products of the reaction ScF_3 + Ca-Zn alloy were calculated, with varying Ca/Zn compositions at 1300 K. Since at this temperature the compounds $CaZn_2$, $CaZn_5$ and $CaZn_{11}$ are in liquid state, the calculations give them as Ca/Zn liquid phase. Furthermore, consumptions amounts of reducing agents and content of product obtained in these reactions are calculated. Graphical presentation of calculations will be shown below on few examples but consumption amounts of Ca and Zn as well as Sc content in product for some additional reduction alloy compositions which connecting line goes through same subsystems, are summarized in section 5.6 (Table 4).

5.1   Reduction of ScF_3 with Ca

As shown with triangulation of the Ca-Sc-F system (Figure 1) and 1, ScF_3 can be reduced by Ca. Calculations with the module "Equilib" in software *FactSage®* also show the possible ScF_3 reduction with Ca (Figure 3), during which Sc(s) and CaF_2(s) in solid state are formed, meaning that no clear separation of reduced Sc and formed slag is possible at considered process temperature. In order to enable separation, the formation of a Zn-Sc alloy is striven, which further supports ScF_3 reduction by formation of ScZn. This alloy is in its liquid state at investigated temperature and facilitates easy separation of alloy and slag. For direct reduction of 1 g of ScF_3, necessary amount of Ca is 0.59 g or 1.337 g of calcium is consumed for production of 1 g of scandium.
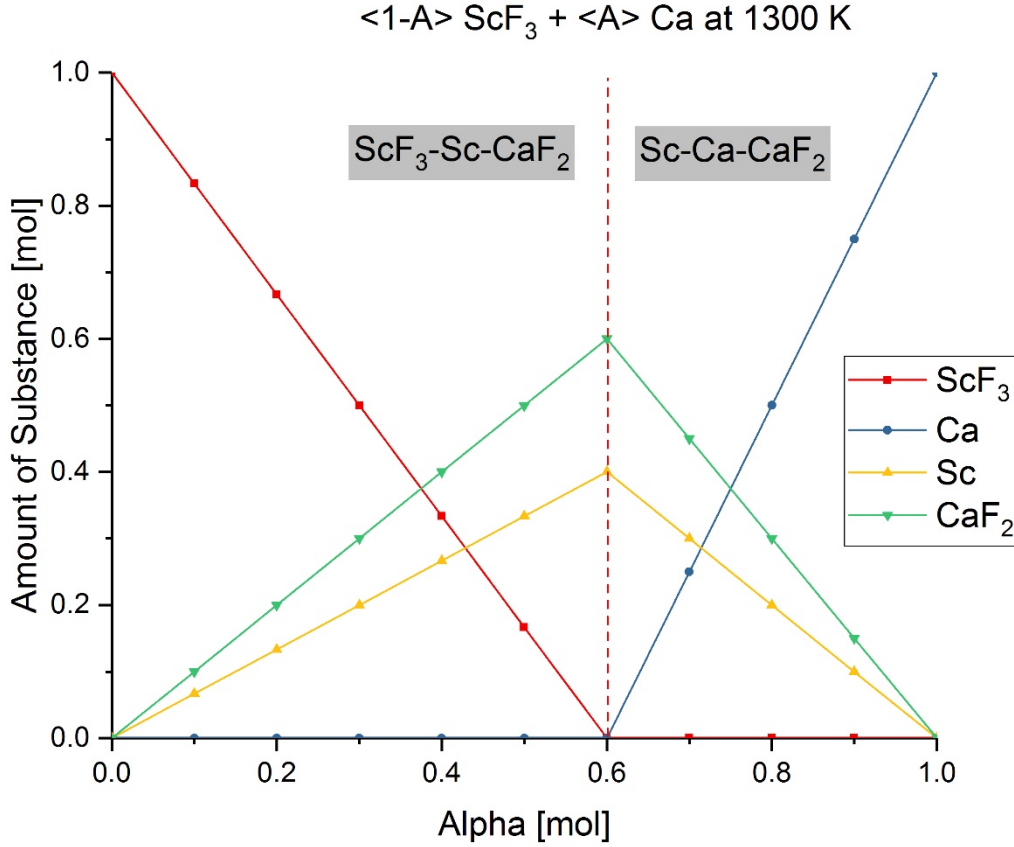
**Figure 3:** ScF$_3$ reduction with Ca at 1300 K (Alpha = mol Ca) calculated with *FactSage®* software

5.2 Reduction of ScF$_3$ with Ca$_3$Zn alloy

During ScF$_3$ reduction, the connecting line between ScF$_3$ and reducing alloy (0.75 Ca + 0.25 Zn) passes three subsystems with increasing quantity of the reducing alloy added to ScF$_3$ which are: ScF$_3$-CaF$_2$-Sc-ScZn, CaF$_2$-Sc-Ca-ScZn and CaF$_2$-Ca-Zn-ScZn. Complete ScF$_3$ reduction occurs on the quasi-ternary plane CaF$_2$-Sc-ZnSc (Figure 2, Figure 4) to Sc(s) und ZnSc(s), Due to this, ScF$_3$ reduction with (0.75 Ca + 0.25) alloy can be described by following reaction:

$$2 \ ScF_3 + Ca_3Zn = 3 \ CaF_2 + Sc + ScZn \tag{2}$$

For extraction of 1 g of scandium, it is necessary to employ 1.337 g of calcium and 0.727 g of zinc calculated both in *FactSage®* and from equilibrium reaction, where scandium content in reaction product amounts 57.9 wt.-%.

With further addition of Ca$_3$Zn alloy the composition reaches quasi-ternary plane CaF$_2$-Ca-ZnSc (Figure 4), at which the free Sc is completely bonded as ZnSc:

$$3 \ CaF_2 + Sc + ScZn + Ca_3Zn = 3 \ CaF_2 + 2 \ ZnSc + 3 \ Ca \tag{3}$$
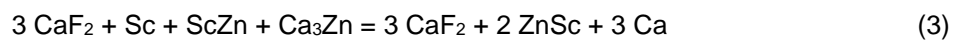
The consumption of calcium and zinc increases up to 1.783 g Ca and 1.455 g Zn but Sc amount in the end product decreases to 29.89 wt.-%.
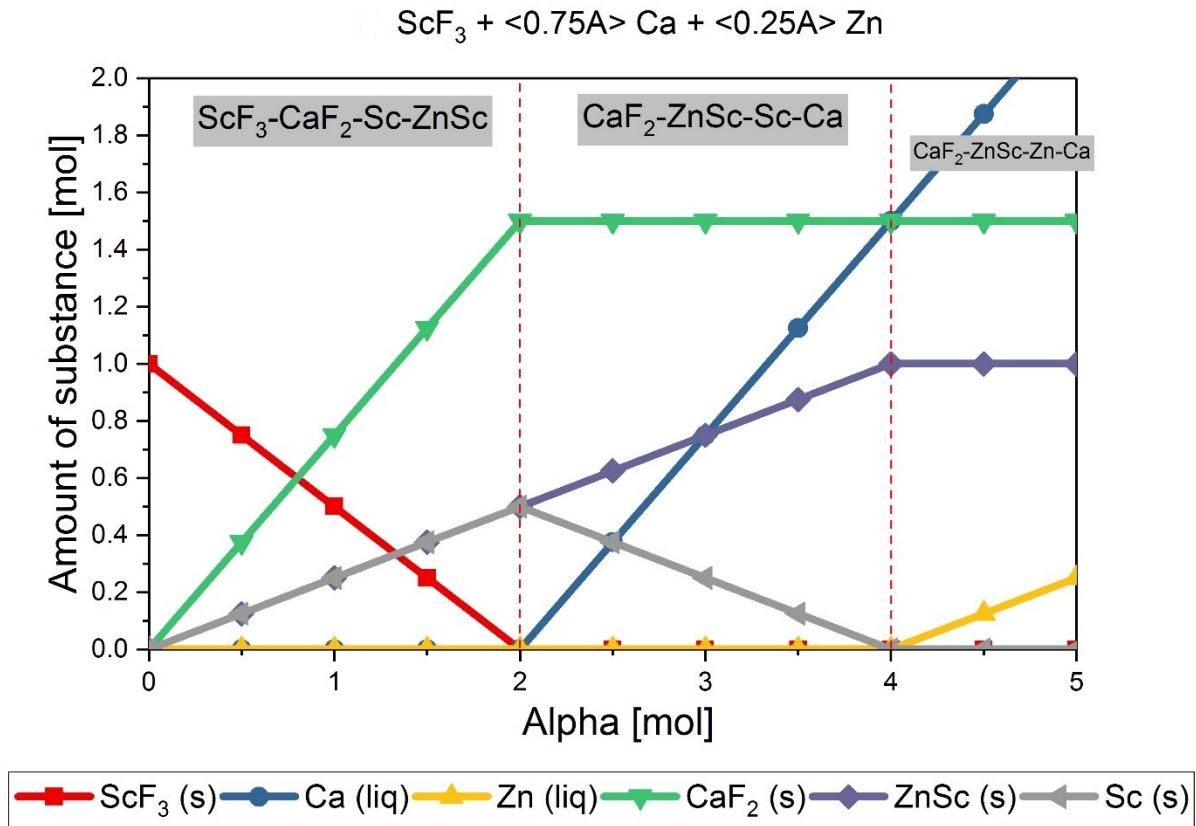

Figure 4: ScF$_3$ reduction by 0.75 Ca : 0.25 Zn alloy as a function of amount of reducing agent at 1300 K. Subsystems are depicted with grey background

5.3 Reduction of ScF3 with Ca0.6Zn0.4 alloy

With further decrease of Ca amount in reducing alloy, connecting line ScF$_3$-Ca$_{0.6}$Zn$_{0.4}$ crosses the quasi-ternary plane ScF$_3$-CaF$_2$-ZnSc (Figure 2, Figure 5). Complete reduction takes place on CaF2-ZnSc tie line following the reaction:

$$2ScF_3 + 3Ca + 2Zn = 3CaF_2 + 2ZnSc \tag{4}$$

Consumption of Ca and Zn needed for extraction of 1 g of Sc is 1.337 g and 1.455 g, respectively. Scandium content in ScZn product reaches 40.74 %. Addition of reducing alloy shifts the products in CaF$_2$-ZnSc-Ca-Zn subsystem where scandium concentration decreases due to dilution by Ca and Zn.
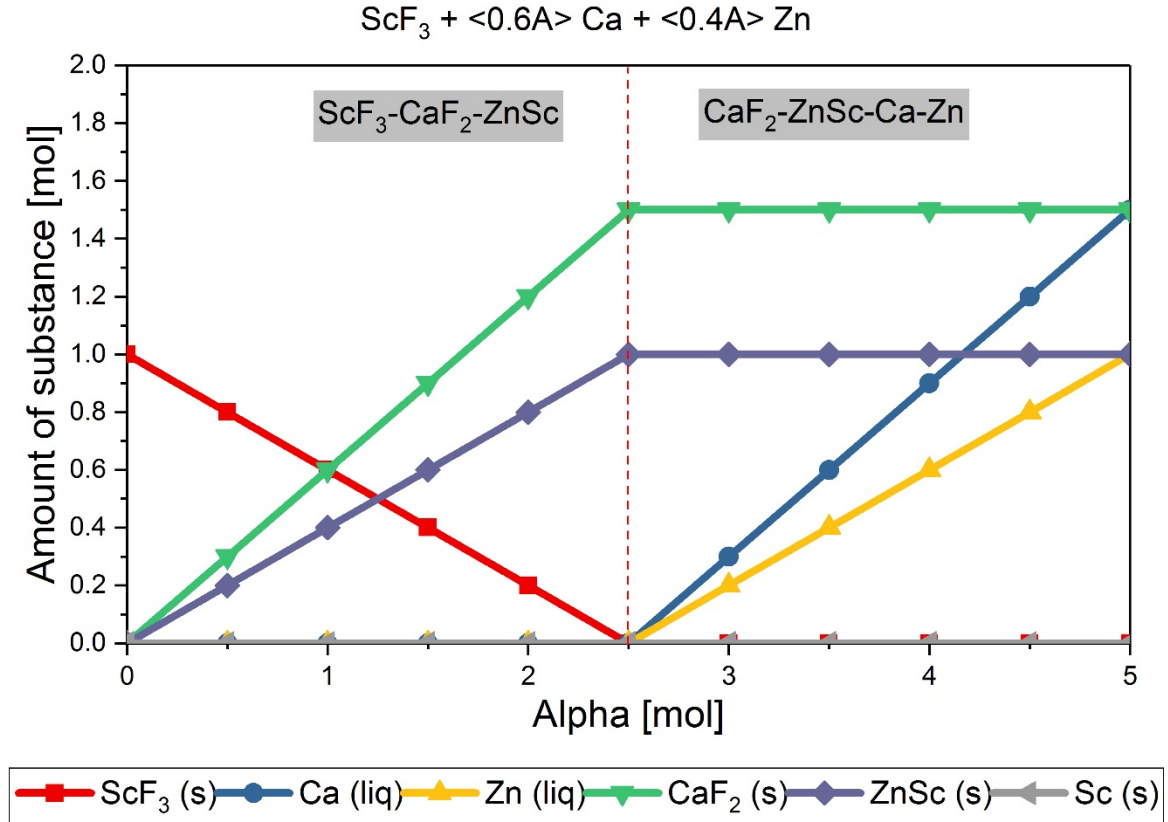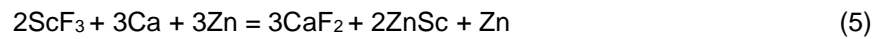
Figure 5: ScF$_3$ reduction by 0.6 Ca : 0.4 Zn alloy as a function of amount of reducing agent at 1300 K. Subsystems are depicted with grey background

5.4 Reduction of ScF$_3$ with Ca$_{0.5}$ Zn$_{0.5}$ alloy

Small addition of Zn to reducing alloy leads the connecting line firstly through the subsystem ScF$_3$-CaF$_2$-ZnSc-Zn and then through CaF$_2$-ZnSc-Ca-Zn, whereas the complete reduction occurs on quasiternary plane CaF$_2$-ZnSc-Zn (Figure 2, Figure 6), which can be described with reaction:

$$2ScF_3 + 3Ca + 3Zn = 3CaF_2 + 2ZnSc + Zn \qquad (5)$$

Based on this reaction the consumption of Ca is the same as in previous cases but Zn consumption increases to 2.182 g/ g Sc and scandium amount in product is 31.43 %. These amounts are the same as those calculated with *FactSage®.*

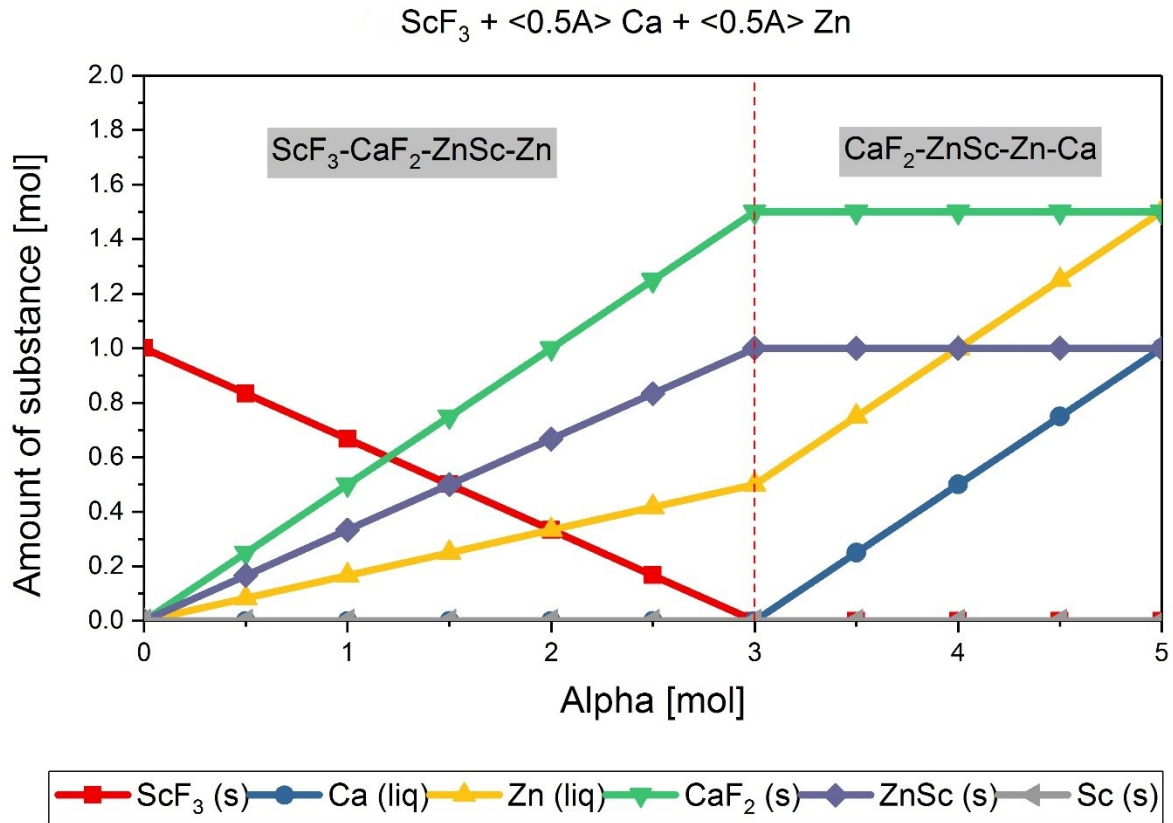**Figure 6:** ScF$_3$ reduction by 0.5 Ca : 0.5 Zn alloy as a function of amount of reducing agent at 1300 K. Subsystems are depicted with grey background

5.5 Reduction of ScF$_3$ with CaZn5 alloy

Every further zinc addition to reducing alloy leads to the same products only with different amounts of reduction agents and decreased scandium concentration in obtained alloy product. Connecting line ScF$_3$-CaZn$_5$ passes through the same subsystems as previous one (Figure 6). Reduction reaction is described as:

$$2ScF_3 + 3CaZn_5 = 3CaF_2 + 2ScZn + 13Zn \tag{6}$$
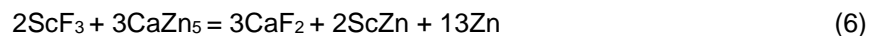
Calcium consumption remains the same and 10.907 g of zinc is needed to obtain 1 g of scandium. Scandium concentration in ScZn product is only 8.4 %. These amounts are confirmed by calculations with *FactSage®* confirming the accuracy of the investigated method.

5.6 Summary of ScF$_3$ reduction with Ca-(Zn)

Based on the obtained tetrahedron the reaction subsystems for different compositions of reducing alloys are recognized, providing the information on products and their composition. Obtained reactions for reduction of ScF$_3$ are summarized in Table 3. The amount of calcium and zinc needed for this reduction calculated from these equations and by *FactSage®* as well as scandium content in reaction product are given in Table 4.

Table 3: ScF$_3$ reduction reactions with different reducing alloy compositions and calculated calcium and zinc consumptions for producing 1 g of scandium based on those reactions and *FactSage®*

Reducing alloy	Reaction
Ca	$2ScF_3 + 3Ca = 3CaF_2 + 2Sc$
Ca$_3$Zn	$2ScF_3 + Ca_3Zn = 3CaF_2 + Sc + ScZn$
	$3CaF_2 + Sc + ScZn + Ca_3Zn = 3CaF_2 + 2ZnSc + 3Ca$
Ca$_5$Zn$_3$	$10ScF_3 + 3Ca_5Zn_3 = 15CaF_2 + Sc + 9ZnSc$
	$15CaF_2 + 3Sc + 9ZnSc + Ca_5Zn_3 = 15CaF2 + 12ZnSc + 5Ca$
Ca$_{0,6}$Zn$_{0,4}$	$2ScF_3 + 3Ca + 2Zn = 3CaF_2 + 2ZnSc$
CaZn	$2ScF_3 + 3CaZn = 3CaF_2 + Zn + 2ScZn$
CaZn$_2$	$2ScF_3 + 3CaZn_2 = 3CaF_2 + 2ScZn + 4Zn$
CaZn$_5$	$2ScF_3 + 3CaZn_5 = 3CaF_2 + 2ScZn + 13Zn$

During ScF$_3$ reduction with Ca, reduction is accompanied by the formation of CaF$_2$ and Sc. Using an Ca-Zn alloy, Ca reduces ScF$_3$ and the emerging Sc combines with Zn to a compound (ScZn), but Sc is diluted in the product by zinc and its content inevitably decreases with increasing Zn consumption. Adding Zn to the reducing agent Ca is helpful when a lower liquidus temperature of the reduction product is desired, however, additional purification steps are necessary for obtaining a highly concentrated Sc phase.

Table 4: Required quantities of reducing agents as a function of their composition and attainable Sc contents in the product during ScF$_3$ reduction calculated by *FactSage®* and equilibrium reactions

Reducing alloy	g Ca/g Sc	g Ca/ g ScF$_3$	g Zn/g Sc	g Zn/ g Sc F$_3$	Sc in product [wt.-%]
Ca	1.337	0.59	-	-	100
Ca$_3$Zn	1.337	0.59	0.727	0.321	57.90
	1.783	0.59	1.455	0.643	29.89
Ca$_5$Zn$_3$	1.337	0.59	1.307	0.600	42.32
	1.486	0.66	1.455	0.668	35.39
Ca$_{0,6}$Zn$_{0,4}$	1.337	0.59	1.455	0.642	40.74
CaZn	1.337	0.59	2.182	0.962	31.43
CaZn$_2$	1.337	0.59	4.356	1.924	18.65
CaZn$_5$	1.337	0.59	10.907	4.810	8.40

Conclusion

By tetradration of quaternary system Sc-Ca-Zn-F the series of adequate reactions within the stated systems are determined and reduction mechanisms of ScF$_3$ with Ca/Zn alloys as a function of reducing alloy compositions and their amounts is investigated. Consumptions of Ca and Zn for ScF$_3$ reduction is calculated by established reactions and with module "Equilib" in thermochemical software *"FactSage® 7.0"*, where quite good data agreement is noticed. Scandium will be in every case completely reduced (100%) but the phase separation is challenging since the products are in solid state. With addition of zinc an scandium-zinc alloy is formed which can be in liquid state at considered temperature of 1300 K.

Decreased working temperature leads to better preservation of expensive tantalum crucibles used in metallothermic reduction of Sc. For reduction of ScF_3 calcium consumption remains same but zinc consumption increases with increase of its content in reducing alloy. Simultaneously, with increase of zinc content, scandium content in end product decreases. Thus, the reduction of ScF_3 with Ca in regard to highest possible Sc content is desirable and with reduction alloy compositions below 1:1 ratio regarding liquid phase formation/separation.

The investigations are solely based on determination of ScF_3 reaction mechanisms by Ca/Zn reducing alloys, considering pure compounds. Detailed problems concerning separation of Sc alloy and slag phases are not studied in this context. Contribution of mixed phases and their activities on reaction products and their content will be the subject of further studies. Moreover, other reducing agents, respectively aluminium and magnesium are to be considered.

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